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Advanced Quantum Mechanics II

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Course Information

Assessment

Assignments 30%, Exam 70% (closed book).

Teaching Format

I will assume you have read the reading material for the day. A précis of the material will be given, with problems set and discussed in lectures.

Course Outline

I. Background

  1. Equations of motion, Symmetries and Conservation Laws
  2. Pictures of quantum dynamics

II. Quantum Optics

  1. Elementary quantum systems
  2. Quantum theory of the electromagnetic field
  3. Fundamental processes in quantum optics
  4. The Density Operator
  5. Dissipation in open quantum systems

III. Ultra-cold Atoms

  1. Scattering Theory
  2. Second Quantization
  3. Degenerate Bose gases

Reference Material

Many excellent texts exist, and this course uses material sourced from

1. *Introduction to Quantum Mechanics*, D. J. Griffiths, Prentice-Hall 2005.
2. *Modern Quantum Mechanics*, J. J. Sakurai, Addison-Wesley 1994.
3. *Advanced Quantum Mechanics*, F. Schwabl, Springer 2008.
4. *Statistical Methods of Quantum Optics*, H. J. Carmichael, Springer 1999.
5. *Quantum Optics*, D. F. Walls and G. J. Milburn, Springer 1995.

6. *Quantum Noise*, C. W. Gardiner and P. Zoller, Springer 2009.
7. *Quantum Statistical Properties of Radiation*, W. H. Louisell, Wiley Classics Library 1990.
8. *Condensed Matter Field Theory*, A. Altland and B. Simons, Cambridge University Press 2010.
9. *Bose-Einstein Condensation*, L. Pitaevskii and S. Stringari, Clarendon Press, Oxford 2003.

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Part I

Background

1 Postulates and Symmetries

1.1 Postulates of quantum mechanics

1. The state of the quantum mechanical system is completely specified at each point in time by a state ket $|\psi, t\rangle$ in *Hilbert space*. In position space, this function $\psi(\mathbf{r}, t) \equiv \langle \mathbf{r}|\psi, t\rangle$ depends on the particle position $\mathbf{r}$, and has the property that

   $$|\psi(\mathbf{r}, t)|^2 d^3\mathbf{r} = (\text{Prob. particle lies in volume } d^3\mathbf{r}, \text{ at position } \mathbf{r} \text{ and time } t). \tag{1.1}$$

   The probabilistic interpretation requires that $\psi(\mathbf{r}, t)$ be normalizable $\int d^3\mathbf{r}|\psi(\mathbf{r}, t)|^2 = 1$, single-valued, and finite.

2. To every observable A in classical mechanics there corresponds a linear, Hermitian operator $\hat{A}$ in quantum mechanics. Requiring that observable expectation values must be real constrains $\hat{A}$ to be Hermitian. If the result of measuring $\hat{A}$ is a, then a must be one of the eigenvalues of $\hat{A}|a\rangle = a|a\rangle$, with eigenfunction $|a\rangle$.

   In practice, the spectrum of eigenvalues can be discrete (bound states), or continuous (unbound states), and the discrete eigenvalue spectra are the origin of the notion of *quantum*.

3. The expectation value of the observable $\hat{A}$ is

   $$\langle \hat{A}\rangle = \langle \psi, t|\hat{A}|\psi, t\rangle, \tag{1.2}$$

   and if the system is in an eigenstate of $\hat{A}$ with eigenvalue a, then every measurement of $\hat{A}$ will give a. Given a complete set of orthogonal eigenvectors $1 = \sum_j |a_j\rangle\langle a_j|$, an arbitrary state may be represented as

   $$|\psi, t\rangle = \sum_j c_j|a_j\rangle, \tag{1.3}$$

   where the probability of finding the result a_j is $P(a_j) = |\langle a_j|\psi, t\rangle|^2 = |c_j|^2$, giving the measurement result

   $$\langle \hat{A}\rangle = \sum_j a_j|c_j|^2 = \sum_j a_j P(a_j). \tag{1.4}$$

   Furthermore, a measurement that leads to eigenvalue a_j *collapses* the state onto the eigenstate $|a_j\rangle$.

4. The state ket of the system evolves in time according to the time-dependent Schrödinger equation

   $$i\hbar\frac{\partial}{\partial t}|\psi, t\rangle = \hat{H}|\psi, t\rangle. \tag{1.5}$$

   where $\hat{H}$ is the *Hamiltonian* of the system. If $|\psi, 0\rangle$ is in an eigenstate of $\hat{H}$ with eigenvalue E, then $|\psi, t\rangle = e^{-iEt/\hbar}|\psi, 0\rangle$.

In what follows we will often omit the "hats" on operators, restoring them if the operator character is not entirely clear from the context.

1.2 Bases in Hilbert space

At this point is useful to remind ourselves of the basic aspects of representing quantum states in Hilbert space and important differences between discrete and continuous spectra of eigenvalues. We assume we have a complete set of eigenkets of an operator $\hat{A}$, with discrete eigenvalue spectrum, and operator $\hat{x}$ with continuous eigenvalue spectrum. Obvious examples are the discrete energy levels of of a simple harmonic oscillator, or the continuous range of allowed values of the position of a particle. In either case, the states provide a complete representations of the Hilbert space of a single particle, but with different properties. Let us compare the properties of these bases:

$$
\begin{array}{rlr}
\textbf{Discrete} & \textbf{Continuous} & \\
\hat{A}|a\rangle = a|a\rangle & \hat{x}|x\rangle = |x\rangle, & (1.6a)\\
\langle a|b\rangle = \delta_{ab} & \langle x|x'\rangle = \delta(x-x'), & (1.6b)\\
1 = \sum_{a} |a\rangle\langle a| & 1 = \int dx\, |x\rangle\langle x|, & (1.6c)\\
|\psi\rangle = \sum_{a} |a\rangle\langle a|\psi\rangle & |\psi\rangle = \int dx\, |x\rangle\langle x|\psi\rangle, & (1.6d)\\
\langle\psi|\phi\rangle = \sum_{a} \langle\psi|a\rangle\langle a|\phi\rangle & \langle\psi|\phi\rangle = \int dx\, \langle\psi|x\rangle\langle x|\phi\rangle, & (1.6e)\\
\hat{O} = \sum_{a,b} |a\rangle\langle a|\hat{O}|b\rangle\langle b| & \hat{O} = \int dx \int dx'\, |x\rangle\langle x|\hat{O}|x'\rangle\langle x'|, & (1.6f)\\
\hat{A} = \sum_{a} |a\rangle\langle a|a, & \hat{x} = \int dx\, |x\rangle\langle x|x. & (1.6g)
\end{array}
$$

We see that (1.6f) gives a general representation of any operator, while for the operator satisfying (1.6a), (1.6g) shows that the representation is *diagonal*. Notice also that from (1.6b) we see that the continuum states have an interesting and unavoidable pathology, namely that they are not normalizable in the usual sense familiar for bound states, since apparently $\langle x|x\rangle = \infty$. We should not be alarmed by this! The continuum states are merely a convenient representation, and we will never be in a position of having to test their normalisation experimentally. Even more reassuringly, the delta function will almost always be accompanied by an integral over one of its arguments, removing the apparent pathology [Reminder: the basic property of the Dirac delta function is $\int dx' f(x')\delta(x-x') = f(x)$].

1.3 Symmetries in classical mechanics

In classical mechanics there is a correspondence between continuous symmetries and conservation laws. In particular, for every continuous symmetry of the equations of motion, there is a corresponding conservation law (*Noether's theorem*). In general there are two kinds of symmetries: *discrete* and *continuous*.

Important examples of continuous symmetries are

Symmetry		Conservation Law
Time invariance	↔	Energy conservation
Space translational invariance	↔	Momentum conservation,

However, in general time and position are not on an equal footing:

1. Time is *not* an observable.
2. There is no Hermitian operator with eigenvalues corresponding to time.
3. Time is a parameter of the theory, not a measurable quantity.

1.4 Continuous Symmetries

Figure 1.1: Emmy Noether (1882-1935), a german mathematician known for major contributions in abstract algebra and theoretical physics. Perhaps most famously, Noether's theorem states that *any differentiable symmetry of the system Lagrangian has an associated conservation law*.

Continuous symmetries involve physical variables that may be continuously varied. In this section we investigate the consequences of continuous symmetries in describing quantum systems.

1.4.1 Infinitesimal unitary transformations

The fundamental representation of such an operation is the infinitesimal transformation. Let an *infinitesimal unitary transformation* depend on a real parameter ε and differ from unity only at first order according to the definition

$$\boxed{U_G(\varepsilon) = 1 - \frac{i\varepsilon}{\hbar}G \qquad (1.7)}$$

where the operator G is called the *generator* of the infinitesimal transformation. The factor $-i/\hbar$ is chosen for convenience. When such a transformation operator acts on a state ket

$$|\psi, \varepsilon\rangle = U_G(\varepsilon)|\psi, 0\rangle, \tag{1.8}$$

conservation of probability imposes $U_G^\dagger(\varepsilon)U_G(\varepsilon) = 1$, and the transformation is *unitary*. At lowest order in ε this condition is satisfied if the parameter ε is real and G is Hermitian:

$$\begin{aligned} U_G^\dagger(\varepsilon)U_G(\varepsilon) &= \left(1 + \frac{i\varepsilon}{\hbar}G^\dagger\right)\left(1 - \frac{i\varepsilon}{\hbar}G\right) = 1 + \frac{i\varepsilon}{\hbar}(G^\dagger - G) + O(\varepsilon^2) && (1.9) \\ &= 1, && (1.10) \end{aligned}$$

provided $G = G^\dagger$. Acting on a state vector or an operator gives

$$|\psi, \varepsilon\rangle = |\psi, 0\rangle - \frac{i\varepsilon}{\hbar}G|\psi, 0\rangle, \tag{1.11}$$

$$A_\varepsilon = U_G(\varepsilon)AU_G^\dagger(\varepsilon) = A + \frac{i\varepsilon}{\hbar}[A, G], \quad \text{at linear order,} \tag{1.12}$$

so that if $[G, A] = 0$, then $A_\varepsilon = A$, and the operator is invariant.

1.4.2 Finite unitary transformations

Successive applications of the infinitesimal transformation enables finite transformations to be built

$$U_G(\alpha) = \lim_{N\to\infty} \prod_{k=1}^{N} \left(1 - \frac{i\alpha}{\hbar N} G\right) = \lim_{N\to\infty} \left(1 - \frac{i\alpha}{\hbar} G\right)^N = e^{-i\alpha G/\hbar}. \tag{1.13}$$

Transforming an operator A

$$e^{i\alpha G/\hbar} A e^{-i\alpha G/\hbar} = A + \frac{i\alpha}{\hbar}[G, A] + \frac{(i\alpha/\hbar)^2}{2!}[G, [G, A]] + \dots \tag{1.14}$$

we see that the operator is invariant under the transformation provided $[G, A] \equiv 0$. However, note that (1.13) requires that the operators commute upon successive applications of G. Time evolution is an important situation where this condition does not hold.

1.4.3 Space translation

The homogeneity and isotropy of space underpins invariance of the equations of motion under space translations in classical mechanics. In quantum mechanics, this symmetry is generated by the momentum operator $\mathbf{p}$. We can deal with all degrees of freedom at once since the operators commute, $[x_j, p_k] = i\hbar\delta_{jk}$. Space translation is given by the choice

$$G = \hat{\mathbf{p}}, \tag{1.15}$$

$$\varepsilon = \delta\mathbf{x}, \quad \text{so that} \tag{1.16}$$

$$U_p(\varepsilon) = 1 - \frac{i\hat{\mathbf{p}} \cdot \delta\mathbf{x}}{\hbar}. \tag{1.17}$$

and for small displacements we can write the action on the ket in the basis of eigenkets of position $\hat{\mathbf{r}}|\mathbf{r}\rangle = \mathbf{r}|\mathbf{r}\rangle$ as

$$\langle\mathbf{r}|\left(1 - \frac{i\hat{\mathbf{p}} \cdot \delta\mathbf{x}}{\hbar}\right)|\psi\rangle = \psi(\mathbf{r}) - \delta\mathbf{x} \cdot \nabla\psi(\mathbf{r}) = \psi(\mathbf{r} - \delta\mathbf{x}) = \langle\mathbf{r} - \delta\mathbf{x}|\psi\rangle, \tag{1.18}$$

where we use $\langle\mathbf{r}|\mathbf{p}|\psi\rangle = -i\hbar\nabla_{\mathbf{r}}\langle\mathbf{r}|\psi\rangle$. Thus the role of the translation operator is to translate the state ket by vector $\delta\mathbf{x}$, equivalent to moving the position eigenkets by $-\delta\mathbf{x}$.

For finite displacement by the vector $\boldsymbol{a}$, we have the translation operator

$$\boxed{U_p(\boldsymbol{a}) = \exp\left(-\frac{i\boldsymbol{a} \cdot \hat{\mathbf{p}}}{\hbar}\right)} \tag{1.19}$$

Exercise 1.1: Taylor series

Show that in one dimension (1.19) reproduces the Taylor series for $\psi(x + a)$ at all orders in a.

1.4.4 Commutation relations

In general we can consider finite displacements, and the action of the displacement operator on position eigenstates must give

$$U_p(\boldsymbol{a})|\mathbf{r}\rangle = |\mathbf{r} + \boldsymbol{a}\rangle, \tag{1.20}$$

hence

$$\hat{\mathbf{r}}U_p(\boldsymbol{a})|\mathbf{r}\rangle = (\mathbf{r} + \boldsymbol{a})U_p(\boldsymbol{a})|\mathbf{r}\rangle. \tag{1.21}$$

However

$$U_p(\boldsymbol{a})\hat{\mathbf{r}}|\mathbf{r}\rangle = \mathbf{r}U_p(\boldsymbol{a})|\mathbf{r}\rangle, \tag{1.22}$$

and hence

$$\hat{\mathbf{r}}U(\boldsymbol{a})|\mathbf{r}\rangle = U_p(\boldsymbol{a})(\hat{\mathbf{r}} + \boldsymbol{a})|\mathbf{r}\rangle. \tag{1.23}$$

Since $|\mathbf{r}\rangle$ is arbitrary, we can write this as

$$\boxed{U^\dagger(\boldsymbol{a})\hat{\mathbf{r}}U(\boldsymbol{a}) = \hat{\mathbf{r}} + \boldsymbol{a}.} \tag{1.24}$$

Choosing now the infinitesimal displacement by $\delta\boldsymbol{a}$, and using (1.17), we have

$$[\delta\boldsymbol{a}\cdot\hat{\mathbf{p}}, \hat{\mathbf{r}}] = -i\hbar\delta\boldsymbol{a}, \tag{1.25}$$

and since this is true for any $\delta\boldsymbol{a}$, we find the *fundamental commutation relations*

$$\boxed{[\hat{x}_j, \hat{p}_k] = i\hbar\delta_{jk}.} \tag{1.26}$$

Exercise 1.2: Momentum commutators

Translations can be applied in any order $U_p(\boldsymbol{b})U_p(\boldsymbol{a}) = U_p(\boldsymbol{a})U_p(\boldsymbol{b})$. Show that this implies

$$[\hat{p}_j, \hat{p}_k] = 0 \tag{1.27}$$

Exercise 1.3: Eigeinstates of momentum

Show that $\hat{\mathbf{p}}$ is an observable whose eigenstates $|\mathbf{p}\rangle$ are given by

$$|\mathbf{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}}\int d^3\mathbf{r}e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}|\mathbf{r}\rangle \tag{1.28}$$

1.4.5 Time translation

In classical mechanics the Hamiltonian is the instantaneous system energy, and time translation is a canonical transformation. In quantum mechanics time is a parameter, not an operator, so that formulating time evolution requires additional information outside of the Hilbert space structure, however, we can make an inspired guess based upon the knowledge that the Hamiltonian is the generator of time evolution in classical mechanics. In essence, we use the fact that time evolution is a continuous symmetry, and the invariance of the equations of motion under time translations (Noether's theorem). A unitary operator that generates infinitesimal time translation by δt is given by the choices

$$G = \hat{H}, \tag{1.29}$$

$$\varepsilon = \delta t, \tag{1.30}$$

where $\hat{H}$ is the Hamiltonian. Applying this to the state ket gives

$$\left(1 - i\hat{H}\delta t/\hbar\right)|\psi, t\rangle \equiv |\psi, t\rangle + \delta t\frac{\partial}{\partial t}|\psi, t\rangle, \tag{1.31}$$

where this is taken as the *definition* of time evolution, equivalent to the postulated form (1.5) of the *time-dependent Schrödinger equation*

$$\boxed{i\hbar\frac{\partial}{\partial t}|\psi, t\rangle = \hat{H}|\psi, t\rangle.} \tag{1.32}$$

It is convenient to define a unitary time evolution operator by its action on kets

$$\boxed{|\psi, t\rangle \equiv \hat{U}(t, t_0)|\psi, t_0\rangle,} \tag{1.33}$$

given the special notation $\hat{U}(t, t_0)$. Note however, that for time translation, the composition rule (1.13) cannot be used to find $\hat{U}(t, t_0)$ because the Hamiltonian does not (in general) commute with itself at different times. For the general case, we can use the definition (1.33) in (1.32), and since $|\psi\rangle$ is arbitrary, find the equation of motion for the time evolution operator

$$\boxed{i\hbar\frac{\partial}{\partial t}\hat{U}(t, t_0) = \hat{H}\hat{U}(t, t_0).} \tag{1.34}$$

The general solution of this equation will be presented in the next chapter.

Exercise 1.4: Time-independent Hamiltonian

Show that if $\hat{H}$ is time-independent, then we can find the finite-time operator

$$\hat{U}(t, t_0) = \exp\left(-\frac{i\hat{H}(t - t_0)}{\hbar}\right) \tag{1.35}$$

Exercise 1.5: Time dependent Hamiltonian

Show that for a time dependent Hamiltonian, if $[\hat{H}(t), \hat{H}(t')] = 0$, then the formal solution is

$$\hat{U}(t, t_0) = \exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} dt'\ \hat{H}(t')\right) \tag{1.36}$$

1.4.6 Conservation of momentum

Dynamical conservation of a given quantity arises when the underlying symmetry is related to time evolution. For a particle moving in free space, displacing the system does not alter its time evolution since the evolution is merely translated (provided space is isotropic and homogeneous). Formally, this means that the displaced system evolves to the system obtained by displacing the original system after time evolution. Hence, for any $|\psi\rangle$, we must have

$$U(t, t_0)U_p(\boldsymbol{a})|\psi\rangle = U_p(\boldsymbol{a})U(t, t_0)|\psi\rangle, \quad \text{and hence,} \tag{1.37}$$

$$\boxed{U(t, t_0)U_p(\boldsymbol{a}) = U_p(\boldsymbol{a})U(t, t_0).} \tag{1.38}$$

Making use of the infinitesimal forms of the two operators, we find

$$[\hat{H}, \hat{p}_j] = 0. \tag{1.39}$$

Consequently, if $|\mathbf{p}\rangle$ is an eigenstate of the momentum operator, then it will remain so under time evolution.

1.4.7 Symmetry operators

The preceding statements can be made more general, by noting that any symmetry must take the form (1.38), and so, given that the symmetry operator must also be unitary and Hermitian, we have, for any symmetry S

$$\boxed{S^\dagger H S = H} \tag{1.40}$$

1.5 Schrödinger's Equation

In the position representation we can obtain a more familiar form of the Schrödinger equation for the wavefuction corresponding to the sate ket $|\psi, t\rangle$:

$$\psi(\mathbf{r}, t) = \langle \mathbf{r}|\psi, t\rangle, \tag{1.41}$$

and so we have, from (1.32),

$$i\hbar\frac{\partial\psi(\mathbf{r}, t)}{\partial t} = \langle \mathbf{r}|H|\psi, t\rangle. \tag{1.42}$$

If the Hamiltonian is $H = \hat{\mathbf{p}}^2/2m + V(\hat{\mathbf{r}})$, then

$$\langle \mathbf{r}|V(\hat{\mathbf{r}})|\psi, t\rangle = V(\mathbf{r}), \tag{1.43}$$

and using (1.18), we have

$$\langle \mathbf{r}|\hat{\mathbf{p}}|\psi, t\rangle = -i\hbar\nabla\psi(\mathbf{r}, t), \tag{1.44}$$

and hence

$$\langle \mathbf{r}|\frac{\hat{\mathbf{p}}^2}{2m}|\psi, t\rangle = -\frac{\hbar^2\nabla^2}{2m}\psi(\mathbf{r}, t), \tag{1.45}$$

leading to the Schrödinger equation in the form

$$\boxed{i\hbar\frac{\partial\psi(\mathbf{r}, t)}{\partial t} = \left(-\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{r})\right)\psi(\mathbf{r}, t).} \tag{1.46}$$

Exercise 1.6: General form of the Schrödinger equation

If the Hamiltonian is a general function $H(\hat{\mathbf{r}}, \hat{\mathbf{p}})$ of momentum and position operators, show that the Schrödinger equation takes the form

$$i\hbar\frac{\partial\psi(\mathbf{r}, t)}{\partial t} = H(\mathbf{r}, -i\hbar\nabla)\psi(\mathbf{r}, t), \tag{1.47}$$

where the ordering of operators is preserved.

1.6 Discrete Symmetries

Perhaps the most important discrete symmetry in quantum mechanics occurs under the operation of particle exchange for indistinguishable particles. Another important example is that of time-reversal, however in this course we will forego a detailed analysis of this symmetry.

1.6.1 Exchange symmetry

In quantum mechanics we deal with indistinguishable particles, and this property of quanta has far reaching consequences. Consider two particles with coordinates $\mathbf{r}_1, \mathbf{r}_2$. We represent the interchange of particles by the permutation operator $\mathcal{P}$ acting on the wavefunction

$$\mathcal{P}\psi(\mathbf{r}_1, \mathbf{r}_2) = \psi(\mathbf{r}_2, \mathbf{r}_1). \tag{1.48}$$

Clearly $\mathcal{P}^2 = 1$. Furthermore, the Hamiltonian is invariant under the permutation, $\mathcal{P}H\mathcal{P}^{-1} = H$, and consequently $\mathcal{P}$ and H commute:

$$[\mathcal{P}, H] = 0, \tag{1.49}$$

and these operators can be simultaneously diagonalised. If ψ is an eigenfunction of H with energy eigenvalue E, $H\psi = E\psi$, then $\mathcal{P}H\psi = E\mathcal{P}\psi$, and hence

$$\mathcal{P}H\psi = (\mathcal{P}H\mathcal{P}^{-1})\mathcal{P}\psi = H\mathcal{P}\psi = E\mathcal{P}\psi, \tag{1.50}$$

so that $\mathcal{P}\psi$ also an eigenfunction of H with the *same* energy. If the energy is not degenerate, then $\mathcal{P}\psi$ and ψ must describe the same sate, and $\mathcal{P}\psi$ can only differ from ψ by a normalization factor. Since $\mathcal{P}^2 = 1$, the factor can be chosen to be ±1, and thus

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \pm\psi(\mathbf{r}_2, \mathbf{r}_1). \tag{1.51}$$

That is, the wavefunction must be either symmetric or antisymmetric under the interchange of particle coordinates. Particles with the symmetric property are called *Bosons* and obey *Bose statistics*, while those with the antisymmetric property are called *Fermions* and obey *Fermi statistics*.

2 Pictures of Quantum Dynamics

2.1 Schrödinger Picture

There is considerable flexibility in quantum mechanics regarding the dynamics we attribute to the various elements of the theory. Consider an observable A, with Schrödinger picture expectation value

$$\langle A(t)\rangle = \langle \psi, t|A(t)|\psi, t\rangle, \tag{2.1}$$

where in general the operator A can contain explicit time dependence even in the Schrödinger picture; we will denote Schrödinger picture operators by the absence of a subscript. However, we have a clear definition for the way state kets evolve, namely via (1.33), (1.34). Thus we can write

$$\boxed{\langle A(t)\rangle = \langle \psi, t_0|U^\dagger(t,t_0)A(t)U(t,t_0)|\psi, t_0\rangle,} \tag{2.2}$$

where the quantity on the left is observable, and independent of the representation of quantum dynamics we choose.

In the Schrödinger picture, time evolution occurs for state-kets, while operators only contain their explicit time dependence:

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle, \tag{2.3}$$

$$\frac{dA}{dt} = \frac{\partial A}{\partial t} \tag{2.4}$$

For the general case where H is time dependent, we must focus on solving the differential equation (1.34). We will see how to do this in Section 2.3, by focusing on the role of an interaction Hamiltonian. The generalisation to arbitrary Hamiltonians is immediate.

2.2 Heisenberg Picture

In the Heisenberg picture we attribute the time evolution to the operators, preserving the state kets. We can define the Heisenberg picture operator When there is no explicit time dependence in the operators, the formal solution to this equation can be written in terms of the time evolution operator (1.33) as

$$\boxed{A_H(t) = U^\dagger(t,t_0)A(t)U(t,t_0).} \tag{2.5}$$

Using (1.34), we find

$$\frac{dA_H}{dt} = -\frac{i}{\hbar}[A_H, H] + U^\dagger(t, t_0)\frac{\partial A}{\partial t}U(t, t_0). \tag{2.6}$$

Noting that A is ultimately just a function of $\hat{x}$ and $\hat{p}$, and these operators transform to $\hat{x}_H(t) = U^\dagger(t, t_0)\hat{x}U(t, t_0)$, etc, we have the *Heisenberg equation of motion*

$$\boxed{\frac{dA_H}{dt} = -\frac{i}{\hbar}[A_H, H] + \frac{\partial A_H}{\partial t}.} \tag{2.7}$$

and all of the time dependence has been moved into the operator evolution, so the kets are now time-invariant.

2.3 Interaction Picture (Dirac Picture)

In practice, it is usually the case that the Hamiltonian can be divided into a system Hamiltonian H_0 describing the bare evolution of each mode of the system in the absence of interactions, and an interaction Hamiltonian V_I describes interactions between modes. In many cases, the system evolution is rather trivial, but may represent a rapid time evolution due to a significant energy. *Dirac* introduced the interaction picture of time evolution that is intermediate between Schrödinger and Heisenberg that simplifies dynamical problems. We write the Hamiltonian in the *Schrödinger* picture as

$$H = H_0 + V(t), \tag{2.8}$$

where we assume that H_0 is independent of time, and the interaction Hamiltonian $V(t)$ may have explicit time dependence. In the *interaction picture* we define the operators and states as

$$A_I(t) = e^{iH_0t/\hbar}A_S e^{-iH_0t/\hbar}, \tag{2.9}$$

$$|\psi_I(t)\rangle = e^{iH_0t/\hbar}|\psi_S(t)\rangle \tag{2.10}$$

giving the time evolution

$$i\hbar\frac{dA_I}{dt} = [A_I(t), H_0], \tag{2.11}$$

$$i\hbar\frac{d}{dt}|\psi_I(t)\rangle = V_I(t)|\psi_I(t)\rangle, \tag{2.12}$$

where

$$V_I(t) \equiv e^{iH_0t/\hbar}V(t)e^{-iH_0t/\hbar} \tag{2.13}$$

is the interaction Hamiltonian in the interaction picture. Thus the operators evolve according to H_0, while the state ket evolution is governed by $V_I(t)$. In terms of the unitary system evolution operator $U_0(t) = e^{-iH_0t/\hbar}$, the interaction picture variables can be written as

$$A_I(t) = U_0^\dagger(t) A_S U_0(t), \tag{2.14}$$

$$|\psi_I(t)\rangle = U_0^\dagger(t)|\psi_S(t)\rangle = U_0^\dagger(t)U(t)|\psi_S(0)\rangle. \tag{2.15}$$

A word of caution: it is common to rather swiftly go into an interaction picture and immediately discard the labels of operators that keep track of the picture. The rationale is similar to that encountered when dropping the "hats" above operators: the context makes it clear that the problem is being solved in an interaction picture. This statement comes with the priviso that one understands the physical system involved — at least at some basic level. It is important to always have in the back of your mind that there is a system Hamiltonian at work causing time evolution with a particular set of energy eigenvalues.

2.3.1 Formal solution via Dyson series

The general problem is now reduced to finding the evolution of the state kets with respect to this modified interaction Hamiltonian. The formal solution of the equation of motion (2.12) is obtained via the Dyson series. Given that time evolution is unitary, there is an operator $U_I(t, t_0)$ that generates time evolution in the interaction picture

$$|\psi_I(t)\rangle = U_I(t, t_0)|\psi_I(t)\rangle, \tag{2.16}$$

and which obeys the equation of motion

$$\frac{dU_I(t, t_0)}{dt} = -\frac{i}{\hbar} V_I(t) U_I(t, t_0), \tag{2.17}$$

with initial condition $U_I(t_0, t_0) = 1$. An implicit solution is found by formally integrating to give

$$U_I(t, t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt_1 V_I(t_1) U_I(t_1, t_0), \tag{2.18}$$

and this solution may be iteratively reused to find

$$U_I(t, t_0) = 1 + \sum_{n=1}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{n-1}} dt_n V_I(t_1) V_I(t_2) \ldots V_I(t_n), \tag{2.19}$$

where the ordering of operators must be carefully accounted for.

This expression is more conveniently expressed in terms of the *time ordered product*, **T**, defined to reorder any operator product so as act with operators in chronological order. Specifically, for any operator product with different time arguments $t_1 > t_2 > t_3$, the action is

$$\mathbf{T}\{A(t_3)B(t_1)C(t_2)\} = B(t_1)C(t_2)A(t_3). \tag{2.20}$$

Noting that, for example

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \mathbf{T}\left\{V_I(t_1)V_I(t_2)\right\} = \int_{t_0}^{t} dt_1 \left(\int_{t_0}^{t_1} dt_2\ V_I(t_1)V_I(t_2) + \int_{t_1}^{t} dt_2\ V_I(t_2)V_I(t_1)\right)$$

$$= 2\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2\ V_I(t_1)V_I(t_2), \tag{2.21}$$

we find in general

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{n-1}} dt_n V_I(t_1)V_I(t_2)\ldots V_I(t_n) = \frac{1}{n!}\mathbf{T}\left\{\left(\int_{t_0}^{t} d\tau\ V_I(\tau)\right)^n\right\}, \tag{2.22}$$

and hence the Dyson series can be rewritten as

$$\boxed{U_I(t,t_0) = \mathbf{T}\left\{\exp\left(-\frac{i}{\hbar}\int_{t_0}^{t} d\tau\ V_I(\tau)\right)\right\}} \tag{2.23}$$

Exercise 2.1: Time ordering the Dyson series

Prove (2.21), and (2.23).

2.4 Canonical Quantization

While there is no rigorous way of proceeding directly from classical mechanics to quantum mechanics, there are two principal procedures, both of which were formulated by *Dirac*. The simplest of these is called *canonical quantization*, and provides a mapping from the Hamiltonian formulation of classical mechanics. The other is the *path integral formulation*, further developed by *Feynman*, and based upon the Lagrangian formulation of classical mechanics. The latter is more technical, and we will not find use for it in this course. It has the advantage of being better suited for relativistic regimes.

The procedure of canonical quantization runs as follows:

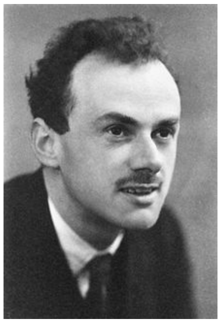

Figure 2.1: In his 1926 doctoral thesis **Paul Dirac** gave a very general and constructive approach to quantizing a classical system. The procedure is called *canonical quantization*, due to the central role played by the canonical coordinates of Hamilton's formulation of classical mechanics.

i) Set up a system of generalised co-ordinates q_i appropriate to the system and identify the Lagrangian $L(q_i, \dot{q}_i)$. This gives a formulation of classical mechanics in terms of the *principle of the stationary action*.

ii) Compute the generalised momenta

$$\boxed{p_i = \frac{\partial L}{\partial \dot{q}_i}} \tag{2.24}$$

iii) These canonical co-ordinates q_i, p_i satisfy the classical *Poisson bracket* relationships $\left\{q_i, p_j\right\}_P = \delta_{ij}$, where for any two functions of the coordinates the bracket is defined as

$$\left\{f(q_i, p_j), g(q_i, p_j)\right\}_P = \sum_j \frac{\partial f}{\partial q_j}\frac{\partial g}{\partial p_j} - \frac{\partial f}{\partial p_j}\frac{\partial g}{\partial q_j}. \tag{2.25}$$

iv) The corresponding quantum operators $\hat{p}_i, \hat{q}_i$ will have the *commutation relations* $[\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij}$.

v) Compute the Hamiltonian

$$\boxed{H(q_i, p_i) = \sum p_i \dot{q}_i - L. \tag{2.26}}$$

vi) The quantized Hamiltonian $\hat{H}$ is the same function of the $\hat{p}_i$ and $\hat{q}_i$ as in classical mechanics — however there may be ambiguities due to choices of operator ordering. The ordering must be chosen to make $\hat{H}$ *Hermitian*.

vii) The Heisenberg equations of motion for operators are computed using the commutation relation $[\hat{q}_i, \hat{p}_j] = i\hbar\delta_{ij}$.

viii) The wavefunction can be chosen as a function of variables q_i, and the operator $\hat{p}_j$ when acting on this wavefunction can be chosen as $-i\hbar\partial/\partial q_j$.

Exercise 2.2: Quantizing the pendulum

1. Carry out the canonical quantization procedure for a simple pendulum consisting of mass m subject to earth's gravity attached to a rigid massless rod of length l, that is fixed at the other end, and allowed to move in a single vertical plane. Take as your canonical coordinate the angle subtended between the rod and the downward direction.
2. Give a *qualitative* account of the eigenfunctions of the Schrödinger equation by describing the limit of large and small energy (Hint: for this purpose you may ignore the fact that the angle is periodic and treat it as an unbounded coordinate).

3 Elementary Quantum Systems

At this point it is worthwhile to review some of the properties of elementary quantum systems. We will outline some of the essential aspects of the simple harmonic oscillator, two level systems, operator algebra, coherent states and numbers states. These concepts have universal application across all of quantum physics.

3.1 Simple Harmonic Oscillator

In classical and quantum mechanics, the Hamiltonian for a single particle in a simple harmonic oscillator potential is

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}. \tag{3.1}$$

The commutation relations $[x, p] = i\hbar$ provide our route to quantisation whereby the classical coordinates are replaced with quantum operators.

3.1.1 Schrödinger picture

In the Schrödinger picture the quantum state $|\psi, t\rangle$ evolves according to the equation of motion (2.3), and the operators are time-invariant. Defining the operators

$$a = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega x + ip), \tag{3.2}$$

$$a^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(m\omega x - ip), \tag{3.3}$$

we have

$$[a, a^\dagger] = 1 \tag{3.4}$$

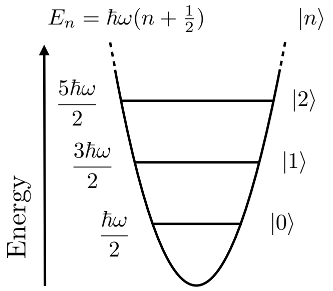

Figure 3.1: Ladder of states for a one dimensional harmonic oscillator.

and the Hamiltonian becomes

$$\boxed{H = \hbar\omega\left(a^\dagger a + \tfrac{1}{2}\right),} \tag{3.5}$$

where the operator $a^\dagger a$ determines the system energy. The eigenstates in the position representation can be labelled by the eigenvalue of this operator, n, and satisfy

$$\hbar\omega(n + \tfrac{1}{2})\psi_n(x) = \left(\frac{-\hbar^2\partial_x^2}{2m} + \frac{m\omega^2 x^2}{2}\right)\psi_n(x) \tag{3.6}$$

with solutions that are well known as products of Hermite polynomials and an overall Gaussian envelope.

3.1.2 Heisenberg picture

Given the Hamiltonian $H_0 = \hbar\omega a^\dagger a$, the Heisenberg picture operators take the form

$$a(t) = e^{i\omega t a^\dagger a} a e^{-i\omega t a^\dagger a}, \tag{3.7}$$

Furthermore $\dot{a}(t) = -i[a, H_0]/\hbar = -i\omega a$, for which the formal solution is $a(t) = e^{-i\omega t}a(0)$. Hence we have

$$\boxed{e^{i\omega t a^\dagger a} a e^{-i\omega t a^\dagger a} = a e^{-i\omega t}.} \tag{3.8}$$

3.2 Fock States or Number States

Given a single spatial mode containing *Bose* particles described by operators a and $a^\dagger$, so that

$$\boxed{[a, a^\dagger] = 1, \quad [a^{(\dagger)}, a^{(\dagger)}] = 0,} \tag{3.9}$$

we can introduce a set of *Fock states* that are defined as eigenstates of the number operator $n = a^\dagger a$

$$\boxed{a^\dagger a|n\rangle = n|n\rangle,} \tag{3.10}$$

and clearly the ground (vacuum) state satisfies $a^\dagger a|0\rangle = 0$. These states form a complete and orthonormal set:

$$\langle n|m\rangle = \delta_{nm}, \tag{3.11}$$

$$\sum_{n=0}^{\infty} |n\rangle\langle n| = 1 \tag{3.12}$$

and thus form a complete set of basis states for the singe-mode Hilbert space for Bosons. The number states are created from the vacuum by successive actions of the creation operator

$$\boxed{|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle.} \tag{3.13}$$

Exercise 3.1: Number states from vacuum states

Show that the definition of the eigenproblem (3.10), together with the commutation relation (3.9) is sufficient to completely determine the action of the creation and annihilation operators on the number states as

$$a|n\rangle = \sqrt{n}|n-1\rangle, \qquad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \tag{3.14}$$

and thus derive (3.13).

3.3 Operator Algebra

3.3.1 Baker-Campbell-Hausdorff theorem

Given any operators for which $[A,[A,B]] = [B,[A,B]] = 0$, there is a very useful factorisation of the exponential (a proof can be found in many texts)

$$e^{A+B} = e^A e^B e^{-[A,B]/2} = e^B e^A e^{[A,B]/2}. \tag{3.15}$$

The special case where the commutator is a c-number often occurs, for example $[q,p] = i\hbar$ or $[a,a^\dagger] = 1$, so the theorem has many applications.

3.3.2 General commutators for Boson operators

For any integer n, it can be shown by induction on n that

$$[a, a^{\dagger n}] = n a^{\dagger n-1} = \frac{\partial a^{\dagger n}}{\partial a^\dagger}, \quad [a^\dagger, a^n] = -n a^{n-1} = -\frac{\partial a^n}{\partial a}. \tag{3.16}$$

Consequently, for any function $f(a,a^\dagger)$ that may be expanded in a power series in a and $a^\dagger$, we also have

$$[a, f(a,a^\dagger)] = \frac{\partial f}{\partial a^\dagger}, \qquad [a^\dagger, f(a,a^\dagger)] = -\frac{\partial f}{\partial a}. \tag{3.17}$$

The corresponding expressions for operators position and momentum operators q, p, related to a, $a^\dagger$ via (3.2), (3.3), with $[q,p] = i\hbar$ are

$$[q, f(q,p)] = i\hbar\frac{\partial f}{\partial p}, \qquad [p, f(q,p)] = -i\hbar\frac{\partial f}{\partial q} \tag{3.18}$$

3.4 Coherent States

Coherent states play a central role in quantum mechanics due to their importance for describing modes containing a large number of bosons. They are states with a maximal coherence, and a classical behaviour, and where first obtained by Schrödinger as minimum uncertainty solutions of the Schrödinger equation that balance the uncertainty equally between X and P. It is difficult to overstate the importance of coherent states. They provide, for example, a first approximation to the quantum state of the coherent light emitted by a laser, of atoms in a dilute gas Bose-Einstein condensate, and of the Cooper pairs of electrons responsible for superconductivity. Coherent states are not eigenstates of any Hamiltonian, rather, they are eigenstates of the annihilation operator that are parametrised by complex eigenvalue α:

$$\boxed{a|\alpha\rangle = \alpha|\alpha\rangle. \qquad (3.19)}$$

In the number state basis, the coherent states take the form

$$\boxed{|\alpha\rangle = e^{-|\alpha|^2/2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle, \qquad (3.20)}$$

involving all possible states $|n\rangle$. This expression gives an indication as to why the corresponding eigenproblem for the creation operator, $a^\dagger|\psi\rangle = \lambda|\psi\rangle$, has no solutions, since the action of the creation operator will remove the vacuum contribution to a number-state expansion of $|\psi\rangle$.

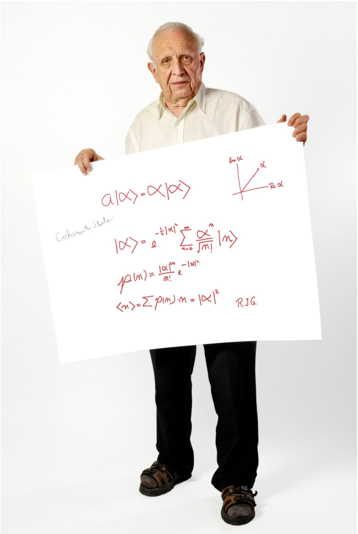
$a|\alpha\rangle = \alpha|\alpha\rangle$
Im α
α
Re α
Coherent State:
$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle$
$p(n) = \frac{|\alpha|^{2n}}{n!}e^{-|\alpha|^2}$
$\langle n\rangle = \sum p(n)\cdot n = |\alpha|^2$
R.J.G.

Figure 3.2: In 1963 **Roy Glauber** introduced *coherent states* in the quantum theory of light. Glauber gave a theory of photodetection in which coherent states are the natural eigenstates of the detection process (photon annilation); he shared the 2005 Nobel Prize in Physics for his discovery.

Exercise 3.2: Number state representation of coherent states

Expand the coherent states in (3.19) in the number state basis and find a recursion relation for the expansion coefficients in terms of a normalisation constant to be determined. Evaluate the normalisation constant, and thus verify (3.20).

The overlap between coherent states

$$|\langle\alpha|\beta\rangle|^2 = e^{-|\alpha-\beta|^2}, \qquad (3.21)$$

shows that they are not orthogonal. The resolution of the identity for these *overcomplete* states reads

$$\frac{1}{\pi}\int d^2\alpha\ |\alpha\rangle\langle\alpha| = 1, \qquad (3.22)$$

where the integral is over the complex plane $\int d^2\alpha \equiv \int_{-\infty}^{\infty} d\alpha_r \int_{-\infty}^{\infty} d\alpha_i$, for $\alpha \equiv \alpha_r + i\alpha_i$.

Using the number state representation, one finds that the number statistics of coherent states are *Poissonian*:

$$\boxed{P(n) \equiv |\langle n|\alpha\rangle|^2 = \frac{\bar{n}^n}{n!}e^{-\bar{n}}, \qquad (3.23)}$$

where $\bar{n} \equiv \langle\alpha|a^\dagger a|\alpha\rangle = |\alpha|^2$.

Exercise 3.3: Poissonian number fluctuations

1. Calculate $\langle\alpha|(a^\dagger a - \bar{n})^2|\alpha\rangle$ and interpret the result in light of (3.23).
2. Use (3.20) to confirm (3.22) by evaluating the integral.

Using the momentum and position operators (3.2), (3.3), it is straightforward to show that coherent states are minimum uncertainty states:

$$\Delta p \Delta q = \frac{\hbar}{2}. \tag{3.24}$$

Using (3.13) is is easily seen that coherent states may be created from the vacuum as

$$|\alpha\rangle = e^{-|\alpha|^2/2} e^{\alpha a^\dagger} |0\rangle. \tag{3.25}$$

Physically, coherent states can be created by exciting a quantum harmonic oscillator with a classical driving field. An example is provided by an optical cavity mode driven by a coherent laser field, with classical amplitude ε (sadly we do not have space in this course for a quantum theory of the laser). The interaction Hamiltonian for this process is

$$H_{int} = i\hbar \left(\varepsilon a^\dagger - \varepsilon^* a \right), \tag{3.26}$$

for which the time-evolution operator is

$$D(\alpha) \equiv e^{\alpha a^\dagger - \alpha^* a}, \tag{3.27}$$

with $\alpha = \varepsilon t$. Continuous driving of the cavity mode will create a large-amplitude coherent state for the oscillator

$$\boxed{|\alpha\rangle = D(\alpha)|0\rangle.} \tag{3.28}$$

Using the Baker-Hausdorf lemma (3.15), one can then show that (3.28) and (3.25) are equivalent. The operator (3.27) is a *displacement* operator, as it displaces the vacuum state to amplitude α on the complex plane.

Exercise 3.4: Coherent states are displaced vacuum states

Prove that (3.28) and (3.25) are equivalent.

Exercise 3.5: Time evolution of a coherent state

Show that for a simple harmonic oscillator evolving according to the system Hamiltonian $H = \hbar\omega a^\dagger a$, an initial coherent state $|\alpha\rangle$ will evolve into an eigenstete of a with coherent amplitude $\alpha(t) = \alpha e^{-i\omega t}$.

3.5 Pauli matrices for two level systems

Two level systems play a fundamental role in physics, underlying the description of electron states of atoms interacting with radiation, and of spin-1/2 fermonic systems generally. The two level atom is described by a two state wave function

$$|\psi\rangle = u_e|e\rangle + u_g|g\rangle \tag{3.29}$$

so that we may identify the state with the two component vector

$$|\psi\rangle \leftrightarrow \begin{pmatrix} u_e \\ u_g \end{pmatrix}, \tag{3.30}$$

and the two-state problem can be described by this basis. The Pauli matrices are defined as

$$\boxed{\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = i\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad (3.31)}$$

which, together with the matrix identity

$$\mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{3.32}$$

form a complete basis for any two level system. At this point a natural step is to introduce the spin *vector* as a vector over the *field* of Pauli matrices:

$$\boldsymbol{\sigma} \equiv [\sigma_x, \sigma_y, \sigma_z], \tag{3.33}$$

thus utilising the identification of each of the Pauli matrices with a particular spatial axis, and giving a compact notation for physical quantities. For example, the system Hamiltonian may be expressed as

$$H_{sys} = \tfrac{1}{2}\hbar\Omega\boldsymbol{\sigma}\cdot\mathbf{n}, \tag{3.34}$$

where **n** is a 3D unit vector. This notation greatly simplifies many calculations. If $\mathbf{n} = (0, 0, 1)$, then

$$H_{sys} = \tfrac{1}{2}\hbar\Omega\sigma_z = \tfrac{1}{2}\hbar\Omega\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{3.35}$$

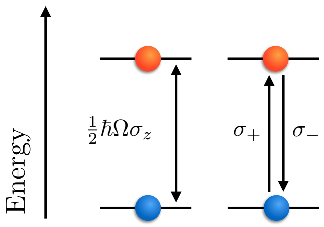

Figure 3.3: Raising and lower operators for a two level atom.

3.5.1 Properties of Pauli matrices

There are a number of useful properties:

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}, \tag{3.36a}$$

$$[\sigma_i, \sigma_j] = 2i\sum_k \epsilon_{ijk}\sigma_k, \tag{3.36b}$$

$$\sigma_i\sigma_j = \delta_{ij} + i\sum_k \epsilon_{ijk}\sigma_k, \tag{3.36c}$$

$$G = \tfrac{1}{2}\left(I\mathrm{Tr}\,(G) + \sum_i \sigma_i\mathrm{Tr}\,(\sigma_i G)\right), \quad \text{for any } 2\times 2 \text{ matrix } G, \tag{3.36d}$$

$$(\boldsymbol{\sigma}\cdot\mathbf{A})(\boldsymbol{\sigma}\cdot\mathbf{B}) = \mathbf{A}\cdot\mathbf{B} + i\boldsymbol{\sigma}\cdot\mathbf{A}\times\mathbf{B}, \tag{3.36e}$$

$$\exp\,(i\theta\boldsymbol{\sigma}\cdot\mathbf{n}) = \cos\theta + i\boldsymbol{\sigma}\cdot\mathbf{n}\sin\theta, \tag{3.36f}$$

$$\exp\,(a + \mathbf{b}\cdot\boldsymbol{\sigma}) = e^a\left(\cosh|\mathbf{b}| + \frac{\boldsymbol{\sigma}\cdot\mathbf{b}}{|\mathbf{b}|}\sinh|\mathbf{b}|\right), \tag{3.36g}$$

where the *Levi-Civita symbol* is defined as

$$\epsilon_{ijk} \equiv \begin{cases} +1 & \text{if } (i,j,k) = (1,2,3) \text{ and cyc. perm,} \\ -1 & \text{if } (i,j,k) = (1,3,2) \text{ and cyc. perm,} \\ 0 & \text{if } i = j \text{ or } j = k \text{ or } k = i. \end{cases} \tag{3.37}$$

Exercise 3.6: Pauli matrix identities

Prove (3.36a)-(3.36f).

It is often convenient to express the two-level system in terms of the raising and lowering operators

$$\sigma_\pm = \tfrac{1}{2}\left(\sigma_x \pm i\sigma_y\right) \tag{3.38}$$

so that, for example

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{3.39}$$

acts to promote the state of a two level atom from the ground to the excited state. These operators have the useful properties

$$\sigma_+^2 = \sigma_-^2 = 0, \quad \sigma_z^2 = 1, \tag{3.40a}$$

$$\sigma_\pm\sigma_\mp = \tfrac{1}{2}(1 \pm \sigma_z), \tag{3.40b}$$

$$[\sigma_+, \sigma_-] = \sigma_z, \tag{3.40c}$$

$$[\sigma_z, \sigma_\pm] = \pm 2\sigma_\pm, \tag{3.40d}$$

$$G = \tfrac{1}{2} I \,\mathrm{Tr}\,(G) + \tfrac{1}{2}\sigma_z \mathrm{Tr}\,(\sigma_z G) + \sigma_+ \mathrm{Tr}\,(\sigma_- G) + \sigma_- \mathrm{Tr}\,(\sigma_+ G)\,. \tag{3.40e}$$

3.5.2 Evolution of an isolated two-level system

It is straightforward to show that the Hamiltonian (3.35) generates the Heisenberg picture time evolution

$$\sigma_\pm(t) = e^{iH_{\text{sys}}t/\hbar}\sigma_\pm e^{-iH_{\text{sys}}t/\hbar} = e^{\pm i\Omega t}\sigma_\pm. \tag{3.41}$$

Exercise 3.7: Free evolution of raising and lowering operators

Prove (3.41).

4 Second Quantization

In this section we introduce the concept of second quantization as a natural extension of canonical quantization to many body systems. For many physical systems the interactions between particles are local or quasi-local in coordinate space, motivating the introduction of *field operators* as a route to quantisation of the single particle Schrödinger wavefunction. This *second quantisation* allows a natural generalization to accommodate *many-body physics*. The essential procedure makes use of a basis of eigenfunctions of a single-particle Schrödinger equation as a suitable expansion of the field operators. For definiteness we confine our discussion to massive particles in this chapter. Quantization of the Electromagnetic Field proceeds along similar lines, as discussed in the next chapter.

4.1 Motivation

Given an orthonormal set of state-kets $|\lambda\rangle$, eigenstates of a single-particle Hamiltonian:

$$H|\lambda\rangle = \epsilon_\lambda|\lambda\rangle, \quad \langle\lambda|\sigma\rangle = \delta_{\lambda,\sigma}, \tag{4.1}$$

this set of states is a complete basis for the one-body Hilbert space:

$$1 = \sum_\lambda |\lambda\rangle\langle\lambda|. \tag{4.2}$$

States in the many-body Hilbert space require correct symmetrisation to account for the quantum statistics of indistinguishable particles, namely, whether they are *Bosons* or *Fermions*. For bosons the wave function must be symmetric under particle exchange, while for fermions it must be antisymmetric. Consider representing the state of two-particles populating only two of these modes $|\lambda_1\rangle$, $|\lambda_2\rangle$. For identical bosons (fermions), we can introduce the index $\zeta = \pm 1$ to describe the statistics of bosons (fermions), and write the correctly symmetrized quantum state as

$$|\lambda_1, \lambda_2\rangle_\zeta = \frac{1}{\sqrt{2}}\left[|\lambda_1\rangle \otimes |\lambda_2\rangle + \zeta|\lambda_2\rangle \otimes |\lambda_1\rangle\right], \tag{4.3}$$

so that the two-body wave function ψ_B (ψ_F), found by projecting onto the coordinate representation $|x_1, x_2\rangle = |x_1\rangle \otimes |x_2\rangle$, is given by

$$\psi_B(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\langle x_1|\lambda_1\rangle\langle x_2|\lambda_2\rangle + \langle x_1|\lambda_2\rangle\langle x_2|\lambda_1\rangle\right], \tag{4.4}$$

$$\psi_F(x_1, x_2) = \frac{1}{\sqrt{2}}\left[\langle x_1|\lambda_1\rangle\langle x_2|\lambda_2\rangle - \langle x_1|\lambda_2\rangle\langle x_2|\lambda_1\rangle\right]. \tag{4.5}$$

The appropriately symmetrized N-particle state can be expressed in the form

$$|\lambda_1, \lambda_2, \ldots, \lambda_N\rangle = \frac{1}{\sqrt{N! \prod_{\lambda_j} n_{\lambda_j}!}} \sum_{\mathcal{P}} \zeta^{(1-\operatorname{sgn}\mathcal{P})/2} |\lambda_{\mathcal{P}1}\rangle \otimes |\lambda_{\mathcal{P}2}\rangle \otimes \cdots \otimes |\lambda_{\mathcal{P}N}\rangle, \tag{4.6}$$

where n_{λ_j} represents the total number of particles in state λ_j (for fermions the exclusion principle forces the additional constraint $n_{\lambda_j} \leq 1$). The summation includes all $N!$ permutations of the quantum numbers $\{\lambda_1, \ldots, \lambda_N\}$, and sgn $\mathcal{P}$ gives the sign of the permutation $\mathcal{P}$[1]. Note that the ordering of the quantum numbers defining $|\lambda_1, \lambda_2, \ldots, \lambda_N\rangle$ must be adhered to.

While describing the symmetrization clearly, this formalism for representing quantum states has serious disadvantages:

i) The practical representation of many-body states requires very large numbers of terms. For example, to calculate the overlap of two states, $(N!)^2$ terms must be computed.

ii) There are very useful statistical ensembles that do not have fixed N, and a more flexible description is desirable.

iii) One often is interested in questions that are more easily formulated in the language of second quantization.

For N particles with positions $\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N$, the system is described by the many-body wavefunction $\phi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N, t) \equiv \langle \mathbf{r}_1, \ldots, \mathbf{r}_N | \phi, t\rangle$. The general problem we consider starts from the expression of the many body Hamiltonian in first-quantization

$$H = \sum_{j=1}^{N} \left[-\frac{\hbar^2}{2m} \nabla_j^2 + V(\mathbf{r}_j) \right] + \frac{1}{2} \sum_{j=1, k \neq j}^{N} U(\mathbf{r}_j, \mathbf{r}_k) + \ldots \tag{4.7}$$

wherein the states evolve according to the many body Schrödinger equation

$$i\hbar \frac{\partial \langle \mathbf{r}_1, \ldots, \mathbf{r}_N | \phi, t\rangle}{\partial t} = i\hbar \frac{\partial \phi(\mathbf{r}_1, \ldots, \mathbf{r}_N, t)}{\partial t} = \langle \mathbf{r}_1, \ldots, \mathbf{r}_N | H | \phi, t\rangle. \tag{4.8}$$

Our aim is to rewrite this formulation in the language of *second-quantization*. This will allow a reformulation of the above description in terms of the action of field operators. The resulting theory is *nonlinear* (note the inherent linearity of (4.8) with respect to the many-body wavefunction). After discussing the free particle kinetic and potential terms, examples of one-body operators, we will see how to find an explicit representation of any two-body operator $U(\mathbf{r}, \mathbf{r}')$.

4.1.1 Many Body Interpretation

There is a direct mapping between the solutions of the free-particle Schrödinger equation, represented by Hamiltonian (3.1), and number state representation for non-interacting Bosons in a single mode defined by (3.9), and (3.10). Note a subtle conceptual distinction: for the solutions of Schrödinger equation in position space $\psi_n(x) \equiv \langle x|n\rangle$, the quantum number n labels the energy of a *single-particle state* with energy $\hbar\omega(n+\frac{1}{2})$. By introducing the number states as above, we now have a representation of a many-body Hilbert space for Bosons in each of a set of *single-particle modes*.

---

[1] sgn $\mathcal{P} = 1(-1)$ if the number of transpositions of two elements that brings the permutation $(\mathcal{P}1, \mathcal{P}2, \ldots, \mathcal{P}N)$ back to its original form $(1, 2, \ldots, N)$ is even (odd).

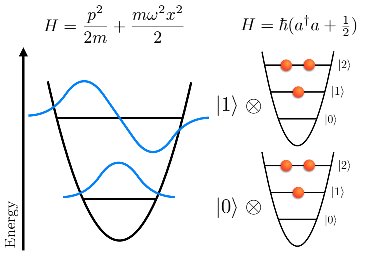

Figure 4.1: Oscillators: solutions of the Schrödinger equation for the harmonic oscillator potential $V(x) = m\omega^2x^2/2$ (left), and the ladder representation of a many-body system (right). The tensor product represents the fact that these states represent different degrees of freedom, motional states (left), and particle number occupation of a *particular* state (right).

4.2 Many-Body Fock Space

We have seen that the number states provide a basis for the single-particle Hilbert space, as any single-particle state can be represented as

$$\boxed{|\psi\rangle = \sum_n |n\rangle\langle n|\psi\rangle = \sum_n c_n|n\rangle. \qquad (4.9)}$$

The natural many-mode generalisation of (3.10) is defined as

$$|n_1,\ldots,n_N\rangle = |n_1\rangle \otimes \ldots |n_N\rangle. \tag{4.10}$$

where these states are now simultaneous eigenstates of the number operators n_σ,

$$\hat{n}_\sigma|n_1,n_2,\ldots\rangle = n_\sigma|n_1,n_2,\ldots\rangle, \tag{4.11}$$

where for brevity we allow σ to run over all of the independent single-particle states, and all possible values of spin or other degrees of freedom required to specify a unique single particle state. For example, for a system of fermions with spatial degrees of freedom described by a set of plane-wave modes $|\mathbf{k}\rangle$ with momentum eigenvalue $\mathbf{k}$, then $n_\sigma \to n_{\mathbf{k},s}$ where s describes the spin state. For photon states, the Fock space includes polarisation so that $n_\sigma \to n_{\mathbf{k},\lambda}$ where $\lambda = 1, 2$ gives two orthogonal polarisations for each electromagnetic plane wave mode with wave vector $\mathbf{k}$. In general, the number operators $\hat{n}_\sigma$ can be chosen to form a complete set of commuting observables for the multimode Fock space. The identity for this Fock space is

$$1 = \sum_{n_j} |n_1,n_2,\ldots\rangle\langle n_1,n_2,\ldots|, \tag{4.12}$$

where the sum runs over all n_j, and all allowed values of each n_j, namely $n_j = 0,1,2,\ldots$ for Bosons, and $n_j = 0,1$ for Fermions.

For many-body states the symmetrization is handled by the commutation relations that the operators satisfy. Defining the generalised commutator

$$\boxed{[A,B]_\zeta \equiv AB - \zeta BA, \qquad (4.13)}$$

where $[A,B]_+ = [A,B] = AB - BA$, and $[A,B]_- = \{A,B\} = AB + BA$, so that $\zeta = +1(-1)$ reproduces the commutation (anti-commutation) relation for Bosons (Fermions). The commutation relations for the raising and lowering operators defining the Fock space are then defined by

$$\boxed{[a_\lambda, a_\sigma^\dagger]_\zeta = \delta_{\lambda\sigma}, \quad [a_\lambda, a_\sigma]_\zeta = [a_\lambda^\dagger, a_\sigma^\dagger]_\zeta = 0 \qquad (4.14)}$$

For bosons the number states of the Fock space are unbounded. For fermions, the double action of the creation operator on the vacuum gives $(a_\sigma^\dagger)^2|0\rangle = 0$, limiting the occupation numbers in (4.11) to 0 or 1, and enforcing Pauli's exclusion principle. Given the definition (4.11) and the commutation relations (4.14), we can find the action of raising and lowering operators on the state kets as

$$a_\sigma^\dagger|n_1,\dots,n_\sigma,\dots\rangle = \zeta^{s_\sigma}\sqrt{n_\sigma+1}|n_1,\dots,n_\sigma+1,\dots\rangle, \tag{4.15}$$

$$a_\sigma|n_1,\dots,n_\sigma,\dots\rangle = \zeta^{s_\sigma}\sqrt{n_\sigma}|n_1,\dots,n_\sigma-1,\dots\rangle \tag{4.16}$$

where $s_\sigma = \sum_{\lambda_j=1}^{\sigma-1} n_{\lambda_j}$, and the ζ^{s_σ} factor now does the work to produce the correct symmetry of the many-body Fock state for identical particles. The many-body Fock states can be created from the vacuum analogously to (3.13) via

$$|n_1,n_2,\dots\rangle = \prod_\sigma \frac{1}{\sqrt{n_\sigma!}}(a_\sigma^\dagger)^{n_\sigma}|0\rangle. \tag{4.17}$$

with the usual constraints on occupation numbers for Bosons and Fermions.

4.3 Change of basis

We first note that any single-particle state can be represented as

$$|\lambda\rangle = a_\lambda^\dagger|0\rangle, \tag{4.18}$$

that is, by creating a state with one particle in a specific single-particle eigenstate $|\lambda\rangle$. Given any two single-particle bases, with creation operators $a_\lambda^\dagger$ and $b_\sigma^\dagger$, we can use the completeness relation (4.2) and (4.18) to change basis according to

$$b_\sigma^\dagger|0\rangle = |\sigma\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\sigma\rangle = \sum_\lambda \langle\lambda|\sigma\rangle a_\lambda^\dagger|0\rangle, \tag{4.19}$$

and similarly for $\langle\sigma| = \langle 0|b_\sigma$. Hence we deduce the general rule for *change of basis*

$$b_\sigma^\dagger = \sum_\lambda \langle\lambda|\sigma\rangle a_\lambda^\dagger, \quad b_\sigma = \sum_\lambda \langle\sigma|\lambda\rangle a_\lambda. \tag{4.20}$$

4.4 Field Operators

One of the most fundamentally important basis representations is the position representation, giving a *continuous field theory*, involving a continuum of quantum numbers to specify the quantum state. We can thus transform from the Fock space to the basis of eigenstates of the position operator

$$\hat{\mathbf{r}}|\mathbf{r}\rangle = \mathbf{r}|\mathbf{r}\rangle \tag{4.21}$$

for which

$$\langle \mathbf{r}|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}'), \tag{4.22}$$

$$1 = \int d^3\mathbf{r}\ |\mathbf{r}\rangle\langle\mathbf{r}|. \tag{4.23}$$

In this case we use (4.20), but we give the new operators a specific notation, and, in terms of the Fock-space operators we have

$$\psi(\mathbf{r}) = \sum_\lambda \langle \mathbf{r}|\lambda\rangle a_\lambda, \quad \psi^\dagger(\mathbf{r}) = \sum_\lambda \langle \lambda|\mathbf{r}\rangle a_\lambda^\dagger. \tag{4.24}$$

Using the fundamental commutation relations (4.14), we can now find the generalised commutation relations

$$\boxed{[\psi(\mathbf{r}),\psi^\dagger(\mathbf{r}')]_\zeta = \delta(\mathbf{r}-\mathbf{r}'), \quad [\psi(\mathbf{r}),\psi(\mathbf{r}')]_\zeta = [\psi^\dagger(\mathbf{r}),\psi^\dagger(\mathbf{r}')]_\zeta = 0,} \tag{4.25}$$

for Bose and Fermi field operators.

4.4.1 Interpretation

The procedure of arriving at the representation (4.24) is known as *second-quantization*, and it can be shown to be equivalent to the first-quantised representation in terms of a many-body wavefunction. Notice that the commutation relations have nothing to do with the *specific* modes of the Fock space underlying the continuous field theory, but merely require that such a basis of single-particle states exists and has the correct orthonormality properties.

The operator $\psi^\dagger(\mathbf{r})$ plays the role of a creation operator for the continuous field theory, by creating a particle at definite position $\mathbf{r}$ as a superposition over all indistinguishable single particle states. Consider the action on the vacuum:

$$\psi^\dagger(\mathbf{r})|0\rangle = \sum_\lambda a_\lambda^\dagger|0\rangle\langle\lambda|\mathbf{r}\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\mathbf{r}\rangle = |\mathbf{r}\rangle. \tag{4.26}$$

However, the state $|\mathbf{r}\rangle$ is not normalizable. A normalised state corresponding to the single-particle wavefunction $\phi(\mathbf{r})$ is

$$|\phi\rangle = \int d^3\mathbf{r}\ \phi(\mathbf{r})\psi^\dagger(\mathbf{r})|0\rangle. \tag{4.27}$$

Exercise 4.1: Field commutators

Prove (4.25) using (4.14), and (4.20).

Exercise 4.2: Normalized state

Assume $\phi(\mathbf{r})$ is normalised to unity. Show, using properties of the field operators, that (4.27) gives a correctly normalised wavefunction.

4.4.2 Plane-wave modes

Let us now consider a specific basis for the Fock space, as defined by the number of particles in each of a set of plane wave modes. For definiteness we consider particles in a large cubical volume of side length L. Assuming periodic boundary conditions on the wave functions, the momenta of the particles can take the values

$$\mathbf{p}_j = \hbar\mathbf{k}_j = \frac{2\pi\hbar}{L}\left\{m_x(j), m_y(j), m_z(j)\right\}, \quad \text{where } m_a(j) = 0, \pm1, \pm2, \pm3, \ldots \tag{4.28}$$

In general, the mode space for the system could involve more quantum numbers to describe each quantum state. In particular, the Fock space for the electromagnetic field requires that each state has definite momentum and polarisation. The box-normalised wave function for a single particle state with wavenumber $\mathbf{k}_j$ is

$$\langle\mathbf{r}|\mathbf{k}_j\rangle = \frac{1}{\sqrt{V}}e^{i\mathbf{k}_j\cdot\mathbf{r}}. \tag{4.29}$$

The field operator now takes the form

$$\psi(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_j e^{i\mathbf{k}_j\cdot\mathbf{r}}a_j. \tag{4.30}$$

The energy of momentum state $\mathbf{p}_j$ is $E_j = \hbar^2\mathbf{k}_j^2/2m$, and the total energy and momentum operators are

$$H = \sum_j \frac{\hbar^2\mathbf{k}_j^2}{2m}a_j^\dagger a_j, \tag{4.31}$$

$$\boldsymbol{P} = \sum_j \hbar\mathbf{k}_j a_j^\dagger a_j, \tag{4.32}$$

for a system with total particle number

$$N = \sum_j a_j^\dagger a_j. \tag{4.33}$$

4.4.3 Properties of Field Operators

We have seen that using the commutation (anti-commutation) rule (4.14) for Bosons (Fermions) we can write down the fundamental commutation relations (4.25) for both Boson and Fermion field operators. However, for either Bosons or Fermions:

i) *Total number operator.—*

$$N = \int d^3\mathbf{r}\ \psi^\dagger(\mathbf{r})\psi(\mathbf{r}), \tag{4.34}$$

ii) *Hamiltonian.—*

$$H = \int d^3\mathbf{r}\ \psi^\dagger(\mathbf{r})\left(-\frac{\hbar^2\nabla^2}{2m}\right)\psi(\mathbf{r}), \tag{4.35}$$

iii) *Total momentum.—*

$$\boldsymbol{P} = \int d^3\mathbf{r}\ \psi^\dagger(\mathbf{r})\,(-i\hbar\nabla)\,\psi(\mathbf{r}), \tag{4.36}$$

iv) *Hamiltonian commutators.*— For commutators only, the following hold

$$[\psi(\mathbf{r}), H] = -\frac{\hbar^2\nabla^2}{2m}\psi(\mathbf{r}), \tag{4.37}$$

$$[\psi^\dagger(\mathbf{r}), H] = \frac{\hbar^2\nabla^2}{2m}\psi^\dagger(\mathbf{r}). \tag{4.38}$$

Exercise 4.3: Free particle

Prove (4.34)-(4.38). Use the basis transformation (4.20) when deriving (4.34)-(4.36).

4.5 Many-Body States

So far we have concentrated on single-particle states in second-quantization. For a general N-body state, the equation of motion is the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\phi, t\rangle = H|\phi, t\rangle. \tag{4.39}$$

Let us consider a two-body state in the second-quantized formalism, defined by

$$|\mathbf{r}_1, \mathbf{r}_2\rangle = \frac{1}{\sqrt{2}}\psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)|0\rangle. \tag{4.40}$$

We then find that, for either Bosons or Fermions, this state has

i) Overlap

$$\langle\mathbf{r}_1, \mathbf{r}_2|\mathbf{r}'_1, \mathbf{r}'_2\rangle = \tfrac{1}{2}\left\{\delta(\mathbf{r}_1 - \mathbf{r}'_1)\delta(\mathbf{r}_2 - \mathbf{r}'_2) + \zeta\delta(\mathbf{r}_1 - \mathbf{r}'_2)\delta(\mathbf{r}_2 - \mathbf{r}'_1)\right\}, \tag{4.41}$$

ii) Identity

$$I = \int d^3\mathbf{r}_1 \int d^3\, \mathbf{r}_2|\mathbf{r}_1, \mathbf{r}_2\rangle\langle\mathbf{r}_1, \mathbf{r}_2|, \tag{4.42}$$

iii) The Schrödinger picture wavefunction

$$\begin{aligned}\phi(\mathbf{r}_1, \mathbf{r}_2, t) &\equiv \langle\mathbf{r}_1, \mathbf{r}_2|\phi, t\rangle \\ &= \langle 0|\psi(\mathbf{r}_1)\psi(\mathbf{r}_2)|\phi, t\rangle,\end{aligned} \tag{4.43}$$

with exchange symmetry $\phi(\mathbf{r}_1, \mathbf{r}_2, t) = \zeta\phi(\mathbf{r}_2, \mathbf{r}_1, t)$.

iv) Equation of motion

$$i\hbar\frac{\partial\phi(\mathbf{r}_1, \mathbf{r}_2)}{\partial t} = \left(-\frac{\hbar^2\nabla_1^2}{2m} - \frac{\hbar^2\nabla_2^2}{2m}\right)\phi(\mathbf{r}_1, \mathbf{r}_2, t), \tag{4.44}$$

using (4.37).

The generalisation to normalised N-particle states is rather obvious. The states are

$$\boxed{|\mathbf{r}_1, \mathbf{r}_2 \ldots \mathbf{r}_N\rangle = \frac{1}{\sqrt{N!}}\psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)\ldots\psi^\dagger(\mathbf{r}_N)|0\rangle,} \tag{4.45}$$

with identity

$$I = \int d^3\mathbf{r}_1 \ldots \int d^3\mathbf{r}_N \; |\mathbf{r}_1, \ldots, \mathbf{r}_N\rangle\langle\mathbf{r}_1, \ldots, \mathbf{r}_N|, \tag{4.46}$$

so that the state

$$\phi(\mathbf{r}_1, \ldots \mathbf{r}_N, t) = \langle 0| \frac{\psi(\mathbf{r}_1) \ldots \psi(\mathbf{r}_N)}{\sqrt{N!}} |\phi, t\rangle \tag{4.47}$$

has normalization

$$\int d^3\mathbf{r}_1 \ldots d^3\mathbf{r}_N |\phi(\mathbf{r}_1, \ldots, \mathbf{r}_N, t)|^2 = 1. \tag{4.48}$$

Thus the creation of many-body position eigenstates is expressed in terms of field operators acting on the vacuum.

4.6 Interactions between particles

4.6.1 One-body operators

Thus far we have met one-body operators, and have seen how to create many body states. Let us briefly revisit the process of constructing many-body operators. A convenient way of constructing many-body operators is to start from a Fock space in which the operator is diagonal, and then transform to an arbitrary basis. For our state kets defined in (4.1), we define the number operator

$$\hat{n}_{\lambda_j} = \hat{a}^\dagger_{\lambda_j} \hat{a}_{\lambda_j}, \tag{4.49}$$

which will define the Fock space via (4.10). Consider an operator in the extended Fock space (4.10), that is *diagonal* in this representation. The operator has a particularly simple representation in the many-body Fock space as

$$\hat{O} = \sum_{n_{\lambda_j}} |n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle\langle n_{\lambda_1}, n_{\lambda_2}, \ldots| \hat{O} \sum_{n_{\lambda_k}} |n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle\langle n_{\lambda_1}, n_{\lambda_2}, \ldots|, \tag{4.50}$$

$$= \sum_{n_{\lambda_j}} |n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle\langle n_{\lambda_1}, n_{\lambda_2}, \ldots| O_{\lambda_1, \lambda_2, \ldots}, \tag{4.51}$$

where

$$O_{\lambda_1, \lambda_2, \ldots} \equiv \langle n_{\lambda_1}, n_{\lambda_2}, \ldots |\hat{O}| n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle. \tag{4.52}$$

We now define a one-body operator $\hat{O}^{(1)}$ in a natural way, namely that for such an operator only one of the n_{λ_j} is changed in (4.52).

Furthermore, since the operator is diagonal, the matrix elements in the Fock space are

$$\langle n'_{\lambda_1}, n'_{\lambda_2}, \ldots |\hat{O}^{(1)}| n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle = \sum_j O^{(1)}_{\lambda_j} n_{\lambda_j} \langle n'_{\lambda_1}, n'_{\lambda_2}, \ldots | n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle$$

$$= \langle n'_{\lambda_1}, n'_{\lambda_2}, \ldots | \sum_j O^{(1)}_{\lambda_j} \hat{n}_{\lambda_j} | n_{\lambda_1}, n_{\lambda_2}, \ldots\rangle, \tag{4.53}$$

for arbitrary n_{λ_j}, and hence we deduce the diagonal form of an arbitrary one-body operator

$$\hat{O}^{(1)} = \sum_{\lambda} \langle \lambda | \hat{O}^{(1)} | \lambda \rangle \hat{a}^{\dagger}_{\lambda} \hat{a}_{\lambda}, \tag{4.54}$$

consistent with the expressions (4.31), (4.32), (4.33). Transforming to an arbitrary basis representation we arrive at the *general form of a one-body operator*

$$\hat{O}^{(1)} = \sum_{\lambda\mu} \langle \lambda | \hat{O}^{(1)} | \mu \rangle a^{\dagger}_{\lambda} a_{\mu}. \tag{4.55}$$

4.6.2 Two-body operators

Two-body operators are required to represent pairwise interactions between particles. Particle indistinguishability makes inclusion of two-body potentials rather cumbersome within first quantization. In the language of second-quantization the formulation is considerably more straightforward.

Initially we consider two particles at $\mathbf{r}_n$ and $\mathbf{r}_m$ subject to a symmetric two-body potential $U(\mathbf{r}_m, \mathbf{r}_n) \equiv U(\mathbf{r}_n, \mathbf{r}_m)$. Thus, our two-body operator is conveniently represented in the position basis, and we wish to find an operator $\hat{U}$ in second-quantized form whose action on a many-body state gives an identical result:

$$\hat{U} | \mathbf{r}_1, \ldots, \mathbf{r}_N \rangle = \sum_{n=1}^{N} \sum_{m>n}^{N} U(\mathbf{r}_n, \mathbf{r}_m) | \mathbf{r}_1, \ldots, \mathbf{r}_N \rangle = \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1, m\neq n}^{N} U(\mathbf{r}_n, \mathbf{r}_m) | \mathbf{r}_1, \ldots, \mathbf{r}_N \rangle. \tag{4.56}$$

By analogy with the general form of one-body operators, working in the position representation one might be tempted to guess the form

$$\hat{U} = \frac{1}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \; \psi^{\dagger}(\mathbf{r}) \psi^{\dagger}(\mathbf{r}') U(\mathbf{r}, \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}), \tag{4.57}$$

and indeed, we can confirm that this is correct. We proceed by applying the field operators to (4.45), and making use of (4.25), $\psi(\mathbf{r})\psi^{\dagger}(\mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') + \zeta \psi^{\dagger}(\mathbf{r}')\psi(\mathbf{r})$:

$$\begin{aligned} \psi^{\dagger}(\mathbf{r})\psi^{\dagger}(\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r}) | \mathbf{r}_1, \ldots, \mathbf{r}_N \rangle \sqrt{N!} &= \psi^{\dagger}(\mathbf{r})\psi^{\dagger}(\mathbf{r}')\psi(\mathbf{r}')\psi(\mathbf{r})\psi^{\dagger}(\mathbf{r}_1) \ldots \psi^{\dagger}(\mathbf{r}_N) | 0 \rangle, \\ = \sum_{n=1}^{N} \zeta^{n-1} \delta(\mathbf{r} - \mathbf{r}_n) \psi^{\dagger}(\mathbf{r}_n) \psi^{\dagger}(\mathbf{r}') \psi(\mathbf{r}') \psi^{\dagger}(\mathbf{r}_1) \ldots \psi^{\dagger}(\mathbf{r}_{n-1}) \psi^{\dagger}(\mathbf{r}_{n+1}) \ldots \psi^{\dagger}(\mathbf{r}_N) | 0 \rangle \end{aligned} \tag{4.58}$$

We now use an identity for both Bosons and Fermions that allows us to move the number-density operator in the above product:

$$\psi^{\dagger}(\mathbf{r}')\psi(\mathbf{r}')\psi^{\dagger}(\mathbf{r}_1) = \psi^{\dagger}(\mathbf{r}_1) \left[\zeta \psi^{\dagger}(\mathbf{r}')\psi(\mathbf{r}') + \delta(\mathbf{r}' - \mathbf{r}_1) \right]. \tag{4.59}$$

We can thus write (4.58) as

$$\sum_{n=1}^{N}\zeta^{n-1}\delta(\mathbf{r}-\mathbf{r}_n)\psi^\dagger(\mathbf{r}_n)\sum_{m\neq n}^{N}\delta(\mathbf{r}'-\mathbf{r}_m)\psi^\dagger(\mathbf{r}_1)\ldots\psi^\dagger(\mathbf{r}_{n-1})\psi^\dagger(\mathbf{r}_{n+1})\ldots\psi^\dagger(\mathbf{r}_N)|0\rangle$$
$$=\sum_{n=1}^{N}\sum_{m\neq n}^{N}\delta(\mathbf{r}-\mathbf{r}_n)\delta(\mathbf{r}'-\mathbf{r}_m)|\mathbf{r}_1,\ldots,\mathbf{r}_N\rangle\sqrt{N!}. \tag{4.60}$$

Thus, multiplying (4.60) by $U(\mathbf{r},\mathbf{r}')/(2\sqrt{N!})$ and integrating, we find that (4.57) gives a position representation of any two-body operator. In an entirely analogous manner to the derivation of (4.55) we can expand in an arbitrary basis and find the general representation of a two-body operator

$$\boxed{\hat{O}_2=\sum_{\mu\mu'\lambda\lambda'}O_{\mu\mu'\lambda\lambda'}a^\dagger_\mu a^\dagger_{\mu'}a_\lambda a_{\lambda'},} \tag{4.61}$$

where $O_{\mu\mu'\lambda\lambda'}\equiv\frac{1}{2}\langle\mu|\otimes\langle\mu'|\hat{O}_2|\lambda\rangle\otimes|\lambda'\rangle$.

Exercise 4.4: Two-body operators

1. Prove (4.59), and hence derive (4.57).
2. Derive (4.61) along similar lines to the proof of (4.55).

4.6.3 Two-body Schrödinger equation

Consider the Hamiltonian

$$H=H_0+H_I,\quad\text{where} \tag{4.62}$$
$$H_0=\int d^3\mathbf{r}\,\psi^\dagger(\mathbf{r})\left(-\frac{\hbar^2\nabla^2}{2m}\right)\psi(\mathbf{r}), \tag{4.63}$$
$$H_I=\frac{1}{2}\int d^3\mathbf{r}_1\int d^3\mathbf{r}_2\,\psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r}_2)U(\mathbf{r}_1,\mathbf{r}_2)\psi(\mathbf{r}_2)\psi(\mathbf{r}_1). \tag{4.64}$$

In many cases of physical interest there is no dependence of U on the absolute coordinate, $U(\mathbf{r}_1,\mathbf{r}_2)\equiv U(\mathbf{r}_1-\mathbf{r}_2)$, and we can then show that the Schrödinger equation is of the form

$$\boxed{i\hbar\frac{\partial\phi(\mathbf{r}_1,\mathbf{r}_2,t)}{\partial t}=\left(-\frac{\hbar^2\nabla_1^2}{2m}-\frac{\hbar^2\nabla_2^2}{2m}+U(\mathbf{r}_1-\mathbf{r}_2)\right)\phi(\mathbf{r}_1,\mathbf{r}_2,t)} \tag{4.65}$$

Exercise 4.5: Two-body Schrödinger equation

1. Derive (4.65).
2. Show that a one-particle state evolving according to (4.62) does not interact.

4.6.4 Two-body interaction in momentum space

For any two-body interaction for which $U(\mathbf{r},\mathbf{r}') = U(\mathbf{r}-\mathbf{r}') = U(|\mathbf{r}-\mathbf{r}'|)$, a straightforward change of basis using (4.30) in (4.64) gives the momentum space representation

$$\hat{U} = \frac{1}{2}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} U_{1234} a^\dagger_{\mathbf{k}_1} a^\dagger_{\mathbf{k}_2} a_{\mathbf{k}_3} a_{\mathbf{k}_4} \tag{4.66}$$

where

$$\begin{aligned} U_{1234} &= \frac{1}{V^2}\int d^3\mathbf{r}\int d^3\mathbf{r}'\, e^{i(\mathbf{k}_3-\mathbf{k}_2)\cdot\mathbf{r}+i(\mathbf{k}_4-\mathbf{k}_1)\cdot\mathbf{r}'}\, U(\mathbf{r}-\mathbf{r}') \\ &= \delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}\tilde{U}(\mathbf{k}_2-\mathbf{k}_3) \end{aligned} \tag{4.67}$$

where

$$\tilde{U}(\mathbf{k}) = \frac{1}{V}\int d^3\mathbf{r}\; U(\mathbf{r})\; e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{4.68}$$

The Kronecker-delta function in (4.67) expresses the fact that momentum is conserved in the two-body collision. Notice that U_{1234} has no symmetry in $(\mathbf{k}_1,\mathbf{k}_2)$ or in $(\mathbf{k}_3,\mathbf{k}_4)$, yet due to the summation over all $\mathbf{k}$ and the commutation relations, the effective interaction terms are

1. *Bosons.*— The symmetrized form $(U_{1234}+U_{2134})/2$, meaning that only even angular momentum partial waves interact.
2. *Fermions.*— The antisymmetrized form $(U_{1234}-U_{2134})/2$ occurs, meaning that only odd angular momentum partial waves interact. Thus at sufficiently low energies Fermions in the same spin state do not interact.

Exercise 4.6: Momentum space two-body interaction

Show that the two-body interaction (4.64) can be written in the form (4.67) when the interaction is translationally invariant and exchange symmetric.

Part II

Quantum Optics

5 Quantum Theory of the Electromagnetic Field

5.1 Quantization of the Electromagnetic Field

We follow the treatment in [1], and take as our starting point the source-free Maxwell equations

$$\nabla \cdot \mathbf{B} = 0, \tag{5.1}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{5.2}$$

$$\nabla \cdot \mathbf{D} = 0, \tag{5.3}$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t}, \tag{5.4}$$

where $\mathbf{B} = \mu_0 \mathbf{H}, \mathbf{D} = \epsilon_0 \mathbf{E}$, and ϵ_0, μ_0 are the electric perimttivity and magnetic permeability of free space, and $c = (\mu_0 \epsilon_0)^{-1/2}$ is the speed of light in vacuum. The EM field can be represented in terms of the vector and scalar potentials $\mathbf{A}$ and ϕ, as

$$\mathbf{E} = -\nabla \phi - \frac{\partial \mathbf{A}}{\partial t}, \tag{5.5}$$

$$\mathbf{B} = \nabla \times \mathbf{A}, \tag{5.6}$$

however there is no unique choice for these potentials as the measurable fields (5.5)-(5.6) are invariant under the *gauge transformation*

$$\mathbf{A} \to \mathbf{A} + \nabla \chi, \tag{5.7}$$

$$\phi \to \phi - \frac{\partial \chi}{\partial t}. \tag{5.8}$$

For the purposes of quantum optics the convenient choice is the *Coulomb gauge* condition

$$\nabla \cdot \mathbf{A} = 0, \quad \phi = 0. \tag{5.9}$$

From (5.6) and (5.4) we find the wave equation for the vector potential

$$\frac{1}{c^2} \frac{\partial^2 \mathbf{A}(\mathbf{r}, t)}{\partial t^2} = \nabla^2 \mathbf{A}(\mathbf{r}, t). \tag{5.10}$$

Quantization of the field can proceed by finding a set of eigenmodes of this classical equation and quantizing the mode amplitudes of the field in this basis. Thus we apply the procedure of *second quantization*. Since the wave equation is separable, we can separate the vector potential as $\mathbf{A}(\mathbf{r},t) = \mathbf{A}^{(+)}(\mathbf{r},t) + \mathbf{A}^{(-)}(\mathbf{r},t)$, where

$$\mathbf{A}^{(\pm)}(\mathbf{r},t) = \sum_k c_k \mathbf{u}_k(\mathbf{r}) e^{\mp i\omega_k t}, \tag{5.11}$$

where the mode functions satisfy

$$\left(\nabla^2 + \frac{\omega_k^2}{c^2}\right)\mathbf{u}_k(\mathbf{r}) = 0, \tag{5.12}$$

and, from (5.9), must also satisfy the Coulomb gauge condition

$$\nabla \cdot \mathbf{u}_k(\mathbf{r}) = 0. \tag{5.13}$$

As usual, dealing with the continuum introduces ultra-violet divergences in the theory. We will thus consider a finite volume V, on which the mode functions form a complete orthonormal basis:

$$\int_V d^3\mathbf{r}\; \mathbf{u}_k^*(\mathbf{r}) \cdot \mathbf{u}_{k'}(\mathbf{r}) = \delta_{k,k'}, \tag{5.14}$$

and have a precise form determined by the boundary conditions assumed on V. For a cubical volume $V = L^3$ with periodic boundary conditions, the modes may be written as

$$\mathbf{u}_k(\mathbf{r}) = u_k(\mathbf{r})\hat{\mathbf{e}}_{\mathbf{k}}^{\lambda} \equiv L^{-3/2} e^{i\mathbf{k}\cdot\mathbf{r}} \hat{\mathbf{e}}_{\mathbf{k}}^{\lambda} \tag{5.15}$$

representing travelling-wave solutions of the wave equation. Here the unit vector $\hat{\mathbf{e}}_{\mathbf{k}}^{\lambda}$ is a unit polarisation vector, which according to (5.13), must satisfy

$$\hat{\mathbf{e}}_{\mathbf{k}}^{\lambda} \cdot \mathbf{k} = 0, \tag{5.16}$$

describing two orthogonal axes transverse to the direction of propagation. The mode index k denotes all the quantities required to specify a particular mode, namely $k = (\lambda, \mathbf{k})$, where $\lambda = 1, 2$, and

$$\hat{\mathbf{e}}_{\mathbf{k}}^{\lambda} \cdot \hat{\mathbf{e}}_{\mathbf{k}}^{\lambda'} = \delta_{\lambda,\lambda'}. \tag{5.17}$$

The allowed values of $\mathbf{k}$ are

$$k_x = \frac{2\pi n_x}{L}, \quad k_y = \frac{2\pi n_y}{L}, \quad k_z = \frac{2\pi n_z}{L}, \qquad n_x, n_y, n_z = 0, \pm 1, \pm 2, \ldots \tag{5.18}$$

and from (5.12) the dispersion relation is (independent of polarisation)

$$\omega_k = c|\mathbf{k}|. \tag{5.19}$$

The vector potential and electromagnetic field can be written as

$$\mathbf{A}(\mathbf{r},t) = \sum_k \left(\frac{\hbar}{2\omega_k \epsilon_0}\right)^{1/2} \left[c_k \mathbf{u}_k(\mathbf{r}) e^{-i\omega_k t} + c_k^* \mathbf{u}_k^*(\mathbf{r}) e^{i\omega_k t}\right], \tag{5.20}$$

$$\mathbf{E}(\mathbf{r},t) = i\sum_k \left(\frac{\hbar\omega_k}{2\epsilon_0}\right)^{1/2} \left[c_k \mathbf{u}_k(\mathbf{r}) e^{-i\omega_k t} - c_k^* \mathbf{u}_k^*(\mathbf{r}) e^{i\omega_k t}\right], \tag{5.21}$$

where now we have chosen normalisation so that the c-number amplitudes c_k are dimensionless. The dimensionless amplitudes may be chosen as our canonical coordinates, and quantization is accomplished by the replacement $c_k \to a_k$, $c_k^* \to a_k^\dagger$, where the operators have boson commutation relations

$$[a_k, a_{k'}] = [a_k^\dagger, a_{k'}^\dagger] = 0, \quad [a_k, a_{k'}^\dagger] = \delta_{k,k'}. \tag{5.22}$$

We can now write the quantized fields in terms of these operators as

$$\mathbf{A}(\mathbf{r},t) = \sum_k \left(\frac{\hbar}{2\omega_k \epsilon_0}\right)^{1/2} \left[a_k \mathbf{u}_k(\mathbf{r}) e^{-i\omega_k t} + a_k^\dagger \mathbf{u}_k^*(\mathbf{r}) e^{i\omega_k t}\right], \tag{5.23}$$

$$\mathbf{E}(\mathbf{r},t) = i \sum_k \left(\frac{\hbar\omega_k}{2\epsilon_0}\right)^{1/2} \left[a_k \mathbf{u}_k(\mathbf{r}) e^{-i\omega_k t} - a_k^\dagger \mathbf{u}_k^*(\mathbf{r}) e^{i\omega_k t}\right], \tag{5.24}$$

and similarly (although more cumbersome) for **B**. Starting from the classical Hamiltonian of the electromagnetic field

$$H_{EM} = \frac{1}{2} \int_V d^3\mathbf{r} \left(\epsilon_0 \mathbf{E}^2 + \mu_0^{-1} \mathbf{H}^2\right), \tag{5.25}$$

and using (5.24) and the equivalent for **H**, and (5.13) and (5.14), we arrive at

$$H_{EM} = \sum_{\mathbf{k},\lambda} \hbar\omega_{\mathbf{k}} \left(a_{\mathbf{k},\lambda}^\dagger a_{\mathbf{k},\lambda} + \tfrac{1}{2}\right). \tag{5.26}$$

Thus the quantum Hamiltonian for the free-space electromagnetic field is that of a set of independent harmonic oscillators. Acting on the vacuum with the Hamiltonian, we find

$$H_{EM}|0\rangle = \sum_{\mathbf{k},\lambda} \frac{\hbar\omega_{\mathbf{k}}}{2} |0\rangle = \infty, \tag{5.27}$$

and thus it would appear that the electromagnetic vacuum contains infinite energy. This embarrassing divergence is a consequence of the way we have quantised the Hamiltonian, and can be removed by normal ordering. However, the physical effects of vacuum fluctuations are fundamental to numerous quantum phenomena, acting to seed spontaneous quantum processes. In particular, the vacuum energy initiates spontaneous emission of an excited atom, and can be measured via the *Casimir force* that acts to push two parallel conducting plates together.

Reflecting upon the origin of (5.27), notice that it is the process of canonical quantization that is ultimately to blame for this embarrassing divergence. It is conventional in quantum field theory to introduce and work with the normally ordered Hamiltonian

$$: H_{EM} := \sum_{\mathbf{k},\lambda} \hbar\omega_{\mathbf{k}}\, a_{\mathbf{k},\lambda}^\dagger a_{\mathbf{k},\lambda} \tag{5.28}$$

which removes the infinite (constant) vacuum correction to the ground state energy, and has no observable effect on dynamical predictions. This is equivalent to insisting that the vacuum state has zero energy:

$$H_{EM}|\text{vac}\rangle = 0. \tag{5.29}$$

While the ground state energy can always be shifted by a convenient constant, the physical effects of zero-point fluctuations are nevertheless fundamentally important in quantum field theory.

Exercise 5.1: Harmonic oscillator Hamiltonian

Prove (5.26). You may find the identity $\nabla \times (\nabla \times \mathbf{A}) = \nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}$ useful.

5.2 Atom-Light Interactions

The correct quantum formulation of the interaction of matter with electromagnetic radiation is the most significant application of the method of canonical quantization. In this section we shall outline the inclusion of electromagnetic forces within the classical Lagrangian and Hamiltonian formalisms, and then proceed to the so-called minimal coupling Hamiltonian.

5.2.1 Classical electromagnetic forces

The force on particle of charge e located at $\mathbf{r}(t)$ and moving with instantaneous (non relativistic) velocity $\mathbf{v}(t) \equiv \dot{\mathbf{r}}(t)$ is given by the *Lorentz force law*

$$\boldsymbol{F} = e\boldsymbol{E} + e\mathbf{v} \times \boldsymbol{B}. \tag{5.30}$$

The electrostatic part can be derived from a potential, while the magnetic part can be derived from a velocity dependent potential within the Lagrangian formalism. The correct Lagrangian[1] giving the equation of motion for (5.30) is

$$\boxed{L = T - e\phi(\mathbf{r}(t), t) + e\boldsymbol{A}(\mathbf{r}(t), t) \cdot \mathbf{v},} \tag{5.31}$$

where, in the absence of sources,

$$\boldsymbol{E} = -\nabla\phi - \frac{\partial \boldsymbol{A}}{\partial t}, \tag{5.32}$$

$$\boldsymbol{B} = \nabla \times \boldsymbol{A}. \tag{5.33}$$

The *canonical momentum* is

$$\boxed{\mathbf{p} \equiv \nabla_{\mathbf{v}} L = m\mathbf{v} + e\boldsymbol{A},} \tag{5.34}$$

and this differs in a fundamental way from the kinetic momentum of a free particle. Carrying out the transformation (2.26), the Hamiltonian is given by

$$\boxed{H = \frac{(\mathbf{p} - e\boldsymbol{A})^2}{2m} + e\phi(\mathbf{r}, t).} \tag{5.35}$$

Note that the magnetic force does not contribute to the energy as it is always perpendicular to the velocity, doing no work on the particle.

---

[1] The proof is somewhat intricate, but highly instructive. See, for example, [2].

Exercise 5.2: Gauge Invariance

Introduce the transformation

$$\boldsymbol{A} \to \boldsymbol{A} + \nabla\chi, \quad \phi \to \phi - \frac{\partial\chi}{\partial t}. \tag{5.36}$$

1. Show that the Lagrangian is changed by the total time derivative $e d\chi/dt$, and hence the equations of motion are preserved.
2. Show that the canonical momenta derived for the new Lagrangian are correct.
3. Does the gauge transformation change the Hamiltonian?

Exercise 5.3: Particle in a uniform magnetic field

The vector potential for a uniform magnetic field $\boldsymbol{B}$ is given by $\boldsymbol{A} = \frac{1}{2}\boldsymbol{B} \times \mathbf{r}$.

1. Explain why the angular momentum is still given by $\boldsymbol{L} = \mathbf{r} \times \mathbf{p}$ with $\mathbf{p}$ defined by (5.34).
2. Using the expressions for $\boldsymbol{L}$ and $\boldsymbol{A}$, show that the interaction can be interpreted in terms of the magnetic moment $\boldsymbol{\mu} = e\boldsymbol{L}/2m$, provided the term proportional to $\boldsymbol{A}^2$ can be neglected.
3. Under what physical conditions can the $\boldsymbol{A}^2$ term be neglected?

5.2.2 Minimal coupling

We describe the electron-photon interaction using the *minimal coupling Hamiltonian*

$$H = \frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 + e\phi(\mathbf{r}) + H_{EM}, \tag{5.37}$$

where $\phi(\mathbf{r})$ is the Coulomb potential for an atom with nucleus localised at $\mathbf{r} = \mathbf{r}_0$, $\mathbf{p}$ is the momentum for electron with mass m, and $\mathbf{A}$ is the electromagnetic vector potential. The EM-field is quantized, and described by (5.26). To develop a quantum mechanical treatment of both electron and photon fields, we quantize the electron wave field by expanding over an orthonormal basis of unperturbed electron wavefuctions $\phi_n(\mathbf{r})$ with energies E_n as

$$\psi(\mathbf{r}) = \sum_n c_n\phi_n(\mathbf{r}) \tag{5.38}$$

where the electron operators are Fermionic

$$[c_n, c_m^\dagger]_- = \delta_{nm}, \quad [c_n^{(\dagger)}, c_m^{(\dagger)}]_- = 0, \tag{5.39}$$

and the index n runs over all quantum numbers required to specify the electronic state. We now have the Hamiltonian

$$H = H_e + H_{EM} + H_{Int}, \tag{5.40}$$

where

$$H_e = \int d^3\mathbf{r}\, \psi^\dagger(\mathbf{r})\left(-\frac{\hbar^2\nabla^2}{2m} + eV(\mathbf{r})\right)\psi(\mathbf{r}) \tag{5.41}$$

describes the motion of the electron in the nuclear electrostatic potential, and H_I describes the interaction between the electron and the light field. The interaction can be decomposed as

$$H_{Int,1} = -\frac{e}{2m}\int d^3\mathbf{r}\, \psi^\dagger(\mathbf{r})\,(\mathbf{p}\cdot\boldsymbol{A} + \boldsymbol{A}\cdot\mathbf{p})\,\psi(\mathbf{r}), \tag{5.42}$$

$$H_{Int,2} = \frac{e^2}{2m}\int d^3\mathbf{r}\, \psi^\dagger(\mathbf{r})\boldsymbol{A}^2\psi(\mathbf{r}). \tag{5.43}$$

Provided the EM-field intensity is not large enough to favour two-photon processes in the vacuum, the contribution from $H_{Int,2}$ can be neglected, leaving $H_I \equiv H_{Int,2}$. Noting that

$$\mathbf{p} \cdot \boldsymbol{A}(\mathbf{r}) - \boldsymbol{A}(\mathbf{r}) \cdot \mathbf{p} = -i\hbar\nabla \cdot \boldsymbol{A}(\mathbf{r}) = 0 \tag{5.44}$$

in the Coulomb gauge, we can then write the Hamiltonian as

$$H_{EM} = \sum_k \hbar\omega_k a_k^\dagger a_k, \tag{5.45}$$

$$H_e = \sum_n E_n c_n^\dagger c_n, \tag{5.46}$$

$$H_I = \hbar \sum_{nlk} c_n^\dagger c_l \left(\kappa_k^{nl} a_k + \kappa_k^{nl*} a_k^\dagger\right), \tag{5.47}$$

where, as in (5.11), k refers to both wave vector and polarisation of the EM mode with annihilation operator a_k, and the coefficients are

$$\kappa_k^{nl} = -\frac{e}{m}\sqrt{\frac{1}{2\hbar\omega_k\epsilon_0}} \int d^3\mathbf{r}\ \phi_l^*(\mathbf{r})\,(\mathbf{u}_k(\mathbf{r}) \cdot \mathbf{p})\,\phi_n(\mathbf{r}). \tag{5.48}$$

5.2.3 Electric dipole approximation

For most systems of interest there is a separation of length scales. The atomic scale is of order $\sim 10^{-11}$m, while the wavelength of an optical photon is of order $\sim 10^{-6}$m. Thus the mode functions $\phi_n(\mathbf{r})$ vary much more rapidly than $u_k(\mathbf{r})$, which may be evaluated at $\mathbf{r}_0$ and taken out of the integral. We then have

$$\int d^3\mathbf{r}\ \phi_l^*(\mathbf{r})[\mathbf{u}_k(\mathbf{r}) \cdot \mathbf{p}]\phi_n(\mathbf{r}) = u_k(\mathbf{r}_0)\hat{\mathbf{e}}_{\mathbf{k}}^{\lambda} \cdot \langle l|\mathbf{p}|n\rangle, \tag{5.49}$$

Since $\mathbf{p} = [\mathbf{r}, \mathbf{p}^2]/2i\hbar$, and the unperturbed electron wave functions are energy eigenstates, we can evaluate the matrix elements as

$$e\langle l|\mathbf{p}|n\rangle = \frac{m}{i\hbar}\langle l|\frac{\mathbf{r}\cdot\mathbf{p}^2 - \mathbf{p}^2\cdot\mathbf{r}}{2m}|n\rangle = im\Omega_{nl}\boldsymbol{d}_{nl}, \tag{5.50}$$

where

$$\Omega_{nl} = \frac{E_l - E_n}{\hbar}, \tag{5.51}$$

and

$$\boldsymbol{d}_{nl} \equiv e\langle l|\mathbf{r}|n\rangle \tag{5.52}$$

is the *electric dipole operator*. Hence, in the dipole approximation, the coupling matrix elements are

$$\kappa_k^{nl} = -i\sqrt{\frac{1}{2\hbar\omega_k\epsilon_0}}\Omega_{nl}u_k(\mathbf{r}_0)\hat{\mathbf{e}}_{\mathbf{k}}^{\lambda} \cdot \boldsymbol{d}_{nl} \tag{5.53}$$

5.2.4 Interaction picture

To gain some insight as to the essential terms in the interaction we transform to the interaction picture with respect to $H_0 = H_e + E_{EM}$, and find

$$a_k(t) = e^{-i\omega_k t} a_k, \qquad c_n(t) = e^{-iE_n t/\hbar} c_n, \tag{5.54}$$

and the interaction Hamiltonian takes the form

$$H_I = \hbar \sum_{nlk} c_n^\dagger c_l e^{-i\Omega_{nl} t} \left(\kappa_k^{nl} a_k e^{-i\omega_k t} + \kappa_k^{nl*} a_k^\dagger e^{i\omega_k t} \right). \tag{5.55}$$

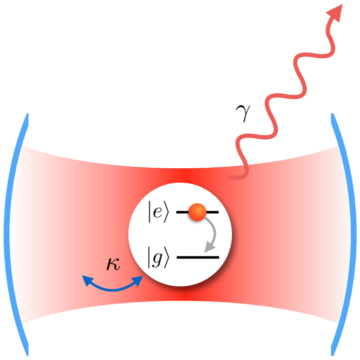

Figure 5.1: Two-level atom in an optical cavity. By tuning the cavity mode frequency to the atomic transition frequency, the system enters the *Jaynes Cummings regime*, whereby the rate of spontaneous emission into the continuum, γ, is negligible compared to the atom-cavity coupling rate, κ.

5.2.5 Rotating wave approximation

When the atomic transition is near-resonant with a particular optical frequency, $\Omega_{nl} \approx \omega_k$, and the off-resonant terms in (5.55) that are proportional to $e^{-(i\Omega_{nl}+\omega_k)t}$ oscillate with very high frequency compared to the near-resonant terms. These terms correspond to processes that involve high energy, such as the simultaneous excitation of the atom and emission of a photon. In the *rotating wave approximation* (RWA) these terms are neglected.

5.2.6 Two-Level Atom

We can make a drastic approximation and consider just two levels of the atom, the ground state $|g\rangle$ and excited state $|e\rangle$ separated by energy $\hbar\Omega_{g,e} \equiv \hbar\Omega$. Using the properties of Pauli matrices, the two level atom Hamiltonian can be represented in terms of raising and lowering operators. One can easily establish the mappings $c_2^\dagger c_1 \to \sigma_+$, $c_1^\dagger c_2 \to \sigma_-$, and $c_2^\dagger c_2 - c_1^\dagger c_1 \to \sigma_z$. In terms of these pseudo-spin 1/2 operators, the two level atom in the RWA and dipole approximations is described by the Schrödinger picture Hamiltonian

$$\boxed{H = \tfrac{1}{2}\hbar\Omega\sigma_z + \sum_k \hbar\omega_k a_k^\dagger a_k + \hbar \sum_k \left(\kappa_k a_k \sigma_+ + \kappa_k^* a_k^\dagger \sigma_- \right), \qquad (5.56)}$$

where the couplings are reduced to

$$\kappa_k = -i\sqrt{\frac{1}{2\hbar\omega_k\epsilon_0}}\,\Omega u_k(\mathbf{r}_0)\hat{\mathbf{e}}_{\mathbf{k}}^{\lambda} \cdot \boldsymbol{d}_{g,e}. \tag{5.57}$$

5.3 Cavity Quantum Electrodynamics

With careful engineering, an optical cavity can be used to manipulate the couplings between particular cavity modes and specific atomic transitions. A regime of fundamental interest for quantum optics occurs when a single mode is strongly coupled to a single two-level atomic transition. This can be achieved with a small cavity mode volume and a large dipole moment.

5.3.1 Jaynes Cummings Regime

The simplest situation that arises involves a two-level atom interacting with a single mode of the electromagnetic field *on resonance* ($\omega_k = \omega \equiv \Omega$), whereby the system is described by the *Jaynes-Cummings Hamiltonian*

$$\boxed{H = \hbar\Omega\left(a^\dagger a + \tfrac{1}{2}\sigma_z\right) + \hbar\kappa(\sigma_+ a + a^\dagger\sigma_-) \equiv H_0 + H_I \qquad (5.58)}$$

where the arbitrary phase of the mode $u_k(\mathbf{r}_0)$ has been chosen to make the coupling real:

$$\kappa = \sqrt{\frac{(\hat{\mathbf{e}}^\lambda_\mathbf{k}\cdot \boldsymbol{d}_{e,g})^2\Omega}{\hbar\epsilon_0 V}}. \tag{5.59}$$

The first term in (5.58) represents the free evolution of the two-level atom and optical mode, and the second describes raising and lowering of the electron energy state via absorption and emission of a photon respectively.

Note that since $[H_0, H_I] = 0$ we can move into the ineraction picture without altering H_I. For an atom initially in the excited state, the Hamiltonian couples the n-photon cavity state $|e, n\rangle$ to the state $|g, n+1\rangle$. The quantum state can be written as

$$|\psi_n(t)\rangle = c_{e,n}(t)|e, n\rangle + c_{g,n+1}(t)|g, n+1\rangle, \tag{5.60}$$

giving the equations of motion in the interaction picture

$$\dot{c}_{e,n}(t) = -i\Omega_n c_{g,n+1}(t), \tag{5.61}$$

$$\dot{c}_{g,n+1}(t) = -i\Omega_n c_{e,n}(t), \tag{5.62}$$

with $\Omega_n = \kappa\sqrt{n+1}$, and the general solution

$$c_{e,n}(t) = c_{e,n}(0)\cos\Omega_n t - ic_{g,n+1}(0)\sin\Omega_n t, \tag{5.63}$$

$$c_{g,n+1}(t) = c_{g,n+1}(0)\cos\Omega_n t - ic_{e,n}(0)\sin\Omega_n t. \tag{5.64}$$

For an initial atomic excited state with the cavity in the number state $|n\rangle$, the probability of finding the atom in the excited state at a later time is

$$p_e(t) = |\langle e, n|\psi_n(t)\rangle|^2 = |c_{e,n}(t)|^2 = \cos^2\Omega_n t, \tag{5.65}$$

and hence the atomic state undergoes cyclic emission and reabsorption from the cavity mode. Note that if we compute the eigenstates of H_I, they are the *dressed states*

$$|\pm, n\rangle = \frac{1}{\sqrt{2}}\left(|e, n\rangle \pm |g, n+1\rangle\right) \tag{5.66}$$

with eigenvalues $\pm i\Omega_n$, and thus the interaction lifts the degeneracy between states $|e, n\rangle$ and $|g, n+1\rangle$ by introducing an energy splitting $\Delta_n = 2\Omega_n$. The degeneracy is lifted even for an unoccupied cavity mode, and the separation $\Delta_0 = 2\kappa$ is known as the *vacuum Rabi splitting*, a consequence of the mode structure imposed by the cavity.

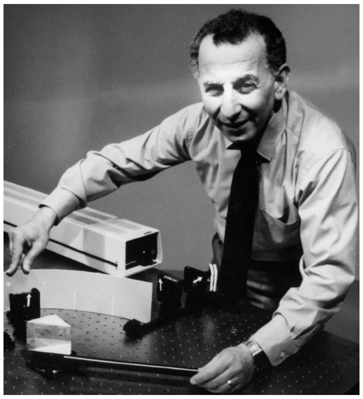

Figure 5.2: A pioneer in laser physics and atom-light interactions, **Shaoul Ezekiel (1935-2015)** developed the first realization of a two-level atom in 1977, and measured the resonance fluorescence spectrum of the atom subject to an intense laser field.

5.3.2 Quantum Collapses and Revivals

Since we know that probabilities of individual number states of the photon field evolve according to (5.65), we can consider the evolution of a coherent state, given by the superposition of number states (3.20). If the atom is initially in the excited

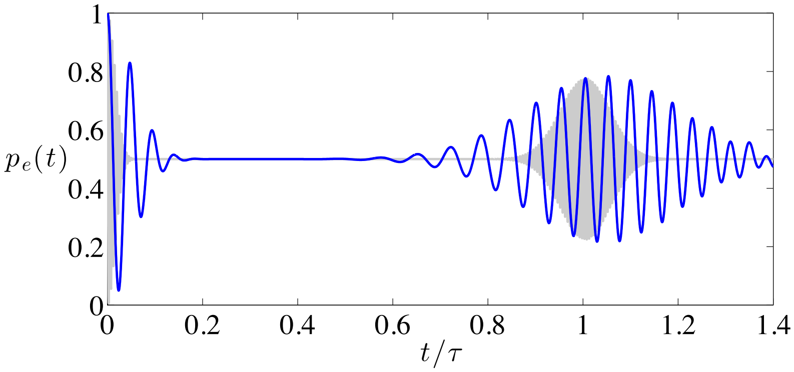

Figure 5.3: Collapses and revivals for a two-level atom on resonance with a single cavity mode, for an initial coherent state with mean photon number $\langle a^\dagger a\rangle = \bar{n} = 10$ (blue) and $\bar{n} = 100$ (gray).

state, and interacting with a cavity mode initially in a coherent state, then (5.65) becomes

$$p_e(t) = \tfrac{1}{2}\left[1 + \sum_{n=0}^{\infty} \frac{e^{-\bar{n}}\bar{n}^n}{n!} \cos\left(2\kappa\sqrt{n+1}t\right)\right]. \tag{5.67}$$

Due to the Poisson distribution of photon number of a coherent state, there will be a spread of Rabi frequencies of order $\sim \sqrt{\bar{n}}$. An approximate evaluation of the sum, valid for times $t < \sqrt{\bar{n}}/\kappa$ gives

$$p_e(t) = \tfrac{1}{2}\left[1 + \cos\left(2\kappa\sqrt{\bar{n}+1}t\right)\exp\left(-\frac{\kappa^2 t^2 \bar{n}}{2(\bar{n}+1)}\right)\right], \tag{5.68}$$

and the oscillations decay under a Gaussian envelope. In fact there is a partial *revival* at $\tau \sim 2\pi\sqrt{\bar{n}}/\kappa$, due to rephasing of the number states, a consequence of *optical coherence*.

Exercise 5.4: Collapse envelope

Derive (5.68) by expanding $\sqrt{n+1}$ around $\sqrt{\bar{n}+1}$.

5.4 Casimir Force

Mode structure can have startling consequences, even *in vaccuo*. In 1948 Casimir presented a paper entitled *On the attraction between two perfectly conducting plates* to the Royal Netherlads Academy of Arts and Sciences. Casimir showed that the abrupt change in the *structure* of the electromagnetic quantum vacuum caused by the plates leads to a force of attraction between them. Although very small, this force has been measured, strikingly demonstrating the existence and physical significance of zero-point fluctuations.

Consider two perfectly conducting parallel plates, of side length $L_x = L_y = L$, and thickness $L_z = d$. The conducting surfaces impose boundary conditions on the modes of the EM field that are allowed between the plates, and most significantly, the internal mode structure differs from the continuum of modes exterior to the interstitial plate volume. The allowed frequencies are given by

$$\omega_{lmn} = \pi c \left(\frac{l^2}{L^2} + \frac{m^2}{L^2} + \frac{n^2}{d^2} \right)^{1/2}, \tag{5.69}$$

where $l, m, n = 0, 1, 2, \ldots$. The zero-point energy in the box is then

$$\begin{aligned} E_0(d) &= \sum_{l,m,n=0}^{\infty} (\tfrac{1}{2})^{\delta_{l0}+\delta_{m0}+\delta_{n0}} (2) \tfrac{1}{2} \hbar \omega_{lmn} \\ &= \sum_{l,m,n=0}^{\infty} (\tfrac{1}{2})^{\delta_{l0}+\delta_{m0}+\delta_{n0}} \pi \hbar c \left(\frac{l^2}{L^2} + \frac{m^2}{L^2} + \frac{n^2}{d^2} \right)^{1/2}, \end{aligned} \tag{5.70}$$

where the factor of 2 accounts for two independent polarisations per mode, and the Kronecker delta factors account for the modes where any one of l, m, n is zero, since there is then only one independent polarisation. When $L \gg d$, the sums over l and m may be replaced by integrals to give

$$E_0(d) = \frac{\hbar c L^2}{\pi} \sum_{n=0}^{\infty} (\tfrac{1}{2})^{\delta_{n0}} \int_0^\infty dx \int_0^\infty dy \left(x^2 + y^2 + \frac{\pi^2 n^2}{d^2} \right)^{1/2}. \tag{5.71}$$

If d is taken to be very large, a similar replacement can be made to give

$$E_0(d \to \infty) = \frac{\hbar c L^2}{\pi^2} \frac{d}{\pi} \int_0^\infty dx \int_0^\infty dy \int_0^\infty dz \left(x^2 + y^2 + z^2 \right)^{1/2}. \tag{5.72}$$

The potential energy of the system when the plates are separated by distance d is $U_0(d) = E_0(d) - E_0(d \to \infty)$, the energy required to bring the plates together from a large separation to distance d:

$$\begin{aligned} U_0(d) = \frac{L^2 \hbar c}{\pi^2} \Bigg[& \sum_{n=0}^{\infty} (\tfrac{1}{2})^{\delta_{n0}} \int_0^\infty dx \int_0^\infty dy \left(x^2 + y^2 + \frac{\pi^2 n^2}{d^2} \right)^{1/2} \\ & - \frac{d}{\pi} \int_0^\infty dx \int_0^\infty dy \int_0^\infty dz \left(x^2 + y^2 + z^2 \right)^{1/2} \Bigg]. \end{aligned} \tag{5.73}$$

Changing to polar coordinates, and to the convenient variable $s = r^2$, we have

$$U_0(d) = \frac{L^2 \hbar c}{4\pi} \frac{\pi^3}{d^3} \left[\sum_{n=0}^{\infty} (\tfrac{1}{2})^{\delta_{n0}} \int_0^\infty ds\, (s + n^2)^{1/2} - \int_0^\infty dz \int_0^\infty ds\, (s + z^2)^{1/2} \right]. \tag{5.74}$$

Note that this is the difference between two *infinite* zero-point energies. We can cast this in a more tractable form by introducing the function

$$F(u) \equiv \int_0^\infty ds\, (s + u^2)^{1/2}, \tag{5.75}$$

so that

$$U_0(d) = \frac{L^2 \hbar c \pi^2}{4 d^3} \left[\tfrac{1}{2} F(0) + \sum_{n=1}^{\infty} F(n) - \int_0^\infty dz\, F(z) \right]. \tag{5.76}$$

The difference between integration and summation can be evaluated using the Euler-Maclaurin formula [3]

$$\sum_{n=1}^{\infty} F(n) - \int_0^{\infty} dz\, F(z) = -\tfrac{1}{2}F(0) - \tfrac{1}{12}F'(0) + \tfrac{1}{720}F'''(0)\ldots \tag{5.77}$$

obtained under the condition that $F(\infty) \equiv 0$, necessitating the introduction of an ultra-violet cutoff. That the result is independent of the cutoff should not be surprising when we note that (5.75) is smooth for large u so that the difference between summation and integration can only depend on the behaviour of $F(u)$ for small u. For (5.75), the derivatives are $F'(0) = 0$, $F'''(0) = -4$, and $F^{(n)}(0) = 0$ for $n > 3$. Thus

$$U_0(d) = -\frac{\pi^2 \hbar c}{720 d^3} L^2, \tag{5.78}$$

and the Casimir force per unit area $F(d) = -\partial_d U_0(d)$ is

$$\boxed{F(d) = -\frac{\pi^2 \hbar c}{240 d^4}.} \tag{5.79}$$

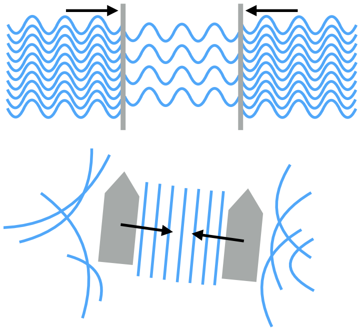

Figure 5.4: Casimir force between two parallel conducting plates. The mode density between the plates is less than that outside, and hence vacuum fluctuation forces acting on either side of each plate do not balance, causing a net attractive force. The force was measured by Sparnaay in 1957. A classical analogue of the force acts to push two boats together. While the latter force does not stem from vacuum fluctuations, it originates from the modified mode structure of surface waves caused by the vessels.

The same result can be derived in terms of the radiation pressure exerted by zero-point virtual photons carrying linear momentum $\frac{1}{2}\hbar\mathbf{k}$ for each polarisation mode with frequency $\hbar\omega_{\mathbf{k}} = c|\mathbf{k}|$. The photons reflected from the exterior of the plates generate slightly higher force than those reflected from the interior. The Casimir force was measured by Sparnaay in 1957. In summarising his impression in 1960, DeWitt captured the impact of the discovery:

> *"What startled me, in addition to the crazy idea that a pair of electrically neutral conductors could attract one another, was the way in which Casimir said the force should be computed, namely, by examining the effect on the zero-point energy of the electromagnetic vacuum cased by the mere presence of the plates. I had always been taught that the zero-point energy of a quantized field was unphysical ..."*

6 Fundamental Processes in Quantum Optics

6.1 Quantum Beam Splitter

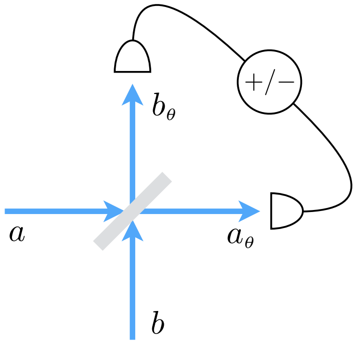

Figure 6.1: An ideal quantum beam splitter — the device acts as a coherent and linear transformation for two input modes. The modes can be in any quantum state, including the vacuum.

A beam splitter is a linear optical element that splits a beam of light in two. The beam splitter acts on incoming modes of the electromagnetic field, creating a new linear combination of the modes as outputs. As a simple and physical model of a lossless beam splitter, consider two distinct input modes described by the Boson annihilation operators a and b. As our starting point we shall describe the transformation introduced by the beam splitter in the Heiseberg picture. The transformation is unitary, and the beam splitter induces a 90° phase shift upon reflection, so that the output modes are described by the destruction operators

$$\boxed{\begin{aligned} a_\theta &= \cos\theta a + i\sin\theta b, && (6.1a)\\ b_\theta &= \cos\theta b + i\sin\theta a. && (6.1b)\end{aligned}}$$

In this linear transformation of the input modes, $T = \cos^2\theta = 1-\sin^2\theta = 1-R$ give the transmittance and reflectance respectively. Expressing the coefficients in terms of an angle θ encodes the fact that the beam splitter is lossless (the transformation is unitary). While this model is introduced along very general lines, in fact it provides a very accurate description of the action of a lossless beamsplitter on input photons.

In direct analogy to the definition of the time evolution operator, the beam splitter transformation is generated by the unitary operator

$$\boxed{S(\theta) = \exp\left(i\theta[a^\dagger b + b^\dagger a]\right), \qquad (6.2)}$$

where we use the notation $S(\theta)$ here, but there is a direct correspondence to $U(t)$ for some effective Hamiltonian.

In terms of the two-mode input state $|\text{in}\rangle$, in the *Schrödinger picture* the output state is determined by the unitary transformation as

$$|\text{out}\rangle = S(\theta)|\text{in}\rangle, \tag{6.3}$$

and the operators are unchanged. In the *Heisenberg picture*, the state kets are preserved, and instead the operators evolve according to

$$\begin{aligned} a_\theta &= S^\dagger(\theta) a S(\theta), && (6.4a)\\ b_\theta &= S^\dagger(\theta) b S(\theta). && (6.4b)\end{aligned}$$

where again, $S(\theta)$ plays the role of time evolution. It is a straightforward task to show that (6.4), and (6.1) are consistent with our postulated form of $S(\theta)$ [In Exercise 7.1 you will confirm that (6.2) is consistent with (6.1)].

Exercise 6.1: Quantum beam splitter transformation in the Heisenberg picture

Confirm (6.4a) and (6.4b) by differentiating and using the form of the transformed operators (6.1a), (6.1b). A constructive proof of (6.2) requires an exponential *ansatz* for $S(\theta)$, that is linear in both creation and annihilation operators, and a similar procedure.

Exercise 6.2: Splitting a coherent state

Working in the Schrödinger picture, show that for coherent state inputs $|\text{in}\rangle = |\alpha\rangle\otimes|\beta\rangle$, the output state is a new product of coherent states $|\text{out}\rangle = |\alpha_\theta\rangle\otimes|\beta_\theta\rangle$, with coherent state amplitudes $\alpha_\theta = \alpha\cos\theta + i\beta\sin\theta$, $\beta_\theta = \beta\cos\theta + i\alpha\sin\theta$. Hence, if a coherent state input is mixed with a vacuum input on a beam splitter, $|\text{in}\rangle = |\alpha\rangle\otimes|0\rangle$, the output state is $|\text{out}\rangle = |\alpha\cos\theta\rangle|i\alpha\sin\theta\rangle$.

6.1.1 Splitting a Single Photon

As an interesting example, consider the action of the beam-splitter on a one-photon input

$$|\text{in}\rangle = |1,0\rangle = a^\dagger|0,0\rangle. \tag{6.5}$$

The beam splitter transforms this into the output state

$$\begin{aligned} |\text{out}\rangle &= S(\theta)|\text{in}\rangle = S(\theta)a^\dagger|0,0\rangle \\ &= S(\theta)a^\dagger S^\dagger(\theta)S(\theta)|0,0\rangle \\ &= a^\dagger_{-\theta}|0,0\rangle = \cos\theta|1,0\rangle + i\sin\theta|0,1\rangle, \end{aligned} \tag{6.6}$$

where we have used the fact that $S(\theta)|0,0\rangle = |0,0\rangle$. Thus the output state is a superposition of two possible paths the photon can take, with a relative phase between transmission and reflection. A photo-detection measurement would report that the photon went *either* along one path *or* along the other.

6.1.2 Hong-Ou-Mandel Effect

Another immediate example is given by the two-photon input state $|\text{in}\rangle = |1,1\rangle$. We have

$$\begin{aligned} |\text{out}\rangle &= a^\dagger_{-\theta}b^\dagger_{-\theta}|0,0\rangle = (\cos\theta a^\dagger + i\sin\theta b^\dagger)(\cos\theta b^\dagger + i\sin\theta a^\dagger)|0,0\rangle, \\ &= |1,1\rangle\cos 2\theta + \frac{i}{\sqrt{2}}(|2,0\rangle + |0,2\rangle)\sin 2\theta. \end{aligned} \tag{6.7}$$

For a 50:50 beam splitter ($\theta = \pi/4$), the photons are transmitted in a pair into either port, while the other port remains in the vacuum state. This is a consequence of destructive interference between the different possible paths occurring in two-photon reflection and transmission.

6.2 Squeezing

Thus far our discussion has focussed on *linear* quantum optics, in the sense that the effective Hamiltonian in (6.2) is at most linear in $a^{(\dagger)}$ or $b^{(\dagger)}$. Nonlinear interactions play a fundamental role throughout physics. The essential nature of nonlinearity is readily apparent in Quantum Optics, where the simplest nonlinear interaction Hamiltonian introduces a fascinating new process, called *squeezing*.

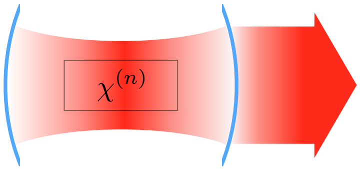

Figure 6.2: Cavity photons undergo interactions induced by a nonlinear crystal.

In free space, the photon-photon interaction process is very weak, requiring specific materials to create nonlinear interactions. Consider an optical cavity with a single mode of frequency ω to which we introduce a nonlinear medium that can generate *parametric down-conversion*. In this process, input photons with frequency 2ω are converted into pairs of photons with frequency ω, coinciding with the cavity mode frequency. This is known as a $\chi^{(2)}$ effect, due to its description in terms of a second-order optical susceptibility. The Hamiltonian for the system comprised of input field and cavity field takes the form

$$H = \hbar\omega a^\dagger a + 2\hbar\omega b^\dagger b + i\hbar\chi^{(2)}\left[ba^{\dagger 2} - b^\dagger a^2\right], \tag{6.8}$$

where the overlap of the spatial mode of the pump field and the cavity mode has been absorbed into $\chi^{(2)}$. We can now make a semi-classical approximation for the pump field, assuming that it is in a coherent state with amplitude β that evolves, in the Schrödinger picture, as $|\beta e^{-i2\omega t}\rangle$. We may then replace $b \to \beta e^{-i2\omega t}$, and, using the parameter χ to absorb both $\chi^{(2)}$ and the classical driving field amplitude, the effective Hamiltonian for the cavity mode can be written as

$$\boxed{H = \hbar\omega a^\dagger a + \frac{i\hbar\chi}{2}\left(a^{\dagger 2}e^{-2i\omega t} - a^2 e^{2i\omega t}\right) \equiv H_0 + H_{\mathrm{Int}}.} \tag{6.9}$$

Moving into the interaction picture with respect to H_0, the interaction Hamiltonian becomes time-independent:

$$H_{\mathrm{Int},I} = \frac{i\hbar\chi}{2}\left(a^{\dagger 2} - a^2\right), \tag{6.10}$$

a consequence of driving the cavity at the specific frequency 2ω. We can now focus on the quantum dynamical problem defined by (6.10). This may be solved by considering the Heisenberg equations of motion

$$\dot a(t) = -\frac{i}{\hbar}[a(t), H_{\mathrm{Int},I}] = \chi a^\dagger(t), \quad \dot a^\dagger(t) = \chi a(t), \tag{6.11}$$

with solutions given by

$$a(t) = a(0)\cosh(\chi t) + a^\dagger(0)\sinh(\chi t), \tag{6.12}$$

and its Hermitian conjugate. Note that the generator of time evolution is

$$U(t) = \exp\left(\chi t[a^{\dagger 2} - a^2]/2\right), \tag{6.13}$$

so that in the Schrödinger picture the state of the cavity mode is

$$|\psi, t\rangle = U(t)|\psi, 0\rangle, \tag{6.14}$$

while in the Heisenberg picture the operator solution (6.12) is equivalent to

$$a(t) = U^{\dagger}(t)a(0)U(t). \tag{6.15}$$

Exercise 6.3:

Differentiate (6.15), and use (6.12) to confirm that (6.13) generates the same time evolution as given by the Heisenberg equations of motion. Comment on the use of time arguments for the operators.

6.2.1 Quadrature Squeezing

To gain some insight into the role of this interaction, we note from (6.12) that $a(t) + a^{\dagger}(t) = [a(0) \pm a^{\dagger}(0)]e^{\pm\chi t}$, so that these choices of operators simplify the time evolution. To ensure the transformation is canonical, we introduce the *quadrature* operators

$$X(t) = a(t) + a^{\dagger}(t), \quad Y(t) = i[a^{\dagger}(t) - a(t)], \tag{6.16}$$

that satisfy

$$[X, Y] = 2i. \tag{6.17}$$

For these operators, the uncertainty principle reads

$$\Delta X \Delta Y \geq 1. \tag{6.18}$$

States that satisfy $\Delta X\Delta Y = 1$ are known as *minimum uncertainty states*, an important example of which are the coherent states. These operators evolve according to

$$X(t) = e^{\chi t}X(0), \quad Y(t) = e^{-\chi t}Y(0), \tag{6.19}$$

and similarly for the uncertainties:

$$\Delta X(t) = e^{\chi t}\Delta X(0), \quad \Delta Y(t) = e^{-\chi t}\Delta Y(0). \tag{6.20}$$

Hence the interaction (6.10) takes any input state and contracts one quadrature, while expanding the other, so as to maintain the initial uncertainty product. Hence, initial minimum uncertainty states become *squeezed*, reducing the uncertainty in one quadrature below the vacuum level, at the expense of the other quadrature. Measurements using squeezed light can thus beat the standard quantum limit, and this principle is behind the pursuit of ultra-precise measurements of gravity waves.

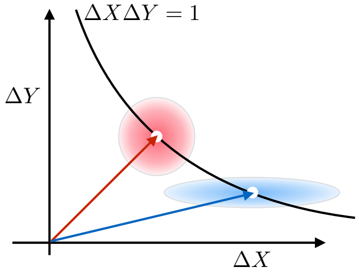

Figure 6.3: The Hamiltonian (6.10) evolves an initial minimum uncertainty state, with equal uncertainties in both quadratures, to a minimum uncertainty state with increased fluctuations in ΔX, and reduced fluctuations in ΔY.

6.2.2 Squeezed Vacuum

Finally, we consider the time evolution of an initial vacuum state. In general there are disentangling theorems for operators of the form (6.13), that recast the time evolution in a convenient form involving normally ordered operator products. For the evolution of an initial vacuum state $|\text{vac}, 0\rangle$, we can make use of the formal solution (6.12) by noting that in general

$$a(0)|\text{vac}, 0\rangle = 0, \tag{6.21}$$

and so

$$U(t)a(0)U^\dagger(t)U(t)|\text{vac},0\rangle = a(-t)|\text{vac},t\rangle = 0. \tag{6.22}$$

For the squeezing evolution

$$\cosh(\chi t)a(0)|\text{vac},t\rangle = \sinh(\chi t)a^\dagger(0)|\text{vac},t\rangle. \tag{6.23}$$

Expanding the ket $|\text{vac},t\rangle$ in number states, we can obtain a recursion relation, eventually giving the result

$$|\text{vac},t\rangle = \mathcal{N}\sum_{n=0}^{\infty}\left(\frac{\tanh(\chi t)}{2}\right)^n \frac{\sqrt{(2n)!}}{n!}|2n\rangle = \frac{1}{\sqrt{\cosh(\chi t)}}\exp\left(\frac{1}{2}\tanh(\chi t)a^{\dagger 2}\right)|0\rangle \tag{6.24}$$

Hence the squeezed vacuum only involves even photon number states, as should be apparent from (6.10).

Exercise 6.4: Squeezed vacuum

Derive (6.24).

6.3 Two-Mode Squeezing

The process described by (6.8) is also referred to as the degenerate parametric amplifier, since both low frequency photons are created in the same mode. The *non-degenerate* parametric amplifier Hamiltonian is

$$H = \hbar\omega_1 a_1^\dagger a_1 + \hbar\omega_2 a_2^\dagger a_2 + i\hbar\chi\left(a_1^\dagger a_2^\dagger e^{-i(\omega_1+\omega_2)t} - a_1 a_2 e^{i(\omega_1+\omega_2)t}\right). \tag{6.25}$$

The system now involves non-degenerate down-conversion of a classical pump field. The interaction Hamiltonian in the interaction picture is

$$H_{\text{Int},I} = i\hbar\chi\left(a_1^\dagger a_2^\dagger - a_1 a_2\right), \tag{6.26}$$

giving equations of motion

$$\dot{a}_1 = \chi a_2^\dagger, \quad \dot{a}_2^\dagger = \chi a_1, \tag{6.27}$$

and the solutions

$$a_1(t) = a_1\cosh(\chi t) + a_2^\dagger\sinh(\chi t), \tag{6.28}$$

$$a_2(t) = a_2\cosh(\chi t) + a_1^\dagger\sinh(\chi t). \tag{6.29}$$

Carrying out the same recursion relation approach as above, where now the expansion is over the two-mode number states $|n,m\rangle = |n\rangle_1 \otimes |m\rangle_2$, we can find the action of the time evolution operator

$$U(t) = \exp\left[\chi t\left(a_1^\dagger a_2^\dagger - a_1 a_2\right)\right] \tag{6.30}$$

on the vacuum state as

$$|\mathrm{vac}, t\rangle = (\cosh \chi t)^{-1} \sum_{n=0}^{\infty} (\tanh \chi t)^n |n, n\rangle. \tag{6.31}$$

If we now compute the reduced density matrix for either mode (see Chapter 7 if you have not encountered the density matrix)

$$\rho_j(t) = \mathrm{tr}_{2-j} \{|\mathrm{vac}, t\rangle\langle \mathrm{vac}, t|\}, \qquad j = 1, 2, \tag{6.32}$$

we find

$$\rho_j(t) = (\cosh \chi t)^{-2} \sum_{n=0}^{\infty} (\tanh \chi t)^{2n} |n\rangle_{j\, j}\langle n|. \tag{6.33}$$

This is recognised as a thermal state with mean photon number $\bar{n} = \sinh^2 \chi t$. The quantum state so created is closely linked to the Hawking effect where correlated pairs of quanta are created near an event horizon, with one particle lost inside the event horizon, while the other escapes. By tracing over a subsystem (in the analogy, the modes interior to the event horizon), the two-photon correlations are lost, generating an incoherent output akin to the thermal radiation emitted from a black hole.

Figure 6.4: John Kerr (1824-1907) was a Scottish physicist and a pioneer in the field of electro-optics. He is best known for the discovery of what is now called the Kerr effect (1877).

Exercise 6.5:

Derive (6.31) and (6.33). Show that this is equivalent to the thermal state with mean occupation $\bar{n} = \sinh^2 \chi t$. **Hint:** since the interaction Hamiltonian creates and destroys *pairs* of quanta and acts on the vacuum, it is sufficient to expand in the basis $|n, n\rangle = |n\rangle_1 \otimes |n\rangle_2$.

6.4 Kerr Effect

A realisation of a fundamentally important interaction Hamiltonian is provided in the context of quantum optics by the *Kerr effect*, occurring when photons interact in a $\chi^{(3)}$ medium. For a single mode system, such as an optical cavity mode, the interaction Hamiltonian in the interaction picture is

$$H_{\mathrm{Int},I} = \frac{\hbar\chi}{2} a^{\dagger 2} a^2. \tag{6.34}$$

This number-conserving evolution leads to *shear* of the quantum state in phase space. An understanding of the Kerr effect provides insights into the quantum evolution of Bose-Einstein condensates, since (6.34) provides a prototypical Hamiltonian describing a single-mode BEC subject to S-wave two-body interactions (scattering theory in the cold-collision regime will be explored in Chapter 9). Notice that $[a^\dagger a, H_{\mathrm{Int},I}] = 0$, and hence the photon number operator is a constant of the motion.

The Heisenberg equation of motion is

$$\frac{da}{dt} = -i\chi a^\dagger a a. \tag{6.35}$$

with solution

$$a(t) = e^{-i\chi a^\dagger a t} a(0). \tag{6.36}$$

While number states do not develop in time (apart from a trivial phase), it is interesting to consider the evolution of an initial coherent state $|\psi, 0\rangle = |\alpha\rangle$, modelling an intense laser field driving the $\chi^{(3)}$ medium, or approximating the quantum state of a Bose-Einstein condensate of atoms occupying a single spatial mode. Using the expansion in number states we have

$$a(t)|\alpha\rangle = \left(e^{-i\chi a^\dagger a t} a(0)\right)|\alpha\rangle = \alpha|\alpha e^{-i\chi t}\rangle, \tag{6.37}$$

recovering a new coherent state with time dependent amplitude. Iterating this expression gives the general result

$$a(t)^p|\alpha\rangle = \alpha^p e^{-i\chi p(p-1)t/2}|\alpha e^{-i\chi p t}\rangle. \tag{6.38}$$

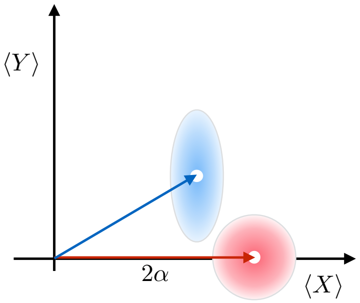

Figure 6.5: Evolution of an initial coherent state according to the Hamiltonian (6.34), whereby initial intensity fluctuations (ΔX) are converted into phase fluctuations (ΔY). The quadrature variances are represented by ellipses, and the quantum state is shown on the phase-space plane defined by the mean quadratures.

Using the overlap of coherent states $\langle\alpha|\beta\rangle = e^{\alpha^*\beta - |\alpha|^2/2 - |\beta|^2/2}$, we find for a coherent initial state

$$\langle a^p(t)\rangle = \alpha^p \exp\left[-i\chi p(p-1)t/2 - |\alpha|^2(1 - e^{-ip\chi t})\right], \tag{6.39}$$

allowing evaluation of the dynamics of observables.

In the Schrödinger picture, a number state will evolve as

$$|n, t\rangle = \exp\left[-i\chi n(n-1)t/2\right]|n\rangle, \tag{6.40}$$

from which we find that an initial coherent state $|\alpha\rangle$ evolves into

$$|\alpha, t\rangle = e^{-|\alpha|^2/2} \sum_{n=0}^{\infty} \frac{\alpha^n}{n!} \exp\left[-i\chi n(n-1)t/2\right]|n\rangle. \tag{6.41}$$

Choosing the phase of the initial state such that α is a real number, and using either (6.39) or (6.41) we can find exact expressions for the mean and variance $V(X) = \langle X^2\rangle - \langle X\rangle^2$ of the quadratures:

$$\langle X(t)\rangle = 2\alpha e^{|\alpha|^2(\cos\chi t - 1)} \cos\left(|\alpha|^2 \sin\chi t\right), \tag{6.42a}$$

$$\langle Y(t)\rangle = 2\alpha e^{|\alpha|^2(\cos\chi t - 1)} \sin\left(|\alpha|^2 \sin\chi t\right), \tag{6.42b}$$

$$\begin{aligned} V(X) = 1 + 2|\alpha|^2 \Big[& 1 + e^{|\alpha|^2(\cos 2\chi t - 1)} \cos\left(\chi t + |\alpha|^2 \sin 2\chi t\right) \\ & - 2e^{2|\alpha|^2(\cos\chi t - 1)} \cos^2\left(|\alpha|^2 \sin\chi t\right)\Big], \end{aligned} \tag{6.42c}$$

$$\begin{aligned} V(Y) = 1 + 2|\alpha|^2 \Big[& 1 - e^{|\alpha|^2(\cos 2\chi t - 1)} \cos\left(\chi t + |\alpha|^2 \sin 2\chi t\right) \\ & - 2e^{2|\alpha|^2(\cos\chi t - 1)} \sin^2\left(|\alpha|^2 \sin\chi t\right)\Big]. \end{aligned} \tag{6.42d}$$

These analytic expressions for the quadratures show an essential effect of the Kerr Hamiltonian, namely that it couples intensity fluctuations to phase fluctuations. For short times $\chi t \ll 1$ one finds that the interaction reduces $V(X)$ below its initial value of 1 while $V(Y)$ is increased, so that intensity fluctuations are reduced at the expense of increased phase fluctuations [Ex 5.6]. This process is illustrated in Figure 6.4.

Exercise 6.6: Evolution of quadratures

1. Prove (6.37), (6.38), and (6.39) for a coherent initial state.
2. Using (6.39), derive (6.42a) and (6.42c).
3. Consider an initial coherent state with α chosen as a real number. Assuming a large amplitude coherent state $|\alpha| \gg 1$, for short times $\chi t \ll 1$, find a linearised expression for $V(X)$, $V(Y)$, and thus show that $V(X)$ decreases while $V(Y)$ increases due to (6.34).

7 The Density Matrix and Quantum Statistics

The most general description of a quantum system includes both quantum *and* statistical uncertainty, enabling the description of any additional uncertainty in specifying the quantum state. Such a formation is provided by the *density matrix* introduced by Von Neumann as a means of describing the statistical state of a quantum system. The density matrix functions as the quantum mechanical analogue of the phase space probability measure of a classical system and provides a natural framework for treating open quantum systems.

If we carry out a measurement of an observable A on a system in a *pure* state $|\psi\rangle$, then we know that, the probability of obtaining the value a is given by $|\langle a|\psi\rangle|^2$, where $A|a\rangle = a|a\rangle$. The reason why we cannot say with certainty what the value of the observable will be is due to the fundamental nature of the disturbance caused by the measuring process itself, rather than any lack of information. We also know that the average value of the observable is given by

$$\langle A\rangle = \langle\psi|A|\psi\rangle \tag{7.1}$$

For the case in which the state of the system is not precisely known (i.e., the system could be in any one of a number of states), we have what is called a *mixed* state. If we know the probabilities, P_a, for the system being in states, $|\psi_a\rangle$, then the average of A is

$$\langle A\rangle = \sum_a P_a\langle\psi_a|A|\psi_a\rangle \tag{7.2}$$

7.1 Density Matrix for Arbitrary States

For a system with state vector $|\psi, t\rangle$, which can be written as a linear combination of the basis eigenkets $|j\rangle$, we define the *density matrix* for the system by the outer product

$$\rho(t) = |\psi, t\rangle\langle\psi, t|. \tag{7.3}$$

Using this, we can rewrite (7.1) as

$$\begin{aligned}\langle A\rangle &= \sum_j \langle\psi, t|j\rangle\langle j|A|\psi, t\rangle = \sum_j \langle j|A|\psi, t\rangle\langle\psi, t|j\rangle = \sum_j \langle j|A\rho(t)|j\rangle \\ &\equiv \mathrm{Tr}\,(A\rho)\,, \end{aligned}\tag{7.4}$$

where the last expression serves to define the *trace* operation as the sum over diagonal matrix elements in any basis. The trace can be applied to any operator. It is easy to show that the trace operation gives the same result in any basis. Consider two distinct complete basis representations $|\lambda\rangle$, $|j\rangle$. Then

$$\mathrm{Tr}\,(A\rho) = \sum_j \langle j|A\rho|j\rangle \tag{7.5}$$

In the $|\lambda\rangle$ basis, this reads

$$\begin{aligned}\mathrm{Tr}\,(A\rho) &= \sum_\lambda \langle\lambda|A\rho|\lambda\rangle = \sum_{j,j',\lambda}\langle\lambda|j\rangle\langle j|A\rho|j'\rangle\langle j'|\lambda\rangle = \sum_{j,j',\lambda}\langle j|A\rho|j'\rangle\langle j'|\lambda\rangle\langle\lambda|j\rangle\\ &= \sum_{j,j'}\langle j|A\rho|j'\rangle\langle j'|j\rangle = \sum_j\langle j|A\rho|j\rangle,\end{aligned} \tag{7.6}$$

where the equivalence is equally valid for continuous eigenvalues provided sums are replaced by integrals. For caculational expedience, we should also note a convenient property of the trace, namely that the trace of any outer product is none other than the inner product:

$$\boxed{\mathrm{Tr}\,(|\psi\rangle\langle\phi|) = \sum_j \langle j|\psi\rangle\langle\phi|j\rangle = \langle\phi|\psi\rangle.} \tag{7.7}$$

In general, the state of the system is not precisely known, i.e., we cannot say with certainty that the system is in the pure state $|\psi, t\rangle$. This uncertainty can be accounted for by the set of statistical probabilities P_a for the system being in states $|\psi_a\rangle$. Then we can rewrite (7.2) as

$$\begin{aligned}\langle A\rangle &= \sum_a\sum_j P_a\langle\psi_a|j\rangle\langle j|A|\psi_a\rangle = \sum_a\sum_j P_a\langle j|A|\psi_a\rangle\langle\psi_a|j\rangle = \sum_j\langle j|A\rho|j\rangle\\ &= \mathrm{Tr}\,(A\rho)\end{aligned} \tag{7.8}$$

where we introduce the general definition of the density operator,

$$\boxed{\rho \equiv \sum_a P_a|\psi_a\rangle\langle\psi_a|.} \tag{7.9}$$

The advantage of using the density operator is that it contains in a rather compact form both the statistical and quantum mechanical information about the system.

7.2 Properties of the Density Operator

For all forms of the density operator, there are a number of general properties:

$$\rho^\dagger = \rho, \tag{7.10a}$$

$$\mathrm{Tr}\,(\rho M) = \mathrm{Tr}\,(M\rho) \tag{7.10b}$$

$$\mathrm{Tr}\,(ABC) = \mathrm{Tr}\,(BCA)\,, \tag{7.10c}$$

$$\mathrm{Tr}\,(\rho) = 1, \tag{7.10d}$$

$$\langle A|\rho|A\rangle \geq 0, \quad \text{for any state } |A\rangle, \tag{7.10e}$$

$$\mathrm{Tr}\left(\rho^2\right) \leq 1. \tag{7.10f}$$

Note that since P_a is real and positive, (7.10e) shows that the diagonal matrix elements of ρ must always be real and positive. Since the trace of ρ is 1, the diagonal matrix elements of ρ in any representation must be real and lie between 0 and 1. The proofs of (7.10a)-(7.10e) follow immediately from the definition. To prove (7.10f) we insert the definition to find

$$\begin{aligned}\mathrm{Tr}\left(\rho^2\right) &= \mathrm{tr}\sum_a P_a|\psi_a\rangle\langle\psi_a| \sum_b P_b|\psi_b\rangle\langle\psi_b| = \sum_j\sum_a\sum_b P_aP_b\langle j|\psi_a\rangle\langle\psi_a|\psi_b\rangle\langle\psi_b|j\rangle \\ &= \sum_a\sum_b P_aP_b|\langle\psi_a|\psi_b\rangle|^2. \qquad (7.11)\end{aligned}$$

However, we know that $\sum_b P_b|\langle\psi_a|\psi_b\rangle|^2 \leq 1$, and hence (7.10f) holds.

7.3 Density Operator Evolution

The equation of motion for the wavefunction $|\psi, t\rangle$ is Schrödinger's equation, using the appropriate Hamiltonian. The equation of motion for the density operator depends whether we are considering an open system or the total system, but the time evolution is rather different to that of operators representing observables. In the Schrödinger picture the density operator evolves in time, while it is time-independent in the Heisenberg picture.

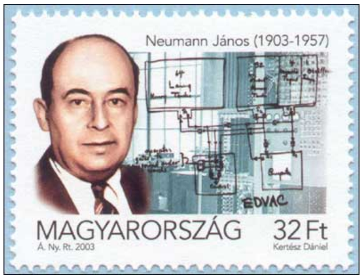

Figure 7.1: John von Neumann (1903-1957) was a pioneer of operator theory in quantum mechanics, among his many contributions to mathematics, physics, and computer science.

7.3.1 Von Neumann equation

In the case we are not dealing with an open system the corresponding equation of motion for the density operator is derived from (7.9) by differentiating and using Schrödinger's equation to obtain *von Neumann's equation* governing the time evolution of the density operator

$$\boxed{i\hbar\frac{\partial\rho}{\partial t} = [H,\rho]. \qquad (7.12)}$$

This description of quantum dynamics has the advantage that it may be readily generalized to treat open quantum systems, and has a close formal analogy with Liouville's equation of motion for the classical phase space distribution.

Von Neumann's equation can be exponentiated to give the formal solution

$$\rho(t) = e^{-iHt/\hbar}\rho(0)e^{iHt/\hbar}. \qquad (7.13)$$

Exercise 7.1: Derivation of von Neumann's equation

Consider (7.9) defined by a set of probabilities P_a at $t = 0$, and derive (7.12) using the Schrödinger equation.

7.3.2 Interaction picture

The density operator evolution in the interaction picture follows from definition (7.9) and the transformation of state kets:

$$\rho_I(t) = U_0^\dagger(t)\rho(t)U_0(t), \tag{7.14}$$

with equation of motion

$$i\hbar\frac{\partial\rho_I(t)}{\partial t} = [V_I(t), \rho_I(t)]. \tag{7.15}$$

7.4 Density Operator in Statistical Mechanics

The density operator is fundamental in the study of quantum statistical mechanics. Any function of the Hamiltonian is a stationary solution of von Neumann's equation, and in particular

$$\boxed{\rho_T \equiv Z(T)^{-1}\exp\left(-\frac{H}{k_B T}\right)} \tag{7.16}$$

is a stationary solution. Normalization forces $Z(T) \equiv \mathrm{Tr}\left(e^{-H/k_B T}\right)$ giving the thermal equilibrium density matrix in the canonical ensemble.

The extension of the Gibbs ensemble to quantum mechanical systems is based upon the *von Neumann entropy* defined as

$$\boxed{S = -k_B \mathrm{Tr}\,(\rho\ln\rho)} \tag{7.17}$$

Exercise 7.2: Canonical ensemble

Show that (7.16) can be obtained by maximising (7.17) at constant T. Work in a basis that diagonalises ρ, and impose the constraints of fixed $E = \langle H\rangle$ and $\mathrm{Tr}\,(\rho) = 1$ using Lagrange multipliers. The first constraint determines one multiplier as proportional to T^{-1} and the second gives a form for $Z(T)$.

7.5 Examples of the Density Operator

7.5.1 Two level systems

A two level system can be written as a two element matrix with basis states,

$$|u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |d\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{7.18}$$

a) Pure State: For an arbitrary ket,

$$|a\rangle = \lambda_a|u\rangle + \mu_a|d\rangle \tag{7.19}$$

the density operator,

$$\rho = \sum_a P_a\Big(|\lambda_a|^2|u\rangle\langle u| \;+\; \lambda_a\mu_a^*|u\rangle\langle d| \;+\; |\mu_a|^2|d\rangle\langle d| \;+\; \lambda_a^*\mu_a|d\rangle\langle u|\Big). \tag{7.20}$$

But since

$$|u\rangle\langle d| = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{7.21}$$

etc., we find

$$\rho = \sum_a P_a \begin{pmatrix} |\lambda_a|^2 & \lambda_a\mu_a^* \\ \lambda_a^*\mu_a & |\mu_a|^2 \end{pmatrix}. \tag{7.22}$$

b) Completely Disordered State: If we require (7.19) to be normalized then $\mathrm{Tr}\,(\rho) = \sum_a P_a(|\lambda_a|^2 + |\mu_a|^2) = 1$ provided $|\lambda_a|^2 + |\mu_a|^2 = 1$. Considering λ_a and μ_a to be completely random, then we can write

$$\begin{aligned} \lambda_a &= e^{i\phi_a}\cos\theta_a \\ \mu_a &= e^{i\chi_a}\sin\theta_a \end{aligned} \tag{7.23}$$

so that

$$\rho = \sum_a P_a \begin{pmatrix} \cos^2\theta_a & \frac{1}{2}e^{i(\phi_a-\chi_a)}\sin(2\theta_a) \\ \frac{1}{2}e^{-i(\phi_a-\chi_a)}\cos(2\theta_a) & \sin^2\theta_a \end{pmatrix} \tag{7.24}$$

If P_a are all the same and θ_a, ϕ_a, χ_a are all *randomly and uniformly distributed* over all values in their ranges $[0, 2\pi)$, then $\sum_a P_a\cos^2\theta_a = \frac{1}{2}$, $\sum_a P_a\sin^2\theta_a = \frac{1}{2}$ and $\sum_a P_a\sin(2\theta_a)e^{i(\phi_a-\chi_a)} = 0$, so that for a *completely disordered* state,

$$\rho = \tfrac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{7.25}$$

c) General State: For a general spin 1/2 system, ρ can be written as a linear combination of the Pauli matrices (3.31), and the 2×2 identity matrix. If $\hat{\boldsymbol{P}}$ is a unit vector—the *polarization vector*—which points in the direction of the particle's spin, then the density operator can be written

$$\rho = \tfrac{1}{2}(1 + \boldsymbol{\sigma}\cdot\hat{\boldsymbol{P}}). \tag{7.26}$$

Exercise 7.3: The polarization vector

Show that the polarization vector is given by $\hat{\boldsymbol{P}} = \langle\boldsymbol{\sigma}\rangle = \mathrm{Tr}\,(\boldsymbol{\sigma}\rho)$.

Exercise 7.4: Spins in a Magnetic Field at Temperature T

Suppose the Hamiltonian is $H = \frac{1}{2}\hbar\mu\mathbf{B}\cdot\sigma$ and we choose the z axis along $\mathbf{B}$, then we can write

$$H = \tfrac{1}{2}\begin{pmatrix} \epsilon & 0 \\ 0 & -\epsilon \end{pmatrix}, \quad \epsilon = \hbar\mu B \tag{7.27}$$

Statistical mechanics tells us that the probability of occupying each of the states is proportional to

$$P(u) \;\propto\; e^{-\epsilon/2kT}, \qquad P(d) \propto e^{\epsilon/2kT}. \tag{7.28}$$

Thus

$$\begin{aligned} \rho &= \frac{|u\rangle\langle u|e^{-\epsilon/2k_BT} + |d\rangle\langle d|e^{\epsilon/2k_BT}}{e^{-\epsilon/2k_BT} + e^{\epsilon/2k_BT}}, \\ &= \frac{1}{1+e^{-\epsilon/k_BT}}\begin{pmatrix} e^{-\frac{\epsilon}{k_BT}} & 0 \\ 0 & 1 \end{pmatrix} \end{aligned} \tag{7.29}$$

7.5.2 Harmonic Oscillator at Temperature T

Using the number state basis, the energy of the state $|n\rangle$ is $(n+\frac{1}{2})\hbar\omega$. In this basis the density operator in the canonical ensemble is *diagonal*, and can be written as

$$\rho = (1-e^{-\hbar\omega/kT})\sum_{n=0}^{\infty} e^{-n\hbar\omega/kT}|n\rangle\langle n| \equiv \sum_{n=0}^{\infty} P(n)|n\rangle\langle n|, \tag{7.30}$$

showing explicitly that ρ is diagonal in the number state basis. Note that $\sum_n P(n) = 1$, as required.

Exercise 7.5: Single mode number fluctuations: photon antibunching

The number fluctuations in a single mode field can be quantified in terms of the normalised second-order correlation function for the number operator $\hat{n}$:

$$g^{(2)} \equiv \frac{\langle\hat{n}^2\rangle}{\langle\hat{n}\rangle^2} = 1 + \frac{V(n)-\bar{n}}{\bar{n}^2}. \tag{7.31}$$

where $V(\hat{A}) \equiv \langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2 = \langle(\hat{A}-\langle\hat{A}\rangle)^2\rangle$, and $\bar{n} = \langle a^\dagger a\rangle$. Starting from (7.30):

1. Express the number distribution for (7.30) in terms of $\bar{n} = \langle n\rangle$.
2. Compute $\langle n(n-1)\rangle$ and thus find the value of $g^{(2)}$ for a thermal state.
3. Do the same for a coherent state, and a number state.

7.6 Equivalence of Ensembles

Consider a system of polarized photons, which can be described by the same formalism as for spin $\frac{1}{2}$ particles. It is not possible to tell the difference between the following ensembles:

i) A mixture of vertically plane-polarized photons in equal proportions, corresponding to the states

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{7.32}$$

ii) A mixture of horizontally plane polarized photons in equal proportions, corresponding to the states

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{7.33}$$

iii) A mixture of circularly plane polarized photons in equal proportions, corresponding to the states

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}, \qquad \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}. \tag{7.34}$$

It is easy to show that all of these correspond to exactly the same density operator

$$\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{7.35}$$

In fact, any pair of orthogonal states mixed together in uniform proportions produces the same density operator, that of a completely disordered state. Here we see that the distinction between the classical probability , governed by the probabilities P_a as introduced in (7.9) and the intrinsic quantum mechanical probability, determined from the state vector, is not at all clear.

7.7 Reduced Density Operator

There is another way in which the state of the system may not be known exactly, and this is when one is dealing with a subsystem of a larger system, which is in a pure state. Such a subsystem is known as an *open quantum system*; that is, a quantum system which communicates in a *quantum* way with the outside world.

Consider a system with sub-systems A, B, and total density matrix ρ. Let $|m, A\rangle$ and $|n, B\rangle$ form complete orthogonal bases for A and B, with eigenvalues denoted by m and n respectively. Consider an operator O_A that is a function of A operators only. Then

$$\begin{aligned} \langle O_A\rangle = \mathrm{Tr}\,(O_A\rho) &= \sum_{m,n}\langle m, A| \otimes \langle n, B|O_A\rho|n, B\rangle \otimes |m, A\rangle \\ &= \mathrm{tr}_A\,(O_A\rho_A)\,, \end{aligned} \tag{7.36}$$

where we identify

$$\boxed{\rho_A \equiv \mathrm{tr}_B\,(\rho) = \sum_n \langle n, B|\rho|n, B\rangle, \tag{7.37}}$$

as the *reduced density matrix* for subsystem A, and $\mathrm{tr}_{A/B}$ denotes the trace over subsystem A/B. Thus we can find the density matrix for a subsystem by "tracing out" the remaining degrees of freedom of the total system. If the total system is in a *separable* pure state $|\psi\rangle = |\phi_A\rangle|\phi_B\rangle$, i.e. the subsystems of not entangled, then we find the rather intuitive result $\rho_A = \mathrm{tr}_B(\rho) = \mathrm{tr}_B(|\phi_A\rangle|\phi_B\rangle\langle\phi_B|\langle\phi_A|) = |\phi_A\rangle\langle\phi_A|$.

Note that ρ_A is clearly Hermitian, and thus it may be diagonalised by a unitary transformation to give a set of eigenvectors $|U, \alpha\rangle$ and eigenvalues P_α, such that $\sum_\alpha P_\alpha = 1$. Hence it may be expressed as

$$\rho_A = \sum_\alpha P_\alpha |U, \alpha\rangle\langle U, \alpha|, \tag{7.38}$$

and is a legitimate density operator in its own right.

8 Dissipation in Open Quantum Systems

8.1 Born-Markov master equation

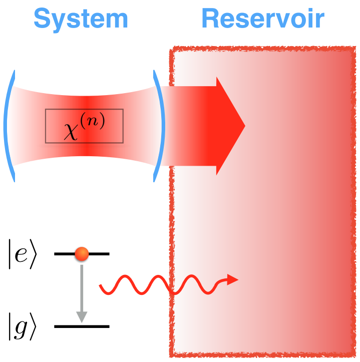

Figure 8.1: An optical cavity and a two level atom coupled to the electromagnetic continuum. The EM-field acts as a reservoir, even at zero temperature where vacuum fluctuations seed spontaneous process. The EM-field vacuum is responsible for natural line width of atomic transitions, and for the irreducible damping of an optical cavity.

When describing real quantum systems, dissipation plays a fundamental role in determining observations. To account for this fundamental physical process, we consider a total system defined by the Schrödinger picture Hamiltonian

$$H = H_S + H_R + V \tag{8.1}$$

where V describes the interaction, and H_S and H_R describe the free evolution of the system and reservoir in the absence of the interaction. In the following we work in the interaction picture, in which $w(t)$ will denote the total density operator, and $V(t) = U_S^\dagger(t) V U_S(t)$ is the interaction Hamiltonian in the interaction picture. The equation of motion is

$$\frac{dw}{dt} = -\frac{i}{\hbar}[V(t), w(t)]. \tag{8.2}$$

Integrating gives the formal solution

$$w(t) = w(0) - \frac{i}{\hbar}\int_0^t dt_1\ [V(t_1), w(t_1)] \tag{8.3}$$

and this may be reintroduced in (8.2) iteratively in the same manner as used to obtain the Dyson series. The first iteration gives

$$\frac{dw}{dt} = -\frac{i}{\hbar}[V(t), w(0)] - \frac{1}{\hbar^2}\int_0^t dt_1\ [V(t), [V(t_1), w(t_1)]]. \tag{8.4}$$

The reduced density operator for the system is given by

$$\rho(t) = \mathrm{tr}_R\Big\{w(t)\Big\}, \tag{8.5}$$

and we can carry out the trace on both sides of (8.4) to give

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}\mathrm{tr}_R\Big\{\ [V(t), w(0)]\ \Big\} - \frac{1}{\hbar^2}\int_0^t dt_1\ \mathrm{tr}_R\Big\{\ \Big[V(t), [V(t_1), w(t_1)]\Big]\ \Big\}, \tag{8.6}$$

an exact implicit equation of motion for the reduced density operator. We now introduce the following simplifications:

i) *Born approximation.*— We assume that the system and reservoir are initially uncorrelated, and remain so throughout the dynamics, so that the density operator factorises as

$$w(t) = \rho(t) \otimes \rho_R, \tag{8.7}$$

and ρ_R is assumed independent of time. This is excellent approximation for many systems of interest, and describes the physical situation when there is a large reservoir upon which the system has little influence.

ii) We assume that the interaction Hamiltonian has zero mean when averaged over the reservoir

$$\mathrm{tr}_R\Big\{V(t)\rho_R\Big\} \equiv 0, \tag{8.8}$$

as can always be arranged by including a non-zero $\mathrm{tr}_R\Big\{V\rho_R\Big\}$ in the system Hamiltonian. This assumption removes the first term in (8.6).

iii) *Markov approximation.*— The trace in (8.6) will involve averages of the form $\langle\Gamma(t)\Gamma^\dagger(t_1)\rangle_R$ where $\Gamma(t)$ is a reservoir operator. We assume that such two-time correlations between reservoir operators decay very rapidly compared to the timescale of evolution of the system. We can then make the replacement

$$\rho(t_1) \to \rho(t) \tag{8.9}$$

in the integrand. This is often an excellent description of the physical system, and a canonical example is given by the damped optical cavity, where photons exit the cavity on a very short timescale.

We thus arrive at the *Born-Markov* equation of motion for the reduced density operator

$$\frac{d\rho}{dt} = -\frac{1}{\hbar^2}\int_0^t dt_1\ \mathrm{tr}_R\Big\{\Big[V(t),[V(t_1),\rho(t)\otimes\rho_R]\Big]\Big\}. \tag{8.10}$$

8.2 Damping to a Quantum Reservoir

Building on our earlier quantization of the electromagnetic field, we generalise (5.56) and consider an interaction Hamiltonian of the form

$$V(t) = \hbar\Big(\Gamma(t)A^\dagger(t) + \Gamma^\dagger(t)A(t)\Big). \tag{8.11}$$

where

$$A(t) = Ae^{-i\omega_0 t}, \tag{8.12}$$

$$\Gamma(t) = \sum_k \kappa_k b_k e^{-i\omega_k t}, \tag{8.13}$$

where our reservoir modes satisfy (4.14), and where the index $k = (\mathbf{k}, \lambda)$ refers to wave vector and an additional degree of freedom. For a two-level atom damped to the EM-field, λ runs over the two independent polarisations for each $\mathbf{k}$. For a reservoir of electrons, λ runs over the two spin-state values for each $\mathbf{k}$ state.

We will assume that the modes are *thermalized*, which means that the quantum density operator is *Gaussian*, with moments

$$\mathrm{tr}_R\left\{\rho_R b_j^\dagger b_k\right\} = \bar{N}(\omega_k)\delta_{jk}, \tag{8.14}$$

$$\mathrm{tr}_R\left\{\rho_R b_j b_k^\dagger\right\} = \left[1+\zeta\bar{N}(\omega_k)\right]\delta_{jk}, \tag{8.15}$$

$$\mathrm{tr}_R\left\{\rho_R b_j b_k\right\} = \mathrm{tr}_R\left\{\rho_R b_j^\dagger b_k^\dagger\right\} = 0, \tag{8.16}$$

and consequently

$$\mathrm{tr}_R\left\{\rho_R \Gamma^\dagger(t)\Gamma(t_1)\right\} = \sum_k |\kappa_k|^2 \bar{N}(\omega_k) e^{-i\omega_k(t_1-t)}, \tag{8.17}$$

$$\mathrm{tr}_R\left\{\rho_R \Gamma(t)\Gamma^\dagger(t_1)\right\} = \sum_k |\kappa_k|^2 \left[1+\zeta\bar{N}(\omega_k)\right] e^{i\omega_k(t_1-t)}, \tag{8.18}$$

$$\mathrm{tr}_R\left\{\rho_R \Gamma(t)\Gamma(t_1)\right\} = \mathrm{tr}_R\left\{\rho_R \Gamma^\dagger(t)\Gamma^\dagger(t_1)\right\} = 0. \tag{8.19}$$

Temporarily adopting the shorthand $B = A(t)$, and $\bar{B} = A(t_1)$ for interaction picture operators, and using (8.19), the master equation now reads

$$\begin{aligned}\frac{d\rho}{dt} = \int_0^t dt_1 \Big\{&\langle\Gamma^\dagger(t_1)\Gamma(t)\rangle_R \left[B^\dagger\rho\bar{B} - \rho\bar{B}B^\dagger\right] + \langle\Gamma(t)\Gamma^\dagger(t_1)\rangle_R \left[\bar{B}\rho B^\dagger - B^\dagger\bar{B}\rho\right] \\ &\langle\Gamma^\dagger(t)\Gamma(t_1)\rangle_R \left[\bar{B}^\dagger\rho B - B\bar{B}^\dagger\rho\right] + \langle\Gamma(t_1)\Gamma^\dagger(t)\rangle_R \left[B\rho\bar{B}^\dagger - \rho\bar{B}^\dagger B\right]\Big\}.\end{aligned} \tag{8.20}$$

We can now write this equation of motion in terms of Schrödinger picture operators, since the time evolution in (8.12), (8.13) is trivial. It is clear from the form (8.17), (8.18), and (8.12) that the correlation functions we require only depend on $\tau = t - t_1$ allowing a change of variables to give the correlation functions [in order of appearance in (8.20)]

$$\int_0^t d\tau\, \langle\Gamma^\dagger(t-\tau)\Gamma(t)\rangle_R e^{i\omega_0\tau} = \int_0^t d\tau\, \sum_k |\kappa_k|^2 \bar{N}(\omega_k) e^{i(\omega_0-\omega_k)\tau}, \tag{8.21}$$

$$\int_0^t d\tau\, \langle\Gamma(t)\Gamma^\dagger(t-\tau)\rangle_R e^{i\omega_0\tau} = \int_0^t d\tau\, \sum_k |\kappa_k|^2 \left[1+\zeta\bar{N}(\omega_k)\right] e^{i(\omega_0-\omega_k)\tau}, \tag{8.22}$$

and their hermitian conjugates. At this point the validity requirement of the Markov approximation can be restated as a condition that the timescale of decay of (8.21), (8.22) is much shorter than the timescale over which the density operator evolves.

Exercise 8.1: Two-time reservoir correlations

Use the form of the interaction operators (8.12), (8.13), and the reservoir correlation functions (8.17), (8.18), (8.19) to derive (8.20) from (8.10).

To further evaluate the correlation functions we can now use the following:

i) *Continuum limit.*— we replace the summations with integration over the density of states:

$$\sum_k |\kappa_k|^2 \bar{N}(\omega_k) e^{i(\omega_0-\omega_k)\tau} \to \sum_\lambda \int d^3\mathbf{k}\; g(\mathbf{k})|\kappa(\mathbf{k},\lambda)|^2 \bar{N}(\omega_\mathbf{k}) e^{i(\omega_0-\omega_\mathbf{k})\tau}, \tag{8.23}$$

where $g(\mathbf{k})$ is density of states for modes with wave vectors $\mathbf{k}$.

ii) *Delta-correlated reservoir.*— as we are presuming a short reservoir correlation time, we can take $t \to \infty$ in the integrals and use the identity

$$\lim_{t\to\infty} \int_0^\infty d\tau\, e^{i\omega\tau} = \pi\delta(\omega) + iP\frac{1}{\omega} \tag{8.24}$$

where P is the *Cauchy principle value*. This identity must be used in the context of an integral over a domain that includes the point $\omega = 0$.

Putting all of this together, the correlation functions (8.21) and (8.22) now become

$$\begin{aligned}\lim_{t\to\infty} \int_0^t d\tau\, \langle \Gamma^\dagger(t-\tau)\Gamma(t)\rangle_R e^{i\omega_0\tau} &= \int_0^\infty d\tau\, \sum_k |\kappa_k|^2 \bar{N}(\omega_k) e^{i(\omega_0-\omega_k)\tau} \\ &= \sum_\lambda \int d^3\mathbf{k}\, g(\mathbf{k})|\kappa(\mathbf{k},\lambda)|^2 \bar{N}(\omega_\mathbf{k}) \int_0^\infty d\tau\, e^{i(\omega_0-\omega_\mathbf{k})\tau} \\ &= \tfrac{1}{2}\gamma\bar{N}(\omega_0) + i\Delta_2, \qquad (8.25) \\ \lim_{t\to\infty} \int_0^t d\tau\, \langle \Gamma(t)\Gamma^\dagger(t-\tau)\rangle_R e^{i\omega_0\tau} &= \tfrac{1}{2}\gamma\left(1+\zeta\bar{N}(\omega_0)\right) + i\Delta_1 + i\zeta\Delta_2, \qquad (8.26)\end{aligned}$$

where

$$\gamma = 2\pi \sum_\lambda \int d^3\mathbf{k}\, g(\mathbf{k})|\kappa(\mathbf{k},\lambda)|^2 \delta(\omega_0-\omega_\mathbf{k}), \tag{8.27}$$

$$\Delta_1 = \sum_\lambda P \int d^3\mathbf{k}\, \frac{g(\mathbf{k})|\kappa(\mathbf{k},\lambda)|^2}{\omega_0-\omega_\mathbf{k}}, \tag{8.28}$$

$$\Delta_2 = \sum_\lambda P \int d^3\mathbf{k}\, \frac{g(\mathbf{k})|\kappa(\mathbf{k},\lambda)|^2\bar{N}(\omega_\mathbf{k})}{\omega_0-\omega_\mathbf{k}}. \tag{8.29}$$

Carrying out these steps, and transforming back to the Schrödinger picture, we finally arrive at the *master equation for damping to a quantum reservoir*

$$\begin{aligned}\frac{d\rho}{dt} &= -\frac{i}{\hbar}[H_S,\rho] - i\Delta_1[A^\dagger A,\rho] - i\Delta_2\left[[A^\dagger,A],\rho\right] && (8.30a)\\ &+ \frac{\gamma}{2}\left(1+\zeta\bar{N}\right)\left(2A\rho A^\dagger - A^\dagger A\rho - \rho A^\dagger A\right), && (8.30b)\\ &+ \frac{\gamma}{2}\bar{N}\left(2A^\dagger\rho A - AA^\dagger\rho - \rho AA^\dagger\right). && (8.30c)\end{aligned}$$

Exercise 8.2: Deriving the master equation

Using (8.25), (8.26) and their hermitian conjugates, derive (8.30) from (8.20).

8.2.1 Interpretation of the Master Equation

i) *System operators.*— We have not specified the operators A, $A^\dagger$, except for the requirement that the time evolution in the interaction picture takes the form

(8.12). For a damped optical cavity the mode operator is that of a simple harmonic oscillator, $A = a$, $A^\dagger = a^\dagger$, with $[a, a^\dagger] = 1$. For a radiatively damped two-level atom, the operators are $A = \sigma_-$, $A^\dagger = \sigma_+$.

ii) *Quantum statistics.*— Depending on the kind of reservoir, set by ζ, we see a clear distinction between *Bose-enhancement* of the damping rate by the factor $\bar{N}(\omega_0)$ for Bosons, and *Pauli blocking* of the damping rate through the factor $[1 - \bar{N}(\omega_0)]$ for Fermions. At $T = 0$, the term (8.30b) is responsible for spontaneous emission of an atom into a vacuum radiation field ($\zeta = -1$), and here Pauli-blocking is evident when $T > 0$.

iii) *Level shifts.*— The shifts incurred from the principal value part of the integrals are important in quantum optical settings, but may often be neglected in dissipative transport phenomena involving massive particles.

iv) *Nonlinear evolution.*— If this system evolution is nonlinear, the derivation can be carried through unchanged, provided the separation of timescales underpinning the Markov approximation still holds. The physical reason is that nonlinear evolution will typically be a small correction to the bare system evolution, over the timescale of the reservoir interaction.

8.3 Pumped, Damped Optical Cavity

As a first example, consider an optical cavity with a single resonant optical mode. The continuum of electromagnetic field modes exterior to the cavity form a quantum environment for the simple harmonic oscillator with system Hamiltonian $H_S = \hbar\omega a^\dagger a$. We will add a coherent driving term (pumping from a laser field) in the form

$$H_D = i\hbar\epsilon(a^\dagger - a), \tag{8.31}$$

where by choosing ϵ to be real we have set the phase of the pump field. In this case $A \to a$, $A^\dagger \to a^\dagger$, $\zeta = 1$, and since $[[a^\dagger, a], \rho] = 0$ it is clear that Δ_2 does not arise, and we may collect the remaining frequency shift as $\bar{\omega} = \omega_0 + \Delta_1$, and find the equation of motion

$$\boxed{\begin{aligned} \frac{d\rho}{dt} &= -i\bar{\omega}[a^\dagger a, \rho] + \epsilon[a^\dagger - a, \rho] && \text{(8.32a)}\\ &+ \frac{\gamma}{2}\left(\bar{N}(\omega_0) + 1\right)(2a\rho a^\dagger - a^\dagger a\rho - \rho a^\dagger a) && \text{(8.32b)}\\ &+ \frac{\gamma}{2}\bar{N}(\omega_0)(2a^\dagger\rho a - aa^\dagger\rho - \rho aa^\dagger). && \text{(8.32c)} \end{aligned}}$$

To see how to work with this master equation, consider first the case $\epsilon = 0$. We then find, in detail:

$$\begin{aligned}\frac{d\langle a\rangle}{dt} &= \mathrm{Tr}\left(\frac{d\rho}{dt}a\right) = -i\bar{\omega}\mathrm{Tr}\left([a^\dagger a, \rho]a\right) + \frac{\gamma}{2}(\bar{N}+1)\mathrm{Tr}\left(2a\rho a^\dagger a - a^\dagger a\rho a - \rho a^\dagger a a\right)\\ &+ \frac{\gamma}{2}\bar{N}\mathrm{Tr}\left(2a^\dagger\rho a a - a a^\dagger \rho a - \rho a a^\dagger a\right) \qquad (8.33)\\ &= -\bar{\omega}\langle a a^\dagger a - a^\dagger a^2\rangle + \frac{\gamma}{2}(\bar{N}+1)\langle 2a^\dagger a^2 - a a^\dagger a - a^\dagger a^2\rangle\\ &+ \frac{\gamma}{2}\bar{N}\langle 2a^2 a^\dagger - a^2 a^\dagger - a a^\dagger a\rangle \qquad (8.34)\\ &= -\left(i\bar{\omega} + \frac{\gamma}{2}\right)\langle a\rangle, \qquad (8.35)\end{aligned}$$

where we use the cyclic property of the trace to get (8.34), and the commutator to get (8.35). Hence, the mean amplitude undergoes exponential decay with rate constant $\gamma/2$. If we consider the photon population, we find

$$\frac{d\langle a^\dagger a\rangle}{dt} = -\gamma\left(\langle a^\dagger a\rangle - \bar{N}(\omega_0)\right), \tag{8.36}$$

with lifetime γ^{-1} and steady state solution $\langle a^\dagger a\rangle = \bar{N}(\omega_0)$, corresponding to thermal equilibrium between the cavity mode and the continuum. It is clear that in the steady state, $\langle a\rangle = 0$. For a single mode with given polarisation λ_1, and cavity output that does not mix polarisation, we can write the damping rate as

$$\gamma = 2\pi\int d^3\mathbf{k}\; g(\mathbf{k})|\kappa(\mathbf{k},\lambda_1)|^2\delta(\omega_0 - |\mathbf{k}|c) = 2\pi\int_0^\infty d\omega\; g(\omega)|\kappa(\omega,\lambda_1)|^2\delta(\omega_0-\omega), \tag{8.37}$$

where we have used the density of states for frequency and the optical dispersion $\omega = |\mathbf{k}|c$. We then find

$$\boxed{\gamma = 2\pi g(\omega_0)|\kappa(\omega_0,\lambda_1)|^2,} \tag{8.38}$$

and the damping rate is set by the density of states and the coupling strength at $\omega \equiv \omega_0$.

Exercise 8.3: Steady state for a zero-temperature environment

Writing (8.32) in the interaction picture with respect to $\bar{\omega}$, for a driven cavity mode damping to a zero temperature environment, $\bar{N} \equiv 0$, $\epsilon > 0$,show that in the steady state $\langle a\rangle = 2\epsilon/\gamma$.

8.4 Two-level Atom

For a two-level atom with states $|1\rangle$ and $|2\rangle$ interacting with the electromagnetic continuum, we set up a correspondence with the Hamiltonian (5.56) by taking $A = \sigma_-$, and $A^\dagger = \sigma_+$, giving the system Hamiltonian

$$H_S = \tfrac{1}{2}\hbar\Omega\sigma_z. \tag{8.39}$$

Here $\zeta \equiv 1$ sets the quantum statistics of the reservoir modes as bosonic.

We obtain the master equation

$$
\boxed{
\begin{aligned}
\frac{d\rho}{dt} &= -i\tfrac{1}{2}\bar{\Omega}[\sigma_z,\rho] && \text{(8.40a)}\\
&+ \frac{\gamma}{2}\left(\bar{N}(\Omega)+1\right)(2\sigma_-\rho\sigma_+ - \sigma_+\sigma_-\rho - \rho\sigma_+\sigma_-) && \text{(8.40b)}\\
&+ \frac{\gamma}{2}\bar{N}(\Omega)\,(2\sigma_+\rho\sigma_- - \sigma_-\sigma_+\rho - \rho\sigma_-\sigma_+)\,, && \text{(8.40c)}
\end{aligned}
}
$$

where $\bar{\Omega} = \Omega + \Delta_1 + 2\Delta_2$ includes the level shifts. Let us now evaluate the terms in this equation.

8.4.1 Damping rate: Einstein A coefficient

Adopting spherical coordinates in **k**-space, the density of states for each λ is given by

$$g(\mathbf{k})d^3\mathbf{k} = \frac{\omega^3 V}{8\pi^3 c^3}d\omega\sin\theta d\theta d\phi. \tag{8.41}$$

We then find, from (8.27) and (5.57), that

$$\gamma = 2\pi\sum_\lambda\int_0^\infty d\omega\int_0^\pi\sin\theta d\theta\int_0^{2\pi}d\phi\frac{\omega^2 V}{8\pi^3c^3}\frac{\omega}{2\hbar\epsilon_0 V}(\hat{\mathbf{e}}_{\mathbf{k}}^{\lambda}\cdot\boldsymbol{d}_{12})^2\delta(\omega-\Omega) \tag{8.42}$$

$$= \frac{\Omega^3}{8\pi^2\epsilon_0\hbar c^3}\sum_\lambda\int_0^{2\pi}d\phi\int_0^\pi\sin\theta d\theta(\hat{\mathbf{e}}_{\mathbf{k}}^{\lambda}\cdot\boldsymbol{d}_{12})^2. \tag{8.43}$$

For each **k** we are free to orient our **k** axes by choosing the k_z axis along $\boldsymbol{d}_{12}$, and $\mathbf{k}\cdot\hat{\mathbf{e}}_{\mathbf{k}}^{\lambda_2} = 0$. We then have $(\mathbf{k}\cdot\hat{\mathbf{e}}_{\mathbf{k}}^{\lambda_1})^2 = d_{12}^2(1-\cos^2\theta)$, and

$$\int_0^{2\pi}d\phi\int_0^\pi\sin\theta d\theta(\hat{\mathbf{e}}_{\mathbf{k}}^{\lambda_1}\cdot\boldsymbol{d}_{12})^2 = d_{12}^2 2\pi\int_0^\pi d\theta\;\sin\theta(1-\cos^2\theta) \tag{8.44}$$

$$= \frac{8\pi}{3}d_{12}^2. \tag{8.45}$$

We thus arrive at the expression for the damping rate

$$\boxed{\gamma = \frac{1}{4\pi\epsilon_0}\frac{4\Omega^3 d_{12}^2}{3\hbar c^3}.} \tag{8.46}$$

this is the *Einstein A coefficient* giving the atomic spontaneous emission rate in laser theory, as should be clear from its role in (8.40b).

8.4.2 Lamb Shift

he term that is independent of temperature, Δ_1, is known as the Lamb shift, an effect of zero-point field fluctuations interacting with the electron. These fluctuations give rise to spontaneous emission and are a source of quantum noise, and of the natural line width of atomic transitions. In fact, the rotating wave approximation that we are currently using does not give the correct non relativistic expression for the Lamb shift, and we must also account for the off-resonant interaction terms. The correct result is given by making the replacement $(\Omega - kc)^{-1} \to (\Omega - kc)^{-1} + (\Omega + kc)^{-1}$ in (8.28).

8.4.3 Stark Shift

The term proportional to $\bar{N}(\Omega)$, Δ_2, gives a temperature-dependent level shift caused by the *AC Stark effect*. The effect is typically not large for optical transitions. In practice it is often a very reasonable approximation to ignore both shifts as they are typically not significant, so that hereafter we take $\bar{\Omega} \equiv \Omega$.

Exercise 8.4: Level shifts

Show that by removing the RWA via the procedure given above, we arrive at the level shifts

$$\Delta_1 = \frac{1}{4\pi\epsilon_0}\frac{2d_{12}^2}{3\hbar\pi c^3} P\int_0^\infty d\omega\,\omega^3\left(\frac{1}{\Omega-\omega}+\frac{1}{\Omega+\omega}\right), \tag{8.47}$$

and

$$\Delta_2 = \frac{1}{4\pi\epsilon_0}\frac{2d_{12}^2}{3\hbar\pi c^3} P\int_0^\infty d\omega\,\omega^3\left(\frac{1}{\Omega-\omega}+\frac{1}{\Omega+\omega}\right)\frac{1}{e^{\hbar\Omega/k_BT}-1}. \tag{8.48}$$

8.4.4 Spontaneous decay

For spontaneous emission we need only consider the regime $T = 0$, and so $\bar{N} = 0$. Neglecting the level shifts, the equation of motion for the atomic coherence $\langle\sigma_-\rangle$ is then found from (8.40) to be

$$\frac{d\langle\sigma_-\rangle}{dt} = \left(-i\Omega - \tfrac{1}{2}\gamma\right)\langle\sigma_-\rangle, \tag{8.49}$$

with solution

$$\langle\sigma_-(t)\rangle = \exp\left[-\left(i\Omega + \tfrac{1}{2}\gamma\right)t\right]\langle\sigma_-(0)\rangle. \tag{8.50}$$

The probability of the atom being in the excited state is $P_2(t) = \rho_{22}(t) = \langle\sigma_+(t)\sigma_-(t)\rangle$. The equation of motion is

$$\frac{dP_2(t)}{dt} = -\gamma P_2(t), \tag{8.51}$$

so that the probability decays exponentially with rate γ. This rate agrees with that found by Wigner and Weisskopf in the theory of natural line width.

Part III

Ultra-Cold Quantum Gases

9 Scattering Theory

Scattering is the study of the unbound states of a system of two interacting particles, in other words, of the continuous spectrum. From a more experimental point of view, it is a way of probing the interactions between particles by measuring their interaction as they pass near each other. The subject is very extensive, and fundamental to the practical applications of quantum mechanics.

9.1 Scattering of Two Particles

We consider the scattering of particles with no internal degrees of freedom, and assume initially that they are distinguishable, with masses m_1 and m_2. We consider here only particles interacting by means of a potential which is a function of the co-ordinate differences. In this case, it is possible to separate completely the centre of mass motion from the relative motion. After this separation, the relative motion is equivalent to a one-body Schrödinger equation for a particle with the *reduced* mass $\mu = m_1 m_2/(m_1 + m_2)$.

9.1.1 Centre of mass coordinates

We consider two particles of masses m_1 and m_2, which satisfy the two-body Schrödinger equation

$$E_{\text{tot}}\Psi(\mathbf{r}_1,\mathbf{r}_2) = \left\{-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V(\mathbf{r}_1 - \mathbf{r}_2)\right\}\Psi(\mathbf{r}_1,\mathbf{r}_2) \tag{9.1}$$

We introduce the variables

$$\mathbf{R} \equiv \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}, \quad \mathbf{r} \equiv \mathbf{r}_1 - \mathbf{r}_2, \quad M \equiv m_1 + m_2, \quad \mu \equiv \frac{m_1 m_2}{m_1 + m_2}. \tag{9.2}$$

From these it follows that

$$\nabla_{\mathbf{R}} = \nabla_{\mathbf{r}_1} + \nabla_{\mathbf{r}_2}, \quad \nabla_{\mathbf{r}} = \frac{m_1\nabla_{\mathbf{r}_2} - m_2\nabla_{\mathbf{r}_1}}{m_1 + m_2}, \tag{9.3}$$

$$-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V(\mathbf{r}_1 - \mathbf{r}_2) = -\frac{\hbar^2}{2M}\nabla_{\mathbf{R}}^2 - \frac{\hbar^2}{2\mu}\nabla_{\mathbf{r}}^2 + V(\mathbf{r}). \tag{9.4}$$

9.1.2 Separation of Variables

If we write the wavefunction as

$$\Psi(\mathbf{r}_1,\mathbf{r}_2) \quad = \quad \Phi(\mathbf{R})\psi(\mathbf{r}), \tag{9.5}$$

then we can separate the Schrödinger equation as

$$-\frac{\hbar^2}{2M}\nabla^2_{\mathbf{R}}\Phi(\mathbf{R}) = E_{\mathrm{CM}}\Phi(\mathbf{R}), \tag{9.6}$$

$$\left\{-\frac{\hbar^2}{2\mu}\nabla^2_{\mathbf{r}} + V(\mathbf{r})\right\}\psi(\mathbf{r}) = \frac{\hbar^2 k^2}{2\mu}\psi(\mathbf{r}), \tag{9.7}$$

$$E_{\mathrm{tot}} = E_{\mathrm{CM}} + \hbar^2 k^2/2\mu. \tag{9.8}$$

The centre of mass equation of motion corresponds to free motion, leaving the description of interactions only in the relative motion Schrödinger equation (9.7).

9.1.3 Scattering Wavefunction and Differential Cross Section

We seek the solution to the relative motion Schrödinger equation

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{9.9}$$

which corresponds to an incoming beam of particles being scattered by a potential $V(\mathbf{r})$ located at the origin. Using $r = |\mathbf{r}|$, the solution must satisfy the following properties

i) There must be a probability of finding a particle moving from left to right along the z-axis. This is the unscattered wave, whose wavefunction is $\exp(ikz)$.

ii) There must be some probability of finding the particle moving away from the scattering centre at the origin, and to conserve particles, this must be of the form $\exp(ikr)/r$ at large r.

iii) Thus, for large r, $\psi(\mathbf{r})$ must have the form

$$\boxed{\psi(\mathbf{r}) \sim e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}.} \tag{9.10}$$

Clearly the dimensions are wrong, and we have been casual regarding normalization. However, an overall normalization factor does not alter any of the arguments that follow (ratios matter, but the absolute magnitudes of the incoming and outgoing waves are immaterial). The dimension of $f(\theta,\phi)$ is clearly length.

iv) Note that $f(\theta,\phi)$ also depends on k, but this argument is often suppressed in presentations of scattering theory. Note that $\hbar^2k^2/2\mu = E$, the total collision energy, and thus the *magnitude* of the momentum is unchanged by a collision with a fixed centre of force.

v) The flux of the *incoming particles* (represented by the wave $\exp(ikz)$) is given by multiplying the particle density (in this case one particle per unit volume since $|\exp(ikz)|^2 = 1$) by the velocity, thus:

$$\begin{aligned} \text{flux in} &= \text{number of particles/unit area/unit time} && (9.11)\\ &= \text{number/unit volume} \times \text{speed} && (9.12)\\ &= v/\text{unit area/unit time.} && (9.13) \end{aligned}$$

vi) The number scattered per unit time into a solid angle $d\Omega$

$$\begin{aligned} &= \text{number/unit volume} \times \text{speed} \\ &\quad \times \text{area on the sphere which subtends } d\Omega \qquad (9.14) \\ &= \frac{|f(\theta,\phi)|^2}{r^2} \times v \times r^2 \times d\Omega = d\Omega |f(\theta,\phi)|^2 v. \qquad (9.15) \end{aligned}$$

vii) Hence

$$\textit{differential cross section} = \frac{\text{number/unit time scattered into } d\Omega}{\text{incoming flux} \times d\Omega}, \qquad (9.16)$$

or, using the standard notation, we have

$$\boxed{\frac{d\sigma}{d\Omega} = |f(\theta,\phi)|^2 \qquad (9.17)}$$

viii) For central forces f depends only on θ, because the system is completely symmetric about the z-axis.

9.1.4 Born Approximation

We can treat scattering using time dependent perturbation theory, in which we take the scattering potential as the perturbation, and the kinetic energy as the free Hamiltonian. We take wavefunctions normalized in a cubic box of volume $\mathcal{V} = L^3$, that is

$$u_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{\mathcal{V}}} e^{i\mathbf{k}\cdot\mathbf{r}}. \qquad (9.18)$$

With a requirement of periodic boundary condition on the edges of the box we also have a discrete spectrum of $\mathbf{k}$ values

$$\mathbf{k} = \frac{2\pi}{L}(n_1, n_2, n_3), \qquad (9.19)$$

where the n_i are integers.

9.1.5 Application of the Dyson Series

We assume the initial state is $|\mathbf{k}_0\rangle$—in the discussion above, $\mathbf{k}_0$ is directed along the z-axis. The wavefunction at time t arising from this initial condition is then given by

$$|\psi, t\rangle_I = |\mathbf{k}_0\rangle - \frac{i}{\hbar}\int_0^t dt' \, V_I(t')|\mathbf{k}_0\rangle. \qquad (9.20)$$

Thus, the amplitude to find momentum **k** in the final state is

$$\begin{aligned}\langle\mathbf{k}|\psi,t\rangle_I &= \delta_{\mathbf{k},\mathbf{k}_0} - \frac{i}{\hbar}\int_0^t dt'\,\langle\mathbf{k}|V_I(t')|\mathbf{k}_0\rangle \\ &= \delta_{\mathbf{k},\mathbf{k}_0} - \frac{i}{\hbar}\int_0^t dt'\,\langle\mathbf{k}|e^{iH_0t'/\hbar}Ve^{-iH_0t'/\hbar}|\mathbf{k}_0\rangle, \\ &= \delta_{\mathbf{k},\mathbf{k}_0} - \frac{i}{\hbar}\int_0^t dt'\,e^{-i(\omega_{\mathbf{k}_0}-\omega_{\mathbf{k}})t'}\langle\mathbf{k}|V|\mathbf{k}_0\rangle, \quad \text{where} \qquad (9.21)\\ \hbar\omega_{\mathbf{k}} &= \frac{\hbar^2\mathbf{k}^2}{2\mu}. \qquad (9.22)\end{aligned}$$

We can do the integral to get the probability for scattering $P(\mathbf{k},\mathbf{k}_0,t)$, with $\mathbf{k}\neq\mathbf{k}_0$, given by

$$\boxed{\begin{aligned}P(\mathbf{k},\mathbf{k}_0,t) &= \frac{4\sin^2\left(\frac{1}{2}(\omega_{\mathbf{k}}-\omega_{\mathbf{k}_0})t\right)}{\hbar^2(\omega_{\mathbf{k}}-\omega_{\mathbf{k}_0})^2}|\langle\mathbf{k}|V|\mathbf{k}_0\rangle|^2, \qquad (9.23)\\ &\to \frac{2\pi}{\hbar^2}\delta(\omega_{\mathbf{k}}-\omega_{\mathbf{k}_0})|\langle\mathbf{k}|V|\mathbf{k}_0\rangle|^2\times t. \qquad (9.24)\end{aligned}}$$

9.1.6 Density of Final States

We need to consider the scattering into a *range* of states residing in the infinitesimal momentum space volume $d^3\mathbf{k}$. From (9.19), the number of states in this range is

$$\begin{aligned}dN \equiv dn_1dn_2dn_3 &= \left(\frac{L}{2\pi}\right)^3 d^3\mathbf{k} = \frac{\mathcal{V}}{8\pi^3}d^3\mathbf{k}, \qquad (9.25)\\ &= \frac{\mathcal{V}}{8\pi^3}k^2\,dk\,d\Omega. \qquad (9.26)\end{aligned}$$

Now note the definition (9.22) of $\omega_{\mathbf{k}}$, so that

$$k\,dk = \frac{\mu\,d\omega_{\mathbf{k}}}{\hbar} \qquad (9.27)$$

so that

$$dN = \frac{\mathcal{V}mk}{8\pi^3\hbar}\,d\omega_{\mathbf{k}}\,d\Omega. \qquad (9.28)$$

The rate of scattering per unit time into *any* $\omega_{\mathbf{k}}$, and into the solid angle element $d\Omega$ is got by integrating with respect to $d\omega_{\mathbf{k}}$ and dividing by t:

$$dw = \frac{\mathcal{V}\mu k}{4\pi^2\hbar^3}|\langle\mathbf{k}|V|\mathbf{k}_0\rangle|^2\,d\Omega. \qquad (9.29)$$

9.1.7 Scattering Matrix Element as the Fourier transform of the Potential

Notice also, with the definition of the wavefunction (9.18) the matrix element is

$$\langle\mathbf{k}|V|\mathbf{k}_0\rangle = \frac{1}{\mathcal{V}}\int d^3\mathbf{r}\,e^{-i\mathbf{q}\cdot\mathbf{r}}V(\mathbf{r}), \qquad (9.30)$$

where **q** is the *momentum transfer* defined by

$$\mathbf{q} \quad\equiv\quad \mathbf{k}-\mathbf{k}_0. \qquad (9.31)$$

9.1.8 Differential Cross Section

To find the differential cross-section, we divide by the incident flux—one particle in the volume $\mathcal{V}$ travelling at a speed $\hbar k/\mu$, i.e., $\hbar k/\mu\mathcal{V}$—and by $d\Omega$, to get

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{\mu^2}{4\pi^2\hbar^4}\left|\int d^3\mathbf{r}\, e^{-i\mathbf{q}\cdot\mathbf{r}}V(\mathbf{r})\right|^2 .} \tag{9.32}$$

At this point, we have arrived at our desired expression, but the physics contained within it is not yet clear. The variable $\mathbf{q}$ encodes both the amount of momentum transfer, and the size of the input momentum. We can identify two regimes where the details of the potential are not so important:

Long wavelength.— Let us assume that $|\mathbf{q}|$ is so small that $\mathbf{q}\cdot\mathbf{r} \ll 1$ inside the range of the potential. Then the exponential factor will be approximately unity over the region of integration, and the differential cross-section becomes *isotropic*. According to (9.17) and (9.10) the outgoing scattered wave is spherically symmetric.

Short wavelength.— In the opposite regime, where $\mathbf{q}\cdot\mathbf{r} \gg 1$ over the range of the potential, the potential varies slowly compared with the rapidly oscillating exponential. We can make a useful change of variables, $\mathbf{r} = \mathbf{u} + \mathbf{v}/2$, $\mathbf{r}' = \mathbf{u} - \mathbf{v}/2$, and in the short wavelength limit find

$$\begin{aligned}\left|\int d^3\mathbf{r}\, e^{-i\mathbf{q}\cdot\mathbf{r}}V(\mathbf{r})\right|^2 &= \int d^3\mathbf{r} \int d^3\mathbf{r}'\, V(\mathbf{r})V(\mathbf{r}')e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}\\ &= \int d^3\mathbf{u} \int d^3\mathbf{v}\; V(\mathbf{u}+\mathbf{v}/2)V(\mathbf{u}-\mathbf{v}/2)e^{i\mathbf{q}\cdot\mathbf{v}}\\ &\to (2\pi)^3 \int d^3\mathbf{u}\; V(\mathbf{u})^2\delta^{(3)}(\mathbf{q}),\end{aligned} \tag{9.33}$$

where it is clear that the differential cross-section has a sharp peak at $\mathbf{k} = \mathbf{k}_0$.

9.2 Born Approximation for Spherically Symmetric Potentials

If the potential has the spherically symmetric form $V(r)$, then, defining $q = |\mathbf{k} - \mathbf{k}_0|$, the *Fourier transformed potential*, in (9.32), becomes (in spherical polar co-ordinates r, α, β)

$$\begin{aligned}\int d^3\mathbf{r}\, e^{-i\mathbf{q}\cdot\mathbf{r}}V(\mathbf{r}) &= \int r^2 \sin\alpha\, dr\, d\alpha\, d\beta\, e^{-iqr\cos\alpha}V(r),\\ &= \frac{4\pi}{q}\int_0^\infty V(r) r \sin qr\, dr,\end{aligned} \tag{9.34}$$

and the cross section becomes

$$\frac{d\sigma}{d\Omega} = \frac{4\mu^2}{\hbar^4 q^2}\left|\int_0^\infty V(r) r \sin qr\, dr\right|^2 . \tag{9.35}$$

Notice that, for spherically symmetric potentials:

i) The cross section depends only on $q = |\mathbf{k} - \mathbf{k}_0|$.

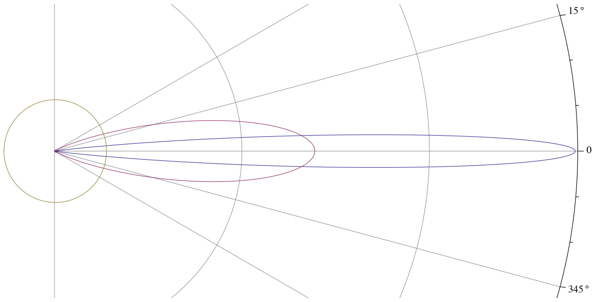

Figure 9.1: Polar plot of the differential cross section (rescaled) for scattering from the potential (9.37). The curves correspond to (from the most circular to the most sharply peaked) to $ka = 0.2, 8, 30$.

ii) The energy conservation enforced by (9.24) requires $|\mathbf{k}_0| = |\mathbf{k}| \equiv k$. Defining the scattering angle θ to be the angle between $\mathbf{k}_0$ and $\mathbf{k}$, we have

$$q \quad = \quad \sqrt{2k^2(1-\cos\theta)} = 2k\sin\frac{\theta}{2}\ . \tag{9.36}$$

9.2.1 Spherical Step

We take

$$V(r) \quad = \quad \begin{cases} 0, & r > a, \\ U_0, & r < a. \end{cases} \tag{9.37}$$

For this potential

$$\int_0^\infty V(r) r \sin qr\, dr = U_0 \int_0^a r \sin qr\, dr = \frac{U_0}{q^2}(\sin qa - qa\cos qa). \tag{9.38}$$

Substituting this in the formula (9.35) for the cross section yields

$$\frac{d\sigma}{d\Omega} = \left(\frac{2\mu U_0 a^3}{\hbar^2}\right)^2 \left(\frac{\sin qa - qa\cos qa}{(qa)^3}\right)^2, \tag{9.39}$$

giving the qualitative result shown in (9.1). For small values of qa the cross section is almost isotropic, while for large qa there is a very strong forward peaking. This is a general feature of all scattering potentials. From the formula (9.32), it can be seen that there will be little contribution to the integral if $\mathbf{q}\cdot\mathbf{r} \ll 1$ inside the range of the potential. When $\mathbf{q} = 0$, the cross section must also be independent of angle for a spherically symmetric potential since the angular dependence of the cross section only arises from the dependence of $\mathbf{q}$ on angle. This limit is of course the limit of long wavelength.

9.2.2 Rutherford Scattering

We consider first scattering from a *screened* Coulomb potential

$$V(r) \quad \to \quad \frac{\beta e^{-\lambda r}}{r}, \tag{9.40}$$

in which case

$$\int_0^\infty V(r) r \sin qr\, dr = \beta \int_0^\infty e^{-\lambda r} \sin qr\, dr = -\frac{\beta q}{q^2 + \lambda^2}. \tag{9.41}$$

The value of the screening constant is quite small—in practice something like it arises from the electrons in an atom, which screen the highly localized charge of the nucleus. For sufficiently large q, we can set $\lambda \to 0$, and then get the *Rutherford scattering* cross section

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{\mu^2 \beta^2}{4(\hbar k)^4 \sin^4(\theta/2)}. \qquad (9.42)}$$

Since $\hbar k$ is the momentum of the incoming particles, this formula does not explicitly contain Planck's constant, and is exactly the same as was derived classically by Rutherford. Even though it is derived using the Born approximation, it is in fact exact. However, the *amplitude* derived this way differs by a non-trivial phase from the exact result, which can be computed exactly by other means not covered in this course.

Figure 9.2: Ernest Rutherford (1871-1937) proposed that the atomic nucleus was a dense charge concentration, confirmed in experiments involving scattering of alpha particles from gold atoms in 1911.

9.2.3 Validity of the Born Approximation

The Born approximation is perturbative, since it omits the higher terms in the Dyson series. The simplest estimate can be made by saying that the term calculated must be "small". This will happen for weak potentials, and when $\mathbf{q}$ is large, since then the exponential oscillates rapidly, and the integral will be small.

Exercise 9.1: Periodic Potentials—the Bragg Formula

Suppose that the scattering potential is *periodic*;

$$V(\mathbf{r}) = V(\mathbf{r} + \mathbf{a}). \tag{9.43}$$

Show that scattering only occurs if $\mathbf{q} \cdot \mathbf{a} = 2n\pi$. Show that this is *Bragg scattering*. Describe the nature of the scattering when there are three periods, $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ as would be the case for any crystal.

Exercise 9.2: Higher Order Born Approximation

The second order Born approximation would be obtained by using the Dyson series to second order. Show how to implement the second order.

9.3 The Method of Partial Waves

In this section we implement the description of scattering from the point of view of the Schrödinger equation, utilizing fully the wave nature of the problem, and especially the description in terms of angular momentum. In this treatment we are able to go beyond the Born approximation and solve the two-body scattering problem exactly.

9.3.1 Eigenfunctions

Because the force is central, H commutes with $\boldsymbol{L}$, and we can find simultaneous eigenstates $\psi_{E,l,m}(\mathbf{r})$, which can be written in terms of spherical harmonics as

$$\psi_{E,l,m}(\mathbf{r}) \quad = \quad L_{k,l}(r) Y^l_m(\theta, \phi), \tag{9.44}$$

and the radial function satisfies the differential equation

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dL_{k,l}}{dr}\right) + \left\{k^2 - U(r) - \frac{l(l+1)}{r^2}\right\} L_{k,l} = 0, \tag{9.45}$$

$$\text{where } U(r) \equiv \frac{2\mu}{\hbar^2} V(r), \qquad E = \frac{\hbar^2 k^2}{2\mu}. \tag{9.46}$$

9.3.2 The Free Particle

In this case $U(r) = 0$, and the equation reduces to a special case of Bessel's equation, the solutions of which are called *spherical Bessel functions*

$$j_l(kr) \quad = \quad \sqrt{\frac{\pi}{2kr}} J_{l+\frac{1}{2}}(kr), \tag{9.47}$$

$$n_l(kr) \quad = \quad \sqrt{\frac{\pi}{2kr}} N_{l+\frac{1}{2}}(kr). \tag{9.48}$$

These have the properties

1. $j_l(kr)$ is *regular* at the origin, while $n_l(kr)$ is *singular* at the origin, and in fact for small l we can give explicit formulae

$$j_0(z) = \frac{\sin z}{z}, \qquad n_0(z) = -\frac{\cos z}{z}, \tag{9.49}$$

$$j_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z}, \qquad n_1(z) = -\frac{\cos z}{z^2} - \frac{\sin z}{z}, \tag{9.50}$$

$$j_2(z) = \left(\frac{3}{z^3} - \frac{1}{z}\right)\sin z - \frac{3}{z^2}\cos z, \qquad n_2(z) = -\left(\frac{3}{z^3} - \frac{1}{z}\right)\cos z - \frac{3}{z^2}\sin z. \tag{9.51}$$

2. For small z we have the expansion

$$j_l(z) \approx \frac{z^l}{1 \cdot 3 \cdot 5 \ldots (2l+1)}, \qquad n_l(z) \approx \frac{1 \cdot 3 \cdot 5 \ldots (2l-1)}{z^{l+1}}. \tag{9.52}$$

3. For large z the solutions approach the asymptotic forms

$$j_l(z) \sim \frac{\sin(z - l\pi/2)}{z}, \qquad n_l(z) \sim -\frac{\cos(z - l\pi/2)}{z}. \tag{9.53}$$

Thus, for a free particle, a general solution to the Schrödinger equation can be written

$$\psi(\mathbf{r}) \quad = \quad \sum_{l,m} a_{l,m} j_l(kr) Y^l_m(\theta, \phi). \tag{9.54}$$

Only the j_l functions occur, since the wavefunction must be finite at the origin.

For an interaction potential with *axial symmetry* $[V(\mathbf{r}) \equiv V(r,\theta)]$, only $m = 0$ can occur, and we can use the relationship between the spherical harmonics and the Legendre polynomials

$$Y_0^l(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta), \tag{9.55}$$

and we can write an expansion of the form

$$\psi(\mathbf{r}) \quad = \quad \sum_l A_l j_l(kr) P_l(\cos\theta). \tag{9.56}$$

A particular case is known as the *Rayleigh plane wave expansion*

$$\boxed{e^{ikz} = \sum_l (2l+1) i^l j_l(kr) P_l(\cos\theta).} \tag{9.57}$$

This expansion is fundamental in scattering theory of almost every kind.

9.3.3 Scattering for a Potential with Finite Range

If $U(r) = 0$ for $r > a$ then outside this range the wavefunction will again be a solution of the equation with $U(r) = 0$, hence outside this range (assuming axial symmetry)

$$\psi(\mathbf{r}) \quad = \quad \sum_l \psi_l(r) P_l(\cos\theta), \tag{9.58}$$

and the *general solution* for the radial wavefunction is a linear combination of the two possible solutions

$$\boxed{\psi_l(r) = A_l \left\{\cos(\delta_l) j_l(kr) - \sin(\delta_l) n_l(kr)\right\},} \tag{9.59}$$

where our choice of coefficients serves to define the *phase shifts* δ_l. Using the long-range approximation for the spherical Bessel functions (9.53) we find the asymptotic form

$$\psi_l(r) \quad \sim \quad \frac{A_l}{kr} \sin(kr - l\pi/2 + \delta_l). \tag{9.60}$$

Thus, for large r,

$$\psi(\mathbf{r}) \quad \sim \quad \sum_l \frac{A_l}{kr} \sin(kr - l\pi/2 + \delta_l) P_l(\cos\theta). \tag{9.61}$$

But we know that for large r

$$\psi(\mathbf{r}) \quad \sim \quad e^{ikz} + f(\theta)\frac{e^{ikr}}{r}, \tag{9.62}$$

$$\sim \quad \sum_l (2l+1) i^l P_l(\cos\theta) \frac{\sin(kr - l\pi/2)}{kr} + f(\theta)\frac{e^{ikr}}{r}. \tag{9.63}$$

We now compare (9.60) with (9.63). By writing the sin functions in terms of complex exponentials, we can equate coefficients of $e^{-ikr}P_l(\cos\theta)$ to get

$$A_l = (2l+1)i^l e^{i\delta_l}. \tag{9.64}$$

Now equate coefficients of e^{ikr}, to get

$$f(\theta) = \frac{1}{2ik}\sum_l \left\{A_l e^{i\delta_l}(-i)^l - (2l+1)\right\} P_l(\cos\theta). \tag{9.65}$$

Collecting terms together we find an expression for $f(\theta)$ in terms of the phase shifts for each partial wave, δ_l, as

$$\boxed{f(\theta) = \frac{1}{2ik}\sum_l (2l+1)\left(e^{2i\delta_l} - 1\right) P_l(\cos\theta)} \tag{9.66}$$

It can be shown that the above analysis requires only that

$$\lim_{r\to\infty} rU(r) = 0 \tag{9.67}$$

and this condition provides a more general *definition* of a finite range potential. For the special case of the Coulomb potential, $U(r) = a/r$, and the condition (9.67) is not satisfied. Coulomb scattering requires a separate analysis, and will not be dealt with in this course.

Exercise 9.3: Asymptotic form a partial wave

Show that (9.59) and (9.53) lead to the expression (9.61).

Exercise 9.4: Equivalent partial wave coefficient

For analysis of (9.66) in the low k limit, prove the useful identity

$$\frac{e^{i2\delta_l} - 1}{2i} = \frac{\tan\delta_l}{1 - i\tan\delta_l}. \tag{9.68}$$

9.3.4 Total Cross Section

The total cross section is given by

$$\sigma = \int d\Omega |f(\theta)|^2 \tag{9.69}$$

$$= \frac{1}{4k^2}\sum_{l,l'}(2l+1)(2l'+1)(e^{-2i\delta_l} - 1)(e^{2i\delta_{l'}} - 1) \times \int_0^\pi 2\pi \sin\theta\, d\theta\, P_l(\cos\theta)P_{l'}(\cos\theta). \tag{9.70}$$

We now use the orthogonality of the Legendre polynomials

$$\int_0^\pi \sin\theta\, d\theta\, P_l(\cos\theta)P_{l'}(\cos\theta) = \frac{2\delta_{ll'}}{2l+1}, \tag{9.71}$$

giving

$$\boxed{\sigma = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l \equiv \sum_l \sigma_l} \tag{9.72}$$

The quantity σ_l is known as the l-wave cross section. From this equation, it can be seen that as far as *total* cross sections are concerned, each partial wave scatters independently. Of course this is not true in terms of differential cross sections.

9.4 Interpretation of the Phase Shifts

The lth radial wavefunction is usually written in terms of

$$u_l(r) \equiv kr\,\psi_l(r) \sim A_l \sin(kr - l\pi/2 + \delta_l). \tag{9.73}$$

The phase shift δ_l is a measure of how far the asymptotic sinusoidal wavefunction is displaced at the origin from the corresponding free asymptotic sinusoidal wavefunction.

9.4.1 Only a finite number of δ_l are significantly different from zero

Classically this follows from an impact parameter interpretation. If the particle has angular momentum l, the wavefunction is only significantly different from zero when $\hbar kr \approx l\hbar$, since $l\hbar$ is the approximate classical value of the angular momentum. This means that if a is the range of the potential, and if $l \gg ka$, this partial wave will not be altered, and its phase shift will be zero. Essentially, if l is very large, the centrifugal term $l(l+1)/r^2$ is very much larger than $U(r)$, and the interaction is dominated by the centrifugal term.

9.4.2 The Optical Theorem

If we calculate $\mathrm{Im} f(0)$, and use $P_l(\cos 0) = 1$,

$$\mathrm{Im} f(0) = \frac{1}{2k} \sum_l (2l+1)(1 - \cos 2\delta_l) = \frac{1}{k} \sum_l (2l+1) \sin^2 \delta_l \tag{9.74}$$

$$= \frac{k\sigma}{4\pi}. \tag{9.75}$$

The imaginary part of the forward amplitude can be looked on as an “absorption”. It measures that proportion of the particles which does not remain in the forward beam. Since particles are conserved, this must be equal to the number scattered, which is measured by the total cross section.

9.4.3 Measurement of Phase Shifts

In practice one can measure the differential cross section, and hence $|f(\theta)|^2$, quite accurately at a number of energies. The phase shifts δ_l are of course energy dependent, and therefore must be determined at every scattering energy, and can only be determined by a fitting procedure, which is considerably assisted by the fact that only a few phase shifts are normally nonzero.

Exercise 9.5: Hard Sphere Potential

The hard sphere potential is defined by

$$U(r) = \begin{cases} \infty, & r < a \\ 0, & r > a. \end{cases} \tag{9.76}$$

Using the boundary condition that the wavefunction should vanish at $r = a$, find the phase shifts for all l.

9.5 Cold collision regime: S-wave scattering

9.5.1 Scattering length and effective range

In very low energy scattering only the S-wave will contribute. Inspection of (9.10) shows that if there is scattering in the limit $k \to 0$, the asymptotic form of the wavefunction for large r must take the form

$$\boxed{\psi \equiv 1 - \frac{a_s}{r},} \tag{9.77}$$

for some constant a_s (not necessarily positive), and a_s then gives the intercept of the asymptotic wavefunction (9.77) with the r axis. On the other hand, in the small k limit the intercept of the far-field wavefunction can be found from (9.59) in terms of the phase shift as

$$\tan\delta_0 = -ka_s. \tag{9.78}$$

Using this expression, and (9.66) we then have

$$\lim_{k\to 0}\frac{e^{2i\delta_0}-1}{2ik} = \lim_{k\to 0}\frac{-a_s}{1+ia_sk} = -a_s. \tag{9.79}$$

The parameter a_s is called the *scattering length*.

The differential cross section is obviously given by

$$\left.\frac{d\sigma}{d\Omega}\right|_{k\to 0} = {a_s}^2. \tag{9.80}$$

A parametrization to higher order is made using a parameter r_0, the effective range, and for various reasons it is made in the form

$$k\cot\delta_0 \approx -\frac{1}{a_s} + \tfrac{1}{2}r_0k^2 + \ldots, \tag{9.81}$$

where the higher order terms are higher powers of k^2. Except for pathological potentials, it can be shown that $k\cot\delta_0$ has a power series in E, which is equivalent to a power series in k^2.

Exercise 9.6: S-wave limit of $f(\theta)$

Using $\tan\delta_0 = -ka_s$, prove (9.79).

9.5.2 S-wave cross section and exchange symmetry

It is clear from (9.80) that the total scattering cross section is

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega} = 4\pi a_s^2, \tag{9.82}$$

so that the collision is essentially that of hard sphere target of radius a_s.

Thus far in this chapter we have not considered the symmetrization of the wavefunction with respect to particle exchange, and have assumed that the particles are distinguishable. For Bosons (Fermions) the wavefunction must be symmetric (antisymmetric) under interchange of the particle coordinates. The exchange operation amounts to changing the sign of the relative coordinate, namely $\mathbf{r} \to -\mathbf{r}$, or $r \to r, \theta \to \pi - \theta, \phi \to \pi + \phi$ for our cylindrical coordinates describing the scattering process. For the cylindrically symmetric potentials that we usually encounter, the exchange symmerized wavefunctions corresponding to (9.10) are

$$\psi = e^{ikz} \pm e^{-ikz} + [f(\theta) \pm f(\pi - \theta)]\frac{e^{ikr}}{r} \tag{9.83}$$

and the amplitude for scattering in the direction specified by θ is $f(\theta) \pm f(\pi - \theta)$, giving the differential cross section

$$\boxed{\frac{d\sigma}{d\Omega} = |f(\theta) \pm f(\pi - \theta)|^2.} \tag{9.84}$$

To find the total cross section we integrate this expression over all *distinct* final states. Hence, we must be careful to only integrate over the range $0 \leq \theta \leq \pi/2$ and $0 \leq \phi \leq 2\pi$, since the range $\pi/2 \leq \theta \leq \pi$ gives identical scattered states due to the symmetry. Thus, if the scattering is purely S-wave, the total cross section is

$$\boxed{\sigma = 8\pi a_s^2} \tag{9.85}$$

for identical Bosons, and σ vanishes for identical Fermions.

9.5.3 Effective potential for identical Bosons

We now return to the two body-problem that formed our starting point, Eq. (9.1). In general the two-body interaction potentials are unknown and must be characterised on a case by case basis for each distinct pair of atoms involved in a pair-wise collision. However, for identical Bosons, a drastic simplification of the theory is now available.

We can look for an effective potential, $V_{\text{eff}}(\mathbf{r})$, to replace the physical two-body interaction. We only require that it must give the same $f(\theta)$, and σ as the physical two-body potential, *in the S-wave limit*. It is straightforward to verify that this is achieved via the effective potential

$$\boxed{V_{\text{eff}}(\mathbf{r}) = g\delta^{(3)}(\mathbf{r}) \equiv \frac{4\pi\hbar^2 a_s}{m}\delta^{(3)}(\mathbf{r}).} \tag{9.86}$$

The atomic collision can be thought of as occurring between atoms with a two-body potential for point-like particles, with a strength characterised by the scattering length. This is sometimes called a *contact interaction*.

Exercise 9.7: Point-like scattering of Bosons

Verify that the value of g given in (9.86) gives the correct values for $d\sigma/d\Omega$ for S-wave scattering, and hence is the correct two-body effective potential for the two-particle Schrödinger equation.

9.6 The Spherical Step

The scattering length depends on the details of the interatomic potential. Consider the spherical step potential (9.37):

$$V(r) = \begin{cases} 0, & r > a, \\ U_0, & r < a. \end{cases} \tag{9.87}$$

The radial wavefunction for any l can be written

$$L_{k,l}(r) = \frac{u_{k,l}(r)}{r}, \tag{9.88}$$

where $u_{kl}(r)$ satisfies the *radial Schrödinger equation*

$$\frac{d^2u_{kl}}{dr^2} + \left\{k^2 - U(r) - \frac{l(l+1)}{r^2}\right\} u_{kl} = 0. \tag{9.89}$$

We consider the case of $l = 0$, and

$$\frac{2\mu U_0}{\hbar^2} = -\beta^2 < 0, \tag{9.90}$$

so that the wavefunction has the form (omitting the subscripts k and 0 for brevity)

$$u(r) = \begin{cases} A\sin(kr+\delta), & r > a, \\ B\sin qr, & r < a. \end{cases} \tag{9.91}$$

where $q^2 = \beta^2 + k^2$. The boundary conditions at $r = a$ lead to two equations from which A and B can be eliminated to give

$$k\cot(ka+\delta) = q\cot qa. \tag{9.92}$$

This equation can be solved for $k\cot\delta$, giving

$$\boxed{k\cot\delta = \frac{q\cot qa + k\tan ka}{1-(q/k)\cot qa\tan ka}.} \tag{9.93}$$

The solution is not straightforward to interpret, but can be used to get the scattering length and effective range.

9.6.1 Relation to Bound States

We consider a situation in which there is one bound state with very small binding energy. The solutions of the Schrödinger equation for k very close to zero look very similar to the bound state solution, except at large distances.

When k is very small, we can write (setting $A = 1$ for convenience)

$$u(r) \approx kr\cos\delta + \sin\delta \tag{9.94}$$

so the the wavefunction crosses the axis at the point

$$r = -\frac{1}{k\cot\delta} = a_s. \tag{9.95}$$

That is, the scattering length represents the place where the $k = 0$ wavefunction crosses the axis.

If the binding energy of the bound state is $E_b = \hbar^2\alpha^2/2\mu$, the logarithmic derivative $u'(a)/u(a)$ for the bound state is $-\alpha$. *If the binding energy and hence αa is very small, a*s the energy changes to zero, the internal wavefunction changes very little, and the logarithmic derivative for $k = 0$ is $k\cot\delta_{k=0} = -1/a_s$.

Thus we can deduce that the scattering length in the case that there is a bound state with very small binding energy is given by

$$a_s \approx \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2\mu E_b}} \tag{9.96}$$

Exercise 9.8: Effective range

Show the effective range in this case is $r_0 \approx a$.

9.7 Green's Function and the Lippman-Schwinger Equation

9.7.1 The Green's Function

The Green's function $G(\mathbf{r}, \mathbf{r}')$ for the free Schrödinger equation is a function which satisfies the equation

$$\left(\nabla^2 + k^2\right) G(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}'). \tag{9.97}$$

There are two solutions to this equation—the one of most interest corresponds to *outgoing waves*, and is

$$\boxed{G_{\mathrm{o}}(\mathbf{r}, \mathbf{r}') = -\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r} - \mathbf{r}'|}.} \tag{9.98}$$

There is another solution, corresponding to *incoming waves*,

$$G_{\mathrm{i}}(\mathbf{r}, \mathbf{r}') = -\frac{e^{-ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r} - \mathbf{r}'|}. \tag{9.99}$$

The easiest way to show these are solutions is to use the relationship

$$\nabla^2 \frac{1}{|\mathbf{r}|} = -4\pi\delta(\mathbf{r}). \tag{9.100}$$

Next convert to polar coordinates, and use

$$\nabla^2 \frac{e^{ikr}-1}{r} = \frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}\left(\frac{e^{ikr}-1}{r}\right), \tag{9.101}$$

$$= -k^2\frac{e^{ikr}}{r}. \tag{9.102}$$

The last equality follows by expanding in power series and differentiating term by term. From (9.100) and (9.101)

$$\left(\nabla^2+k^2\right)\frac{e^{ikr}}{r} = \nabla^2\frac{e^{ikr}-1}{r}+\nabla^2\frac{1}{r}+k^2\frac{e^{ikr}}{r} = -4\pi\delta(\mathbf{r}). \tag{9.103}$$

9.7.2 Use of the Green's Function in Scattering

We will consider the Schrödinger equation in the form

$$\left(\nabla^2+k^2\right)\psi_{\mathbf{k}}(\mathbf{r}) = U(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r}). \tag{9.104}$$

Using the Green's function, the solution can be written

$$\psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{1}{4\pi}\int d^3\mathbf{r}'\,\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}U(\mathbf{r}')\psi_{\mathbf{k}}(\mathbf{r}'). \tag{9.105}$$

(Conventionally $\mathbf{k} = (0, 0, k)$.) This is a form of the integral equation of scattering theory known as the *Lippman-Schwinger equation*.

a) Asymptotic Analysis: If the potential vanishes outside a certain range R, then the asymptotic wavefunction at large distances is computed for $|\mathbf{r}'| < R$, and $|\mathbf{r}| \gg R$. Thus at long distances we can approximate

$$|\mathbf{r}-\mathbf{r}'| \approx \sqrt{x^2-2xx'\cos\theta} \tag{9.106}$$

$$= x - x'\cos\theta. \tag{9.107}$$

We may neglect the second term in the denominator of (9.105), but it must be included in the exponent, giving the result

$$\boxed{\psi_{\mathbf{k}}(\mathbf{r}) \sim \psi^s_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{e^{ik|\mathbf{r}|}}{4\pi|\mathbf{r}|}\int d^3\mathbf{r}'\;U(\mathbf{r}')e^{-i\mathbf{k}'\cdot\mathbf{r}'}\psi_{\mathbf{k}}(\mathbf{r}'). \qquad (9.108)}$$

In this equation $\mathbf{k}'$ is a vector with magnitude k, and parallel to $\mathbf{r}$, that is, in the direction of the scattered particle.

b) Scattering Amplitude: The asymptotic form of the wavefunction shows that the scattering amplitude is given by

$$f(\theta,\phi) = -\frac{1}{4\pi}\int d^3\mathbf{r}'\;U(\mathbf{r}')e^{-i\mathbf{k}'\cdot\mathbf{r}'}\psi_{\mathbf{k}}(\mathbf{r}'). \tag{9.109}$$

Thus, in principle, to get the scattering amplitude on should solve the Lippman-Schwinger equation (9.105) to get $\psi_{\mathbf{k}}(\mathbf{r})$, and then use (9.109).

c) The Born Approximation: The approximation that the scattering is weak enables us to make the replacement

$$\psi_{\mathbf{k}}(\mathbf{r}') \rightarrow e^{i\mathbf{k}\cdot\mathbf{r}'} \tag{9.110}$$

yields the Born Approximation in the form

$$f(\theta,\phi) = -\frac{1}{4\pi}\int d^3\mathbf{r}'\, U(\mathbf{r}')e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}'}. \tag{9.111}$$

Exercise 9.9: Higher Order Born Approximations

How would you write down higher order approximations to the scattering amplitude based on the use of (9.105) and (9.108)?

9.7.3 The *T*-Matrix

The T-matrix or *transition matrix* is defined in terms of the scattering amplitude as

$$\begin{aligned} T_{\mathbf{k}',\mathbf{k}} &= -\frac{2\pi\hbar^2}{\mu} f(\theta,\phi) && (9.112)\\ &= \frac{\hbar^2}{2\mu}\int d^3\mathbf{r}'\, U(\mathbf{r}')e^{-i\mathbf{k}'\cdot\mathbf{r}'}\psi_{\mathbf{k}}(\mathbf{r}') = \int d^3\mathbf{r}'\, V(\mathbf{r}')e^{-i\mathbf{k}'\cdot\mathbf{r}'}\psi_{\mathbf{k}}(\mathbf{r}'). && (9.113)\end{aligned}$$

Exercise 9.10: Equivalence of Descriptions

Use this definition to express $\psi_{\mathbf{k}}(\mathbf{r})$ in terms of $T_{\mathbf{k}',\mathbf{k}}$, and that therefore *everything* about the scattering problem is contained in the T-matrix.

9.7.4 Lippman-Schwinger Equation for the *T*-Matrix

It is not very difficult to derive the Lippman-Schwinger equation for the T-matrix from that for the wavefunction. It takes the form

$$\begin{aligned} T_{\mathbf{k}',\mathbf{k}} &= V_{\mathbf{k}',\mathbf{k}} + \frac{2\mu}{(2\pi)^3\hbar^2}\int d^3\mathbf{q}\, \frac{V_{\mathbf{k}',\mathbf{q}}T_{\mathbf{q},\mathbf{k}}}{k^2 - q^2 + i\epsilon}, && (9.114)\\ V_{\mathbf{k}',\mathbf{k}} &\equiv \int d^3\mathbf{r}\, V(\mathbf{r})e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}. && (9.115)\end{aligned}$$

The $i\epsilon$ is very common in scattering theory—the integral is evaluated in the limit of $\epsilon \to 0$ from the *positive* side.

10 Degenerate Bose Gases

In 1925 the statistical approach proposed for photons by Bose was generalised to massive particles by Einstein. The central result Einstein demonstrated was the existence of a phase transition when the temperature becomes so low that occupation of the system ground state becomes macroscopic.

Despite great efforts in cryogenic helium systems, this state of matter was not achieved until 1995 when a team led by Eric Cornell and Carl Wiemann finally realised a quantum degenerate Bose gas in a magnetic trap, and were able to verify its existence [4]. The discovery, rapidly followed by the first realisation of a quantum-degenerate Fermi gas [5] ushered in a modern era of highly controllable, degenerate, ultra-cold matter-waves.

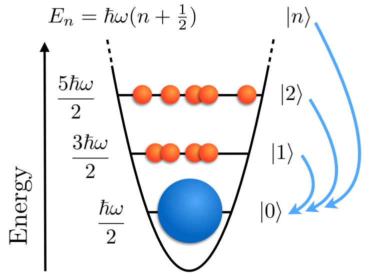

Figure 10.1: In 1925 Einstein predicted that a new phase of quantum degenerate matter would form in a system of Bose particles at low enough temperatures. His argument hinged on the de Broglie wavelength of each boson becoming of order the system size.

10.1 Ideal Gas Phase Transition

A fundamental property of the BEC transition is that is driven by *quantum statistics* and thus does not require an explicit interaction between Bosons to realise it. In practice, interactions provide the thermalisation mechanism required for the system to reach equilibrium, and are hence an essential aspect of any physical realisation.

The phenomenon rests upon a high occupation of a specific quantum state, that, at thermal equilibrium, is necessarily the ground state of the system. We will give an account of the phenomenon applicable to realistic trapped systems created in laboratories such as at Otago.

10.1.1 Grand canonical free energy

In the general, the grand canonical potential for any system can be written as

$$F = -k_B T \ln Z, \tag{10.1}$$

where Z is the grand-canonical partition function. For a system of Bosons distributed over a set of states with energies ϵ_i, this can be written as

$$F = k_B T \sum_i \ln\left(1 - e^{\beta(\mu-\epsilon_i)}\right), \tag{10.2}$$

where $\beta = 1/k_B T$. At sufficiently low temperatures, the chemical potential μ approaches the ground state energy ϵ_0 from below, leading to a macroscopic occupation N_0. Provided the potential confining the atoms is sufficiently smooth, we can use a semi-classical approximation for the excited states, provided we single out the ground state for special treatment — this is necessary if we are to properly account for the situation $N_0 \gg 1$. Using the semiclassical approximation for the excited states, we can make the replacements

$$\sum_i \to \int\int \frac{d^3\mathbf{r}d^3\mathbf{p}}{(2\pi\hbar)^3}, \tag{10.3}$$

$$\epsilon_i \to \epsilon(\mathbf{r},\mathbf{p}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}), \tag{10.4}$$

and integrate over the particle momentum to find

$$\boxed{F = N_0(\epsilon_0 - \mu) - \frac{1}{\beta\lambda_{dB}^3}\sum_{k=1}^{\infty}\frac{e^{k\beta\mu}}{k^{5/2}}G_\beta(k),} \tag{10.5}$$

where

$$G_\beta(k) = \int d^3\mathbf{r}\; e^{-k\beta V(\mathbf{r})}, \tag{10.6}$$

accounts for the trapping geometry, and

$$\lambda_{dB} = \sqrt{\frac{2\pi\hbar^2}{mk_BT}} \tag{10.7}$$

is the thermal de Broglie wavelength. All thermodynamic properties of the trapped system are determined by $G_\beta(k)$ and its derivatives; we can recover the theory of the homogeneous gas by taking $V(\mathbf{r}) \to 0$ and limiting the spatial integration to a finite volume $\mathcal{V}$.

The BEC transition occurs when the chemical potential reaches the ground state energy, and can be written in terms of the thermodynamic relation for the total atom number

$$N = -\frac{\partial F}{\partial \mu}\bigg|_{\mu=\epsilon_0}. \tag{10.8}$$

The next step is a little subtle. We assume that, precisely at the transition point, $N_0 \equiv 0$. This is a paradoxical statement, clarified when we realise that by insisting that the condensate is empty at the transition point, we are really imposing the condition that it is not *macroscopic* when compared with the population of excited states, i.e. $N_0 \ll N_{ex}$. In practice N_0 is necessarily finite, and indeed, larger than the population of any other mode.

At the transition temperature, defined as $T = T_c$, we then have $N \equiv N_{ex}$, often referred to as the *saturation of excited states* precisely because the excited states of the system are unable to hold any more Bosons. At this point

$$N\lambda_{dB}^3 = \sum_{k=1}^{\infty}\frac{1}{k^{3/2}}G_\beta(k), \tag{10.9}$$

where the trap minimum is taken as $\epsilon_0 = V_0 = 0$. For a 3-dimensional harmonic trap

$$V(\mathbf{r}) = \sum_{i=1}^{3}\tfrac{1}{2}m\omega_i^2 x_i^2, \tag{10.10}$$

and we have the simple result

$$G_\beta(k) = \left(\frac{2\pi}{\beta m\bar{\omega}^2 k}\right)^{3/2}, \tag{10.11}$$

where $\bar{\omega}^3 \equiv \omega_x\omega_y\omega_z$ defines the *geometric mean* trapping frequency. Using this result, we arrive at

$$\boxed{k_B T_c = \frac{\hbar\bar{\omega}N^{1/3}}{\zeta(3)^{1/3}}.} \tag{10.12}$$

where

$$\zeta(s) = \sum_{k=1}^{\infty}\frac{1}{k^s} \tag{10.13}$$

is the *Riemann zeta function*, and the numerical factor in (10.12) is close to unity: $\zeta(3)^{-1/3} \simeq 0.94$. Note an interesting feature of (10.12), namely that the thermal de Broglie wavelength does not appear (in contrast to the homogeneous system). Using (10.12) in the total atom number relation (10.8), for $\mu \geq \epsilon_0$, we have the condensate fraction for the trapped ideal gas

$$\boxed{\frac{N_0}{N} = 1 - \left(\frac{T}{T_c}\right)^3.} \tag{10.14}$$

Exercise 10.1: Homogeneous Bose gas

Use (10.9) to find the equivalent of (10.12) and (10.14) for an ideal Bose gas confined to volume $\mathcal{V}$. Express your result in terms of the particle density $n = N/\mathcal{V}$, and λ_{dB}. Comment on the role of confinement.

Exercise 10.2: Trapped gas transition

1. Calculate the ideal gas T_c for $N = 10^6$ atoms of ^{87}Rb held in a harmonic trap with $(\omega_x, \omega_y, \omega_z) = 2\pi(10, 50, 100)\text{s}^{-1}$.
2. Assuming a the same harmonic trap, estimate the number of atoms in the BEC of Figure 10.2.
3. Calculate the condensate fraction at $T = 90$nK.

10.2 Bose-Einstein Condensates in Trapped Alkali Gases

> The mathematics is pretty, but is there any truth to it?
> *Albert Einstein*

The achievement of BEC in a dilute gas of ^{87}Rb in 1995 was an experimental tour-de force. The essential elements required are

1. *Atoms as composite Bosons:* Provided the energies required to probe internal structure are not available, a composite of an even number of Fermions will obey Bose statistics.
2. *Dilute gas:* When cooling a gas, many-body collisions cause droplet formation, and a gas-liquid transition. This must be avoided by keeping the gas extremely dilute.
3. *Optical molasses:* Careful manipulation with off-resonant laser beams generates optical forces that are both *directionally* and *velocity* selective, acting to slow the atoms down in specific directions. The cooling achieved via this process has a limitation due to spontaneous emission, and the laser cooling typically produces $\sim 10^{11}$ atoms at temperatures of order $\sim \mu$K.
4. *Evaporative cooling:* The final phase involves energy-selective removal of atoms, allowing the slower atoms to continuously rethermalize until condensation is achieved at temperatures of order $\sim$ 100nK. Most of the gas is lost during this stage, leaving of order $10^3 - 10^8$ atoms in the dilute gas BEC.

10.2.1 Binary collision Hamiltonian

In the second-quantized theory, a system of identical bosons is described by the field operator, $\hat{\psi}(\mathbf{r})$, that obeys Bose commutation relations

$$[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}'). \tag{10.15}$$

The Hamiltonian can then be written as

$$\boxed{\begin{aligned} H =& H_0 + H_I \\ =& \int d^3\mathbf{r}\ \hat{\psi}^\dagger(\mathbf{r})\left(-\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{r}, t)\right)\hat{\psi}(\mathbf{r}) \\ &+ \frac{1}{2}\int d^3\mathbf{r} \int d^3\mathbf{r}'\ \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')U(\mathbf{r} - \mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r}), \qquad (10.16) \end{aligned}}$$

where $U(\mathbf{r} - \mathbf{r}')$ is the two-body interaction potential, and $V(\mathbf{r}, t)$ describes the external confining potential. In the *cold-collision* regime, the dominant interactions occur pair-wise and for identical Bosons the scattering becomes entirely S-wave. We can thus use the point-like scattering description, and replace the true two-body potential with the effective potential (9.86), making the replacement

$$U(\mathbf{r} - \mathbf{r}') \rightarrow g\delta(\mathbf{r} - \mathbf{r}') \equiv \frac{4\pi\hbar^2 a}{m}\delta(\mathbf{r} - \mathbf{r}'), \tag{10.17}$$

for mass m and s-wave scattering length a, giving

$$H_I = \frac{g}{2}\int d^3\mathbf{r}\ \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}). \tag{10.18}$$

The Heisenberg equation of motion for the field operator is

$$i\hbar\frac{\partial\hat{\psi}(\mathbf{r})}{\partial t} = \left(-\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{r}, t) + g\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\right)\hat{\psi}(\mathbf{r}). \tag{10.19}$$

In general this equation of motion is insoluble, due to the vastness of the Hilbert space it describes.

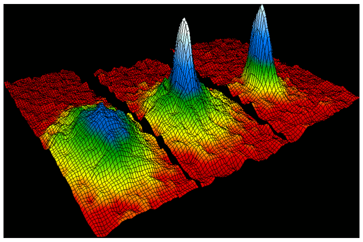

Figure 10.2: Formation of the first Bose-Einstein condensate in a dilute gas of ^{87}Rb atoms, at a transition temperature $T_c \sim$ 200nK. The exotic phase of matter was achieved for the first time in 1995 by the group led by Eric Cornell and Carl Wieman at the Joint Institute for Laboratory Astrophysics (JILA), Boulder, Colorado.

10.2.2 Gross-Pitaevskii equation

It is reasonable to suppose that for a highly occupied Bose field, the field operator may approach a classical state. At temperatures $T \ll T_c$, the atoms condense into a many-body ground state of the interacting system. For a pure BEC with every atom is in the common state, $\phi_0(\mathbf{r}, t)$ the many-body wavefunction factorizes:

$$\phi(\mathbf{r}_1, \ldots, \mathbf{r}_N, t) = \phi_0(\mathbf{r}_1, t) \ldots \phi_0(\mathbf{r}_N, t). \tag{10.20}$$

The total energy of the Hamiltonian (4.7) is then

$$\begin{aligned}\langle\phi|\hat{H}|\phi\rangle = N \int d^3\mathbf{r}\, \phi_0^*(\mathbf{r}) \left[-\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{r})\right] \phi_0(\mathbf{r}) \\ + \frac{N(N-1)}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}'\, U(\mathbf{r}-\mathbf{r}')|\phi_0(\mathbf{r})|^2|\phi_0(\mathbf{r}')|^2.\end{aligned} \tag{10.21}$$

Introducing the form $\phi(\mathbf{r}) = \sqrt{N}\phi_0(\mathbf{r})$, normalised to $N = \int d^3\mathbf{r}\, |\phi(\mathbf{r})|^2$, and using $N \simeq N-1$ for large N, and (10.17), we arrive at the *Gross-Pitaevskii energy* for the condensate wavefunction

$$E(N) = \int d^3\mathbf{r}\, \phi^*(\mathbf{r}) \left[-\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{r})\right] \phi(\mathbf{r}) + \frac{g}{2} \int d^3\mathbf{r}\, |\phi(\mathbf{r})|^4, \tag{10.22}$$

and the equation of motion is, in the Hamiltonian formalism

$$i\hbar \frac{\partial\phi(\mathbf{r}, t)}{\partial t} \equiv \frac{\delta E(N)}{\delta\phi^*(\mathbf{r}, t)}. \tag{10.23}$$

This is the classical Hamiltonian mechanics equivalent of calculating the commutator to derive (10.19) from (10.16).

We thus arrive at the *Gross-Pitaevskii equation* for the condensate wavefunction

$$\boxed{i\hbar \frac{\partial\phi(\mathbf{r}, t)}{\partial t} = \left(-\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{r}, t) + g|\phi(\mathbf{r}, t)|^2\right)\phi(\mathbf{r}, t). \qquad (10.24)}$$

This equation of motion gives a remarkably accurate description of dilute gas BEC's for temperatures $T \ll T_c$. The equation describes a large range of collective phenomena in degenerate Bose gases. Interestingly, this equation would also have been obtained via the heuristic replacement $\hat{\psi} \to \phi$ in the Heisenberg equation of motion (10.19), corresponding to recovering the *classical field* limit of the many body quantum field theory.

10.2.3 Chemical potential

When the system of Bosons is in equilibrium, it has an associated *chemical potential* μ, and the time evolution is a trivial exponential factor

$$\phi(\mathbf{r}, t) \equiv \phi(\mathbf{r})e^{-i\mu t/\hbar}, \tag{10.25}$$

giving the time-independent GPE

$$\mu\phi(\mathbf{r}) = \left(-\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{r}) + g|\phi(\mathbf{r})|^2\right)\phi(\mathbf{r}), \tag{10.26}$$

the solution of which describes the ground state of the system. Suppose now that we have a solution of the stationary GPE, for which we set $N \to N+1$, leading to $\phi \to \phi + \delta\phi$. Then

$$\delta E(N) = \int d^3\mathbf{r}\,\left(\delta\phi^*\left[-\frac{\hbar^2\nabla^2\phi}{2m} + V\phi + g|\phi|^2\phi\right] + \left[-\frac{\hbar^2\nabla^2\phi^*}{2m} + V\phi^* + g|\phi|^2\phi^*\right]\delta\phi\right), \tag{10.27}$$

and since ϕ satisfies (10.26), we find

$$\delta E(N) = \int d^3\mathbf{r}\,(\delta\phi^*\mu\phi + \phi^*\mu\delta\phi) = \mu\delta\int d^3\mathbf{r}\,|\phi(\mathbf{r})|^2 = \mu\delta N. \tag{10.28}$$

Hence μ is the energy associated with adding a particle to the *interacting* system

$$\boxed{\mu(N) = \frac{\partial E(N)}{\partial N}.} \tag{10.29}$$

10.2.4 Thomas-Fermi regime

When the system is well described by (10.26), i.e. near $T = 0$, at any points in space where the interaction and potential terms dominate the energy, it is a very good approximation to neglect the kinetic energy term. In practice this is usually a consistent approximation when $V(\mathbf{r}) \ll \mu$, and in equilibrium this corresponds to avoiding the boundary of the BEC.

Making this *Thomas-Fermi* approximation in (10.26), we have

$$|\phi(\mathbf{r})|^2 = \frac{1}{g}\max\left[\mu - V(\mathbf{r}), 0\right]. \tag{10.30}$$

For a 3D harmonic trap given by (10.10), we can write this as the parabolic density profile

$$|\phi(\mathbf{r})|^2 = \frac{\mu}{g}\max\left[1 - \frac{x_i^2}{R_i^2}, 0\right], \tag{10.31}$$

where $R_i = \sqrt{2\mu/m\omega_i^2}$ are the Thomas-Fermi radii. This approximation breaks down near the BEC edge, where the density is low and the kinetic energy term is required to give a complete description. However, over the bulk of the condensate, the TF-approximation gives quite an accurate description of the interacting BEC. In particular, we may find an explicit form for the chemical potential of N atoms by calculating the norm of the TF-wavefunction:

$$\begin{aligned} N = \int d^3\mathbf{r}\,|\phi_0(\mathbf{r})|^2 &= \frac{\mu}{g}\int_{-R_x}^{R_x} dx \int_{-\sqrt{1-x^2/R_x^2}}^{\sqrt{1-x^2/R_x^2}} dy \\ &\times \int_{-\sqrt{1-x^2/R_x^2-y^2/R_y^2}}^{\sqrt{1-x^2/R_x^2-y^2/R_y^2}} dz\left(1 - \frac{x^2}{R_x^2} - \frac{y^2}{R_y^2} - \frac{z^2}{R_z^2}\right). \end{aligned} \tag{10.32}$$

Changing variables to $(x, y, z) = (uR_x, vR_y, vR_z)$ makes the integral spherically symmetric so that we can write $r^2 = u^2 + v^2 + w^2$, and

$$N = \frac{\mu}{g\bar{\omega}^3}\left(\frac{2\mu}{m}\right)^{3/2} 4\pi \int_0^1 dr\, r^2(1-r^2) = \frac{\mu}{g\bar{\omega}^3}\left(\frac{2\mu}{m}\right)^{3/2} \frac{8\pi}{15}. \tag{10.33}$$

In terms of the geometric mean oscillator length $\bar{a} = \sqrt{\hbar/m\bar{\omega}}$, we find

$$\boxed{\mu(N) = \frac{\hbar\bar{\omega}}{2}\left(\frac{15Na}{\bar{a}}\right)^{2/5}, \tag{10.34}}$$

that, together with (10.31) gives a complete Thomas-Fermi description of the BEC ground state.

Exercise 10.3: Chemical potential

Verify (10.34).

Exercise 10.4: Thomas-Fermi parameters

Calculate the peak density and the Thomas-Fermi radii for a system of $N = 10^5$ atoms of ^{87}Rb in a trap with $(\omega_x, \omega_y, \omega_z) = 2\pi(10, 50, 100)\mathrm{s}^{-1}$. The scattering length of ^{87}Rb may be taken to be $a \simeq 95a_0$, where $a_0 = 5.29 \times 10^{-11}$m is the Bohr radius.

Exercise 10.5: Thomas-Fermi energy

Use (10.29) to show that in the Thomas-Fermi approximation

$$E(N) = \int_0^N \mu(N)dN = \frac{5N\mu(N)}{7} \tag{10.35}$$

10.2.5 Quantum vortices

In 1947 Onsager noticed that if a superfluid (the only such fluid available was Helium at 4K) is described by a common wavefunction, the phase of the wavefunction has profound implications for the kinds of excitations supported by the fluid. The superfluid wavefunction $\phi(\mathbf{r}, t)$ can be decomposed in terms of the density $\rho(\mathbf{r}, t) = |\phi(\mathbf{r}, t)|^2$, and the phase $\Theta(\mathbf{r}, t)$, as

$$\phi(\mathbf{r}, t) = \sqrt{\rho(\mathbf{r}, t)}e^{i\Theta(\mathbf{r},t)}, \tag{10.36}$$

known as the Madelung transformation. For any wavefunction, the phase must be continuous and *single valued* wherever the density is non-zero. Note that, since the interaction term in (10.24) takes the form of a potential, the GPE obeys the same continuity equation as the ordinary Schrödinger equation:

$$\boxed{\frac{\partial\rho(\mathbf{r}, t)}{\partial t} + \nabla \cdot \mathbf{j}(\mathbf{r}, t) = 0, \tag{10.37}}$$

where the current is

$$\mathbf{j}(\mathbf{r},t) = \frac{i\hbar}{2m}\Big([\nabla\phi^*]\phi - \phi^*\nabla\phi\Big) \tag{10.38}$$
$$= \rho(\mathbf{r},t)\mathbf{v}(\mathbf{r},t), \tag{10.39}$$

and in the last line we use the decomposition (10.36), and identify the *superfluid velocity*

$$\boxed{\mathbf{v}(\mathbf{r},t) \equiv \frac{\hbar}{m}\nabla\Theta(\mathbf{r},t).} \tag{10.40}$$

An immediate consequence of this expression is that vorticity must be *quantized*. Let us compute the superfluid circulation around any planar region A of space with boundary ∂A containing a superfluid described by $\phi_0(\mathbf{r},t)$:

$$\Gamma \equiv \oint_{\partial A} \mathbf{v}\cdot \boldsymbol{dl} = \frac{\hbar}{m}\oint_{\partial A} \nabla\Theta(\mathbf{r},t)\cdot \boldsymbol{dl} = n\frac{h}{m}, \tag{10.41}$$

where $n = 0, \pm1, \pm2, \ldots,$ as required by the single-valued phase condition. Note that since (10.40) shows that the velocity is the gradient of a potential, it must also be *curl-free*, $\nabla\times\mathbf{v} \equiv 0$, wherever the phase Θ is well defined. We can use this fact to deduce the form of the *vorticity* defined as

$$\boldsymbol{\omega}(\mathbf{r},t) = \nabla\times\mathbf{v}(\mathbf{r},t). \tag{10.42}$$

From (10.41), (10.40), it is clear that

$$\frac{\hbar}{m}\iint_A (\nabla\times\Theta)\cdot \boldsymbol{dA} = n\frac{h}{m}. \tag{10.43}$$

A particular solution of this equation when the system contains N vortices is

$$\boldsymbol{\omega}(\mathbf{r},t) = \frac{h}{m}\sum_{j=1}^{N}\kappa_j\delta^{(2)}(\mathbf{r}-\mathbf{r}_j), \tag{10.44}$$

where $\kappa_j = \pm1$ gives the sign of the vortex at $\mathbf{r}_j$. The physical requirement that the fluid remain curl free is enforced by the density going to zero at each vortex core. Thus the vorticity is compressed down into a set of infinitesimal points, allowing the superfluid to remain curl free. Notice that in (10.44) we have constrained the vortices to each have a only a single unit of circulation. In principle quantum vortices with any integer circulation are permitted, but in practice vortices with greater than unit charge are highly unstable.

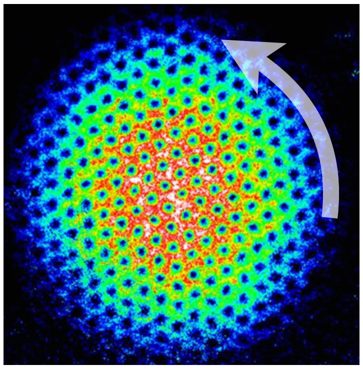

Figure 10.3: False colour map of the particle density of a Bose-Einstein condensate containing a rapidly rotating Abrikosov vortex lattice states created in the Cornell lab at JILA. The system was spun up by evaporatively cooling a rotating thermal gas across the transition temperature, with enhanced evaporation of non-rotating atoms, thus increasing the angular momentum per particle of the remaining atoms. The Abrikosov lattice undergoes uniform rigid body rotation.

Exercise 10.6: Feynman rule for a large vortex lattice

The ground state of the GPE in a rotating frame takes the form of a rigidly rotating hexagonal vortex lattice (Abrikosov lattice, see Figure 10.2.5). In the limit of a large number of vortices such a state acquires a classical *rigid body velocity field*. Assuming a constant area per vortex A/N over the lattice:

1. Carry out the circulation integral (10.41) around a region of radius R containing N quantum vortices with $\kappa_j = 1$.
2. Equate this result to the integral around a classical rigid body rotating with angular frequency Ω. Hence deduce Feynman's rule for the areal density of vortices $n_v = N/A$.

10.2.6 Superfluid hydrodynamics

A fundamental property of superfluids is revealed when we use transformation (10.36) to rewrite the GPE (10.24). For the density we obtain (10.37), and for the superfluid velocity we find

$$\boxed{m\frac{\partial \mathbf{v}(\mathbf{r},t)}{\partial t} = -\nabla V_{\text{eff}}(\mathbf{r},t),} \tag{10.45}$$

where the effective potential is

$$V_{\text{eff}}(\mathbf{r},t) = \tfrac{1}{2}m\mathbf{v}(\mathbf{r},t)^2 + V(\mathbf{r},t) + g\rho(\mathbf{r},t) - \frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho(\mathbf{r},t)}}{\sqrt{\rho(\mathbf{r},t)}}. \tag{10.46}$$

The last term in (10.46) is called the *quantum pressure*, and is significant near abrupt changes in the superfluid density, such as in the vicinity of a vortex core. Away from such structures, the term may be neglected, and the fluid obeys the Euler equation for *inviscid hydrodynamics*.

If we consider small perturbations about a stationary state, we can obtain an equation of motion for long wavelength excitations. Expanding in small fluctuations about the stationary solution of (10.37) and (10.45) around the homogeneous stationary state $\rho(\mathbf{r},t) = n_0 + \delta\rho(\mathbf{r},t)$, and $\mathbf{v}(\mathbf{r},t) = \delta\mathbf{v}(\mathbf{r},t)$, we can show that when the quantum pressure and potential terms in (10.46) are neglected, valid for a homogeneous ground state, the equation of motion for density perturbations is the *wave equation*

$$\boxed{\frac{1}{c^2}\frac{\partial^2\delta\rho}{\partial t^2} = \nabla^2\delta\rho} \tag{10.47}$$

with $c = \sqrt{gn_0/m}$ giving the speed of sound. For trapped systems where the density varies smoothly the sound waves move in a non-uniform density, giving an effective speed of sound that is position dependent.

Exercise 10.7: Deriving the Euler equation

Show that the application of (10.36) to (10.24) yields (10.45).

Exercise 10.8: Wave equation for phonons

Prove that long wavelength density fluctuations obey the wave equation (10.47).

Exercise 10.9: Dark soliton

Solitons are an emergent nonlinear excitation with particle-like properties. In this exercise you will show that the homogeneous 1D GPE

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2\partial_x^2\psi}{2m} + g|\psi|^2\psi, \quad \text{with} \quad g = 4\pi\hbar^2 a/m \tag{10.48}$$

has a dark soliton solution.

1. Rewrite the equation in terms of the rescaled time $\tau = \hbar t/2m$, and $\lambda = 8\pi a$, as

$$i\frac{\partial\psi}{\partial\tau} = -\frac{\partial^2\psi}{\partial x^2} + \lambda|\psi|^2\psi. \tag{10.49}$$

2. Show that for $\lambda > 0$, a particular solution is $\psi(x,\tau) = f(\theta)e^{-i(\sqrt{2}b\theta+4b\tau)}$, with $\theta = x - v\tau$, $b = v^2/8$, and

$$f(\theta) = b\sqrt{2/\lambda}\tanh b\theta. \tag{10.50}$$

   This is the dark soliton solution propagating with velocity v.

10.3 Bogoliubov theory of the weakly interacting Bose gas

The transition to BEC can be understood within an ideal gas treatment of the equilibrium states of a fixed total number of particles N. We have seen that the BEC state can be described by a nonlinear Schrödinger equation. Within such a classical field treatment of the BEC, we find a description of an inviscid superfluid that supports quantum vortices, and acoustic waves.

To gain deeper insight into the role of interactions for the many body *quantum* system, we consider a system of Bosons interacting via s-wave collisions, in a homogeneous geometry with periodic boundary conditions. For a highly occupied BEC subject to weak S-wave interactions, the role of particles outside the condensate can be understood within a perturbative approach and leads to a picture of the emergent effects of quantum mechanics in the bulk system.

10.3.1 Momentum representation

For a system of N identical bosons in a volume V with periodic boundary conditions, recalling (4.66), the Hamiltonian is written in the momentum representation as

$$\boxed{H = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + \sum_{\mathbf{k}_1,\,\mathbf{k}_2,\,\mathbf{q}} U_{\mathbf{q}}\; a^\dagger_{\mathbf{k}_1+\mathbf{q}} a^\dagger_{\mathbf{k}_2-\mathbf{q}} a_{\mathbf{k}_1} a_{\mathbf{k}_2}, \qquad (10.51)}$$

where $[a_{\mathbf{k}}, a^\dagger_{\mathbf{k}'}] = \delta_{\mathbf{k},\mathbf{k}'}$, and

$$U_{\mathbf{q}} = \frac{1}{V}\int d^3\mathbf{r}\; e^{-i\mathbf{q}\cdot\mathbf{r}}\,U(\mathbf{r}), \tag{10.52}$$

for two-body interaction potential $U(\mathbf{r})$.

Figure 10.4: In 1947—1948 **Nikolay Bogoliubov** computed the excitation spectrum for a weakly imperfect Bose gas and used this as a theoretical description for superfluidity of Helium II. Bogoliubov's theory exploits the large occupation of the ground state by linearizing the full field theory around the condensate wavefunction.

10.3.2 Bogoliubov's "Hunting License"

At sufficiently low temperatures a BEC forms, associated with macroscopic occupation N_0 at $\mathbf{k} = 0$,

$$N_0 = \langle a^\dagger_0 a_0 \rangle \lesssim N, \tag{10.53}$$

corresponding to the excited state population

$$N_{ex} = N - N_0 \ll N. \tag{10.54}$$

The dominant interactions are self-interactions between condensate particles, or interactions between condensate and non-condensate particles. Thus we can write the Hamiltonian as

$$\begin{aligned} H = &\sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{U_0}{2} a_0^\dagger a_0^\dagger a_0 a_0 + \sum_{\mathbf{k}\neq 0} (U_0 + U_{\mathbf{k}})\, a_0^\dagger a_0 a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \\ &+ \frac{1}{2} \sum_{\mathbf{k}\neq 0} U_{\mathbf{k}} \left(a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger a_0 a_0 + a_0^\dagger a_0^\dagger a_{\mathbf{k}} a_{-\mathbf{k}} \right) + \mathcal{O}(a_{\mathbf{k}}^3) \end{aligned} \tag{10.55}$$

Terms like $a_0^\dagger a_0^\dagger a_0 a_{\mathbf{k}\neq 0}$ vanish due to momentum conservation. For a highly occupied condensate, we can make the following approximations:

i) The *Bololiubov approximation*, namely, to replace condensate operators with c-numbers

$$a_0 \to \sqrt{N_0}, \qquad a_0^\dagger \to \sqrt{N_0}, \tag{10.56}$$

equivalent to neglecting the commutator $[a_0, a_0^\dagger] = 1$ relative to the eigenvalue $N_0 \gg 1$.

ii) Note that at present the value of N_0 is unknown, and will be determined by the interactions. In the absence of interactions, this occupation approaches $N_0 = N$ at $T = 0$. As we shall see below, interactions introduce *quantum depletion*. However, we can write

$$N = N_0 + \sum_{\mathbf{k}\neq 0} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \tag{10.57}$$

so that, for example

$$\begin{aligned} N_0^2 &= N^2 - 2N \sum_{\mathbf{k}\neq 0} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \sum_{\mathbf{k}\neq 0, \mathbf{q}\neq 0} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} a_{\mathbf{q}}^\dagger a_{\mathbf{q}} \\ &\approx N^2 - 2N \sum_{\mathbf{k}\neq 0} a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \end{aligned} \tag{10.58}$$

where the final expression gives the leading terms in an expansion in powers of N^{-1}.

iii) Initially, we shall approximate the interactions by the simple replacement $U(\mathbf{r}) \to g\delta^{(3)}(\mathbf{r})$, giving $U_{\mathbf{k}} \to g/V$, where $g = 4\pi\hbar^2 a_s/m$. This approximation gives an adequate description of long wavelength excitations, but requires modification for a more complete of ultra-violet behaviour.

Making these replacements, and truncating the summation we arrive at the quadratic Hamiltonian

$$\boxed{H_{\text{Bog}} = \frac{gN^2}{2V} + \sum_{\mathbf{k}\neq 0} \left(\frac{\hbar^2 k^2}{2m} + gn \right) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \frac{gn}{2} \sum_{\mathbf{k}\neq 0} \left(a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + a_{\mathbf{k}} a_{-\mathbf{k}} \right). \qquad (10.59)}$$

This Hamiltonian may be diagonalised via the *Bogoliubov transformation*. Motivated by the coupling between ±**k** in the off-diagonal terms of (10.59), we introduce the ansatz

$$\boxed{\begin{aligned} a_{\mathbf{k}} &= u_{\mathbf{k}}\alpha_{\mathbf{k}} + v^*_{\mathbf{k}}\alpha^\dagger_{-\mathbf{k}}, && (10.60a)\\ a^\dagger_{\mathbf{k}} &= u^*_{\mathbf{k}}\alpha^\dagger_{\mathbf{k}} + v_{\mathbf{k}}\alpha_{-\mathbf{k}}, && (10.60b)\end{aligned}}$$

and impose the condition that the transformation must be *canonical*:

$$[\alpha_{\mathbf{k}}, \alpha^\dagger_{\mathbf{k}'}] = \delta_{\mathbf{k},\mathbf{k}'}, \qquad [\alpha_{\mathbf{k}}, \alpha_{\mathbf{k}'}] = [\alpha^\dagger_{\mathbf{k}}, \alpha^\dagger_{\mathbf{k}'}] = 0. \tag{10.61}$$

This condition ensures that our new operators describe some kind of particle, the precise nature of which is to be determined. The transformation is canonical, provided

$$|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 = 1, \tag{10.62}$$

which resembles the hyperbolic identity. The coefficients can thus be parameterised as $u_{\mathbf{k}} = \cosh(\theta_{\mathbf{k}})$, $v_{\mathbf{k}} = \sinh(\theta_{\mathbf{k}})$, with $\theta_{\mathbf{k}}$ to be determined by the condition that (10.59) is reduced to diagonal form by the new operators, namely

$$gn\left(|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2\right) + \left(\frac{\hbar^2k^2}{2m} + gn\right)2u_{\mathbf{k}}v_{\mathbf{k}} = 0, \tag{10.63}$$

or, using $\cosh(2\theta) = \cosh^2(\theta) + \sinh^2(\theta)$ and $\sinh(2\theta) = 2\cosh(\theta)\sinh(\theta)$,

$$\coth(2\theta_{\mathbf{k}}) = -\frac{\hbar^2k^2/2m + gn}{gn}, \tag{10.64}$$

giving the explicit forms

$$u_{\mathbf{k}} = \left(\frac{\hbar^2k^2/2m + gn}{2\epsilon(k)} + \frac{1}{2}\right)^{1/2}, \qquad v_{\mathbf{k}} = -\left(\frac{\hbar^2k^2/2m + gn}{2\epsilon(k)} - \frac{1}{2}\right)^{1/2}, \tag{10.65}$$

where we have written the coefficients in terms of the *Bogoliubov spectrum*

$$\boxed{\epsilon(k) = \left[\frac{\hbar^2k^2}{2m}\left(\frac{\hbar^2k^2}{2m} + 2gn\right)\right]^{1/2}.} \tag{10.66}$$

After carrying out this diagonalizing transformation, the Hamiltonian reads

$$\boxed{H_{\text{Bog}} = E_0 + \sum_{\mathbf{k}\neq 0}\epsilon(k)\alpha^\dagger_{\mathbf{k}}\alpha_{\mathbf{k}}.} \tag{10.67}$$

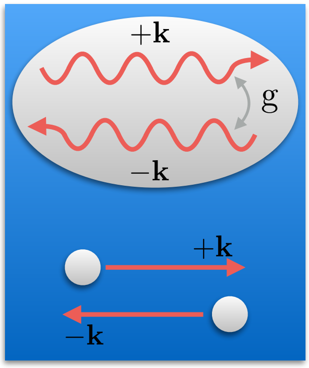

Figure 10.5: Excitations of a weakly interacting Bose gas. For low energy, long wavelength motion, the excitations are *quasiparticles*, a collective phenomena emerging from the interaction of ±**k** plane waves. For high energy, short wavelength excitations, the particles are essentially immune to the interactions, and behave like free particles.

10.3.3 Interpretation of the Bogoliubov Hamiltonian

This result has deep physical implications:

i) *Quasiparticles.*— The spectrum given in (10.66) gives the energy of Bogoliubov *quasiparticles*. At this level of approximation the system of interacting particles is equivalent to a system of *independent* quasiparticles, with energy spectrum modified by the interactions. Quasiparticles are thus an emergent collective phenomena in the many-body system. A more complete treatment of the Hamiltonian necessarily includes interactions between quasiparticles.

ii) *Phonon regime.*— For small momenta we have

$$\epsilon(k) = \hbar k c, \tag{10.68}$$

with the speed of sound given by $c = \sqrt{gn/m}$, as found in (10.47). The Bogoliubov coefficients become

$$|u_{\mathbf{k}}|^2 \to \frac{mc}{2\hbar k}, \quad |v_{\mathbf{k}}|^2 \to \frac{mc}{2\hbar k}, \tag{10.69}$$

describing quasiparticles involving equal mixing between particles with momentum $\pm\mathbf{k}$. Note that what we mean by small k can now be understood as the regime $\hbar^2k^2/2m \ll mc^2$.

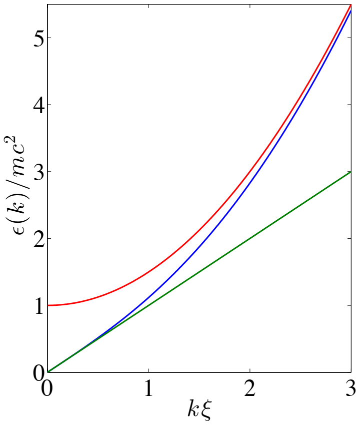

Figure 10.6: Bogoliubov spectrum (blue), with asymptotics for the low (green) and high (red) energy regimes, (10.68) and $\epsilon(k) = \mu + \hbar^2k^2/2m$, respectively. Wavenumbers are shown in units of the healing length $\xi = \hbar/mc$.

iii) *Particle regime.*— For large momenta $\hbar^2k^2/2m \gg mc^2$, we recover particle-like behaviour

$$\epsilon(k) = \frac{\hbar^2k^2}{2m}, \tag{10.70}$$

and now

$$|u_{\mathbf{k}}|^2 \to 1, \quad |v_{\mathbf{k}}|^2 \to 0. \tag{10.71}$$

The quasiparticles behave like non-interacting particles, as should be expected when the particle kinetic energy greatly exceeds the interaction energy. A more careful treatment yields the high energy asymptotic form $\epsilon(k) = \mu + \hbar^2k^2/2m$, as shown in Figure ii.

iv) *Ground state.*— The quasiparticle ground state is given by

$$\alpha_{\mathbf{k}}|\text{vac}\rangle = 0. \tag{10.72}$$

This can be used together with the inverse of the transformation (10.60):

$$\alpha_{\mathbf{k}} = u^*_{\mathbf{k}} a_{\mathbf{k}} - v_{\mathbf{k}} a^\dagger_{-\mathbf{k}}, \tag{10.73a}$$

$$\alpha^\dagger_{\mathbf{k}} = u_{\mathbf{k}} a^\dagger_{\mathbf{k}} - v^*_{\mathbf{k}} a_{-\mathbf{k}}, \tag{10.73b}$$

to find the Bogoliubov ground state.

Exercise 10.10: Bogoliubov vacuum

The ground state has a close formal correspondence to the two-mode squeezing Hamiltonian considered in Section 6.3.

1. Verify that (10.73) is the inverse Bogoliubov transformation.
2. Find a recursion relation for the Bogoliubov ground state in the number state basis for *particles*, $|n_{\mathbf{k}}, n_{-\mathbf{k}}\rangle$, and use it to obtain an explicit form for $|\text{vac}\rangle$. Comment on the role of interactions.

v) *Quantum depletion.*— In general the role of interactions is to deplete the condensate. In thermal equilibrium we can write the population of quasiparticles as

$$N_Q = \sum_{\mathbf{k}\neq 0} \langle \alpha^\dagger_{\mathbf{k}} \alpha_{\mathbf{k}} \rangle = \sum_{\mathbf{k}\neq 0} \frac{1}{e^{\beta\epsilon(\mathbf{k})} - 1}, \tag{10.74}$$

since these excitations are independent, noninteracting, and massless. This population should not be confused with the population of real particles in excited states:

$$N_{ex} = \sum_{\mathbf{k}\neq 0} \langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \rangle = \sum_{\mathbf{k}\neq 0} \langle \alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} \rangle |u_{\mathbf{k}}|^2 + \langle \alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} \rangle |v_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2, \tag{10.75}$$

from which we can pass to the continuum limit in volume V, the write the depletion of the condensate as

$$\boxed{N_0 = N - N_{ex} = N - \frac{V}{(2\pi\hbar)^3} \int d^3\mathbf{k} \left[|v_{\mathbf{k}}|^2 + \frac{|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2}{e^{\beta\epsilon(\mathbf{k})} - 1} \right]} \tag{10.76}$$

from which we see that even at $T = 0$ there is a finite quantum depletion of the condensate.

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Figure 10.7: The phonon regime associated with the linear spectrum (10.68) is the origin of *superfluidity*, a phenomenon first explained by Lev Landau in 1941. Landau managed to get released from his incarceration by the Soviet Secret Service by developing his theory, making good on a promise made to his jailers by Pyotr Kapitsa.

10.4 Degenerate Fermi Gases

At sufficiently low temperatures, the population of a Fermi system will fill up the all of the states to the Fermi energy. Soon after the realisation of BEC, degenerate Fermi gases were achieved [5]. The cooling process is further complicated by the inhibition of S-wave scattering (Pauli-blocking), necessitating the use of *buffer gas cooling* to reach degeneracy.

As shown in Figure 10.8 the quantum degeneracy stops the Fermi gas from shrinking below a minimum size determined by the Pauli exclusion principle. This Fermi pressure is the same force that prevents white dwarf and neutron stars from collapsing to densities sufficient to form black holes [6].

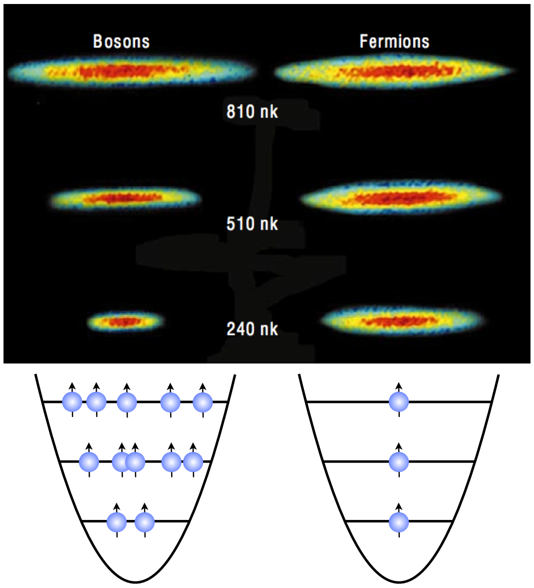

Figure 10.8: Demonstration of Fermi pressure for degenerate quantum gases. Comparison between Bosonic ^{6}Li and Fermionic ^{7}Li, shows the distinctive nature of quantum statistics. The size of the Bose gas shrinks as the temperature is reduced by evaporative cooling. The Fermionic cloud cannot shrink below a certain size determined by the Pauli exclusion principle. Figure adapted from [6]. The schematic bottom left shows the counting statistics of spin-1/2 Fermions. In the Fermionic cloud shown on the right the spin-polarization of Fermions limits the populations to one particle per energy eigenstate of the trap.

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