PHYS571: Lecture Notes
Modern Atomic Physics

by

Han Pu

Department of Physics and Astronomy

Rice University

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Contents

Chapter 1

Two-Level-Atom and Semiclassical Theory

In quantum optics, we are often interested in the dynamics of atoms coupled to an electromagnetic field (laser). Simple models are required to describe many of the most important features of this dynamics. In these models, the field may be described either classically or fully quantum mechanically, while the atomic system is adequately described by a small number of essential states (together with a free-electron continuum in problems involving ionization). This simplest atomic model is of course the two-level-atom.

1.1 Two-Level-Atom

The level structures of a real atom look anything but two-level. So how can a two-level-atom (TLA) be a good approximation? The reason lies in two factors: 1) Resonance excitation and 2) Selection rules.

The absorption cross section of an atom absorbing an off-resonant photon is generally of the order of $1\mathring{A}^2$. But when the frequency of the photon matches with the transition frequency from the initial state to some final state, the cross section can be enhanced by many orders of magnitude. This is why the intensities of the lasers used in labs are much less than that required to produce an electric field with one atomic unit ($8.3 \times 10^{16}\mathrm{W/cm^2}$).

Under the resonance condition, many levels lying far away from the resonance can be simply ignored. In addition, the dipole section rules dictates only certain magnetic sublevels are excited. In most cases, the field therefore only causes transitions between a small number of discrete states, in the simplest of which only two states are involved.

1.2 Semiclassical Theory

In the semiclassical theory of atom-photon interaction, the atom is quantized (it has quantized level structures), while the light field is treated classically. The classical treatment of field is valid when the field contains many photons, hence the quantum mechanical commutation relations are no longer important.

Of course, certain aspects of atom-photon interaction cannot be studied with the semiclassical theory, e.g., the spontaneous emission of an atom.

By treating the field classically, we neglect the quantum correlations of the atomic operators and the field.

Chapter 2

Optical Bloch Equations

2.1 operator physics for a two-level atom

The states for a two-level atom: $|g\rangle$ and $|e\rangle$. They are assumed to have opposite parity (hence dipole transition is allowed) and orthogonal to each other. From these one can construct four independent operators:

$$|g\rangle\langle g|, \;\; |g\rangle\langle e|, \;\; |e\rangle\langle g|, \;\; |e\rangle\langle e|,$$

which form a complete basis. Any arbitrary operator, $\hat{O}$, can then be expanded onto this basis as

$$\hat{O} = O_{gg}\hat{\sigma}_{gg} + O_{ge}\hat{\sigma}_{ge} + O_{eg}\hat{\sigma}_{eg} + O_{ee}\hat{\sigma}_{ee}$$

where $\hat{\sigma}_{ij} = |i\rangle\langle j|$, and $O_{ij} = \langle i|\hat{O}|j\rangle$. In particular, the dipole operator $\hat{\mathbf{d}} = e\hat{\mathbf{r}}$ can be expressed as

$$\hat{\mathbf{d}} = \mathbf{d}_{ge}\hat{\sigma}_{ge} + \mathbf{d}_{eg}\hat{\sigma}_{eg}$$

where we have used the property that states $|g\rangle$ and $|e\rangle$ have opposite parity such that $\langle g|\hat{\mathbf{r}}|g\rangle = \langle e|\hat{\mathbf{r}}|e\rangle = 0$.

2.2 Feynman-Bloch Equations

Assume $\mathbf{d}_{eg} = \mathbf{d}_{ge} = \mathbf{d}$, the total Hamiltonian under the dipole approximation is:

$$H = \hbar\omega_0\hat{\sigma}_{ee} - \hat{\mathbf{d}}\cdot\mathbf{E} = \hbar\omega_0\hat{\sigma}_{ee} - \mathbf{d}\cdot\mathbf{E}(\hat{\sigma}_{ge} + \hat{\sigma}_{eg})$$

Using

$$i\hbar\dot{\hat{O}} = [\hat{O}, H],$$

the equations of motion in Heisenberg picture for $\sigma_{ij} = \langle\hat{\sigma}_{ij}\rangle$ are (note that the equations of motion for operators $\hat{\sigma}_{ij}$ are linear, their respective expectation values σ_{ij} obey exactly the same equations.)

$$\begin{aligned}
i\hbar\dot{\sigma}_{gg} &= -\mathbf{d}\cdot\mathbf{E}(\sigma_{ge} - \sigma_{eg}) && (2.1)\\
i\hbar\dot{\sigma}_{ee} &= \mathbf{d}\cdot\mathbf{E}(\sigma_{ge} - \sigma_{eg}) && (2.2)\\
i\hbar\dot{\sigma}_{eg} &= -\hbar\omega_0\sigma_{eg} - \mathbf{d}\cdot\mathbf{E}(\sigma_{ee} - \sigma_{gg}) && (2.3)\\
i\hbar\dot{\sigma}_{ge} &= \hbar\omega_0\sigma_{ge} + \mathbf{d}\cdot\mathbf{E}(\sigma_{ee} - \sigma_{gg}) && (2.4)
\end{aligned}$$

From these 4 quantities, we can difine

$$\begin{aligned} S_0 &= \sigma_{gg}+\sigma_{ee}, \quad \text{probability} && (2.5)\\ S_1 &= \sigma_{ge}+\sigma_{eg}, \quad \text{dipole moment} && (2.6)\\ S_2 &= i(\sigma_{ge}-\sigma_{eg}), \quad \text{dipole current} && (2.7)\\ S_3 &= \sigma_{ee}-\sigma_{gg}, \quad \text{population inversion} && (2.8)\end{aligned}$$

The equations of motion are

$$\begin{aligned} \dot{S}_0 &= 0 && (2.9)\\ \dot{S}_1 &= -\omega_0 S_2 && (2.10)\\ \dot{S}_2 &= \omega_0 S_1+\frac{2\mathbf{d}\cdot\mathbf{E}}{\hbar}S_3 && (2.11)\\ \dot{S}_3 &= -\frac{2\mathbf{d}\cdot\mathbf{E}}{\hbar}S_2 && (2.12)\end{aligned}$$

Define the Feynman-Bloch vector

$$\mathbf{S}=[S_1,\, S_2,\, S_3]$$

the last three equations of motion can be combined to give

$$\dot{\mathbf{S}}=\mathbf{\Omega}_{\text{opt}}\times\mathbf{S} \tag{2.13}$$

where the vector

$$\mathbf{\Omega}_{\text{opt}}=[-\frac{2\mathbf{d}\cdot\mathbf{E}}{\hbar},\, 0,\, \omega_0]$$

For typical parameters, $\omega_0 \gg |2\mathbf{d}\cdot\mathbf{E}/\hbar|$, so $\mathbf{\Omega}_{\text{opt}}\approx\omega_0\hat{3}$ (designate by $\hat{1}$, $\hat{2}$ and $\hat{3}$ the fixed unit vectors of the three-dimensional coordinate system). Hence, from Eq. (2.13), the "main motion" of $\mathbf{S}$ is then simply constant precession about axis-$\hat{3}$.

Now, for a monochromatic light field,

$$\mathbf{E}(\mathbf{r},t)=\mathbf{E}_0\left(e^{-i\omega t}+c.c.\right)=\mathbf{E}_0\cos\omega t$$

we can decompose $\mathbf{\Omega}_{\text{opt}}$ as

$$\mathbf{\Omega}_{\text{opt}}=\mathbf{\Omega}^{(3)}+\mathbf{\Omega}^{(+)}+\mathbf{\Omega}^{(-)}$$

where

$$\begin{aligned} \mathbf{\Omega}^{(3)} &= \omega_0\,\hat{3} && (2.14)\\ \mathbf{\Omega}^{(\pm)} &= -R\,(\cos\omega t\,\hat{1}\pm\sin\omega t\,\hat{2}) && (2.15)\end{aligned}$$

where $R=2\mathbf{d}\cdot\mathbf{E}_0/\hbar$ is the so-called Rabi frequency.

We can see that $\mathbf{\Omega}^{(\pm)}$ rotate in the $\hat{1}$-$\hat{2}$ plane in opposite directions. $\mathbf{\Omega}^{(+)}$ rotates in phase (co-rotating) with the main motion of $\mathbf{S}$, while $\mathbf{\Omega}^{(-)}$ (counter-rotating) rotates in the opposite direction from the main motion. We expect $\mathbf{S}$ to see a very rapidly alternating effect from $\mathbf{\Omega}^{(-)}$ and a persistent effect from $\mathbf{\Omega}^{(+)}$.

2.3 rotating wave approximation and RWA equations

Taking the hint from the discussion above, let us define a rotating coordinate with rotating axis $\hat{3}$:

$$\begin{aligned} \mathbf{e}_1(t) &= \cos\omega t\,\hat{1} + \sin\omega t\,\hat{2} && (2.16)\\ \mathbf{e}_2(t) &= -\sin\omega t\,\hat{1} + \cos\omega t\,\hat{2} && (2.17)\\ \mathbf{e}_3 &= \hat{3} && (2.18) \end{aligned}$$

Key advantage of rotating frame: automatically separates time scales, allowing more detailed examination of slow but significant changes.

Now we want to derive the new equation of motion, i.e., the counterpart of Eq. (2.13) in the rotating frame. First, we decompose $\mathbf{S}$ in the new frame as

$$\mathbf{S} = u\,\mathbf{e}_1(t) + v\,\mathbf{e}_2(t) + w\mathbf{e}_3$$

where

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} \cos\omega t & \sin\omega t & 0 \\ -\sin\omega t & \cos\omega t & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} S_1 \\ S_2 \\ S_3 \end{pmatrix}$$

Second, we want to decompose $\boldsymbol{\Omega}_{\text{opt}}$. Using

$$\begin{aligned} \boldsymbol{\Omega}^{(3)} &= \omega_0\,\mathbf{e}_3 && (2.19)\\ \boldsymbol{\Omega}^{(+)} &= -R\mathbf{e}_1 && (2.20)\\ \boldsymbol{\Omega}^{(-)} &= -R\left(\cos 2\omega t\,\mathbf{e}_1 - \sin 2\omega t\,\mathbf{e}_2\right) && (2.21) \end{aligned}$$

As one can see, $\boldsymbol{\Omega}^{(-)}$ represents terms rotating at frequency 2ω. These fast rotating terms average quickly to zero. This is the reason that we can neglect these double-frequency terms. This is called the Rotating Wave Approximation (RWA).

Now we seem to be ready to convert Eq. (2.13) into the rotating frame. But before doing so, we should remind ourselves about the Coriolis effect from classical mechanics: the rate of change of a vector $\mathbf{V}$ in a rotating frame is the rate of change of $\mathbf{V}$ in the original fixed frame minus a Coriolis term, which is given by $\omega\hat{a} \times \mathbf{V}$, where $\hat{a}$ is the unit vector in the direction of the axis of rotation and ω is the rate of rotation. Therefore,

$$\left(\dot{\mathbf{S}}\right)_{\text{rot}} = \left(\dot{\mathbf{S}}\right)_{\text{fixed}} - \omega\hat{3} \times \mathbf{S} = \boldsymbol{\Omega}^{\text{RWA}} \times \mathbf{S} \qquad (2.22)$$

where

$$\boldsymbol{\Omega}^{\text{RWA}} = -R\,\mathbf{e}_1 - \Delta\,\mathbf{e}_3$$

with $\Delta = \omega - \omega_0$ being the laser detuning from atomic transition frequency.

The equations for the components of $\mathbf{S}$ in the rotating frame under RWA can be easily extracted:

$$\frac{d}{dt}\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} 0 & \Delta & 0 \\ -\Delta & 0 & R \\ 0 & -R & 0 \end{pmatrix} \begin{pmatrix} u \\ v \\ w \end{pmatrix} \qquad (2.23)$$

It is also instructive to note that the expectation value of the dipole operator

$$\langle \hat{\mathbf{d}} \rangle = \mathbf{d}_{ge}\sigma_{ge} + c.c. = \frac{1}{2}\mathbf{d}_{ge}(S_1 - iS_2) + c.c. = \frac{1}{2}\mathbf{d}_{ge}(u - iv)e^{-i\omega t} + c.c.$$

Hence $(u - iv)$ can be interpreted as the dimensionless part of the dipole moment in the rotating frame. Furthermore,

$$u^2 + v^2 + w^2 = 1$$

2.4 RWA: an alternative formulation

Consider a two-level atom interacting with a classical laser light whose electric field is written as

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0(\mathbf{r}) \left(e^{-i[\omega t + \phi(\mathbf{r})]} + c.c. \right) \tag{2.24}$$

The Hamiltonian that describes the interaction reads

$$H = H_A + H_{AF}$$

where the atomic bare Hamiltonian

$$H_A = \hbar\omega_0\hat{\sigma}_{ee}$$

and the atom-field interaction Hamiltonian

$$H_{AF} = -\hat{\mathbf{d}} \cdot \mathbf{E} = \frac{\hbar}{2}\Omega(\mathbf{r})e^{-i\omega t}\left(\hat{\sigma}_{eg} + \hat{\sigma}_{ge}\right) + \frac{\hbar}{2}\Omega^*(\mathbf{r})e^{i\omega t}\left(\hat{\sigma}_{ge} + \hat{\sigma}_{eg}\right)$$

where $\Omega(\mathbf{r}) = -2\mathbf{d} \cdot \mathbf{E}_0(\mathbf{r})e^{-i\phi(\mathbf{r})}/\hbar$ is the Rabi frequency.

Using

$$i\hbar\dot{\hat{O}} = [\hat{O}, H],$$

the equations of motion in Heisenberg picture for $\sigma_{eg} = (\sigma_{ge})^*$ and $\sigma_{ee} = 1 - \sigma_{gg}$ $(\sigma_{ij} = \langle\hat{\sigma}_{ij}\rangle)$ are

$$i\dot{\sigma}_{eg} = -\omega_0\sigma_{eg} + \frac{\Omega^*(\mathbf{r})}{2}e^{i\omega t}(\sigma_{ee} - \sigma_{gg}) + \frac{\Omega(\mathbf{r})}{2}e^{-i\omega t}(\sigma_{ee} - \sigma_{gg}) \tag{2.25}$$

$$i\dot{\sigma}_{ee} = \frac{\Omega(\mathbf{r})}{2}e^{-i\omega t}(\sigma_{eg} - \sigma_{ge}) + \frac{\Omega^*(\mathbf{r})}{2}e^{i\omega t}(\sigma_{eg} - \sigma_{ge}) \tag{2.26}$$

Define the slowly varying variables (equivalent to changing into a rotating frame)

$$\tilde{\sigma}_{eg} = (\tilde{\sigma}_{ge})^\dagger = e^{-i\omega t}\sigma_{eg}, \;\; \tilde{\sigma}_{ee} = \sigma_{ee}, \;\; \tilde{\sigma}_{gg} = \sigma_{gg}$$

The OBEs become

$$i\dot{\tilde{\sigma}}_{eg} = \Delta\tilde{\sigma}_{eg} + \frac{\Omega^*(\mathbf{r})}{2}(\sigma_{ee} - \sigma_{gg}) + \frac{\Omega(\mathbf{r})}{2}e^{-i2\omega t}(\sigma_{ee} - \sigma_{gg}) \tag{2.27}$$

$$i\dot{\sigma}_{ee} = \frac{\Omega(\mathbf{r})}{2}\left(\tilde{\sigma}_{eg} - e^{-i2\omega t}\tilde{\sigma}_{ge}\right) + \frac{\Omega^*(\mathbf{r})}{2}\left(e^{i2\omega t}\tilde{\sigma}_{eg} - \tilde{\sigma}_{ge}\right) \tag{2.28}$$

Now under RWA, we drop those double-frequency terms and obtain

$$i\dot{\tilde{\sigma}}_{eg} = \Delta\tilde{\sigma}_{eg} + \frac{\Omega^*(\mathbf{r})}{2}(\sigma_{ee} - \sigma_{gg}) \tag{2.29}$$

$$i\dot{\sigma}_{ee} = \frac{\Omega(\mathbf{r})}{2}\tilde{\sigma}_{eg} - \frac{\Omega^*(\mathbf{r})}{2}\tilde{\sigma}_{ge} \tag{2.30}$$

Equivalently, we can start from the RWA interaction Hamiltonian

$$H_{AF}^{\mathrm{RWA}} = -\hat{\mathbf{d}} \cdot \mathbf{E} = \frac{\hbar}{2}\Omega(\mathbf{r})e^{-i\omega t}\hat{\sigma}_{eg} + \frac{\hbar}{2}\Omega^*(\mathbf{r})e^{i\omega t}\hat{\sigma}_{ge}$$

Instead of σ_{ee} and σ_{gg}, it is sometimes convenient to use the *population inversion* defined as

$$w = \sigma_{ee} - \sigma_{gg}$$

and it satisfies

$$\dot{w} = 2\dot{\sigma}_{ee} = \Omega(\mathbf{r})\tilde{\sigma}_{eg} - \Omega^*(\mathbf{r})\tilde{\sigma}_{ge}$$

The OBE's can be solved analytically if $\Omega(\mathbf{r}) = \Omega$ is a constant. But the general solution is quite complicated. For the special initial condition that all the populations are in the ground state, i.e., $w(0) = -1$ and $\tilde{\sigma}_{eg}(0) = \tilde{\sigma}_{ge}(0) = 0$, the solution for the population inversion is

$$w(t) = -\frac{\Delta^2 + |\Omega|^2 \cos \tilde{\Omega} t}{\tilde{\Omega}^2}$$

where $\tilde{\Omega} = \sqrt{\Delta^2 + |\Omega|^2}$ is the generalized Rabi frequency. The oscillation amplitude is given by $2|\Omega|^2/\tilde{\Omega}^2$. The effect of increasing $|\Delta|$ is to increase the oscillation frequency, and to decrease the oscillation amplitude.

2.5 relaxation

Relaxation arises from the collection of weak and effectively random perturbations that practically every atomic oscillator is subject to. These perturbations are conventionally attributed to interaction with the "environment" or "reservoir", which means any very large physical system coupled to a single atom in a weak way over a very wide frequency band. The effect of the atom on each reservoir mode is infinitesimal, insignificant for the reservoir, but with cumulative phase memory over the modes and in this way the atom produces a finite back reaction on itself that has a damping effect on its diagonal (population) and off-diagonal (coherence) atomic dynamics. For example, spontaneous emission of an excited atom arises from the interaction between the atom with the vacuum EM modes. I think a full account of relaxation is out of scope for this course. So let us just take it phenomenologically: adding by hand the decay rates of the excited state population σ_{ee} and coherence σ_{eg}, σ_{ge} as:

$$i\dot{\tilde{\sigma}}_{eg} = -i\frac{\Gamma}{2}\tilde{\sigma}_{eg} + \Delta\tilde{\sigma}_{eg} + \frac{\Omega^*(\mathbf{r})}{2}(\sigma_{ee} - \sigma_{gg}) \tag{2.31}$$

$$i\dot{\sigma}_{ee} = -i\Gamma\sigma_{ee} + \frac{\Omega(\mathbf{r})}{2}\tilde{\sigma}_{eg} - \frac{\Omega^*(\mathbf{r})}{2}\tilde{\sigma}_{ge} \tag{2.32}$$

I take here the decay rate of coherence half that of population. This is the lower limit for the former.

With the addition of relaxation, the above equations allow steady state solutions. In the steady state, we have

$$\tilde{\sigma}_{eg,st} = \frac{\Omega^*(\mathbf{r})}{2\Delta - i\Gamma}\frac{1}{1+s} \tag{2.33}$$

$$\sigma_{ee,st} = \frac{1}{2}\frac{s}{1+s} \tag{2.34}$$

where

$$s = \frac{2|\Omega(\mathbf{r})|^2}{4\Delta^2 + \Gamma^2}$$

is the saturation parameter.

Finally, with relaxation, the equation of motion for Feynman-Bloch vector in the rotating frame becomes:

$$\begin{aligned} \dot{u} &= \Delta v - u/T_2 &(2.35)\\ \dot{v} &= -\Delta u + Rw - v/T_2 &(2.36)\\ \dot{w} &= -Rv - (1+w)/T_1 &(2.37) \end{aligned}$$

with $1/T_2 = \Gamma/2$ and $1/T_1 = \Gamma$. Without the light field (i.e., $R = 0$), we have

$$\begin{aligned} (1+w)_t &= (1+w)_0\, e^{-t/T_1} &(2.38)\\ (u - iv)_t &= (u - iv)_0\, e^{i\Delta t - t/T_2} &(2.39) \end{aligned}$$

With relaxation, the length of the vector $u^2 + v^2 + w^2$ is no longer a constant. Without the light field, it eventually decreases to zero.

Chapter 3

Light Pressure Force and Doppler cooling on two-level atom

3.1 Expressions for the force for a two-level atom at rest

Consider a two-level atom interacting with a classical laser light whose electric field is written as

$$\mathbf{E}(\mathbf{r},t) = \mathbf{E}_0(\mathbf{r})\left(e^{-i[\omega t+\phi(\mathbf{r})]} + c.c.\right) \tag{3.1}$$

The Hamiltonian that describes the interaction reads

$$H = H_A + H_{AL}$$

where the atomic bare Hamiltonian

$$H_A = \frac{\hat{\mathbf{p}}^2}{2m} + \hbar\omega_0|e\rangle\langle e|$$

and the atom-field interaction Hamiltonian under the rotating wave approximation

$$H_{AF} = -\hat{\mathbf{d}}\cdot\mathbf{E} = \frac{\hbar}{2}\Omega(\mathbf{r})e^{-i\omega t}|e\rangle\langle g| + \frac{\hbar}{2}\Omega^*(\mathbf{r})e^{i\omega t}|g\rangle\langle e|$$

where $\Omega(\mathbf{r}) = -2\mathbf{d}\cdot\mathbf{E}_0(\mathbf{r})e^{-i\phi(\mathbf{r})}/\hbar = \tilde{\Omega}(\mathbf{r})e^{-i\phi(\mathbf{r})}$ ($\tilde{\Omega} = -2\mathbf{d}\cdot\mathbf{E}_0/\hbar$ is real) is the Rabi frequency.

The force acting on the atomic center of mass is

$$F(\mathbf{r}) = \left\langle \frac{d\hat{\mathbf{p}}}{dt} \right\rangle = -\frac{\hbar}{2}\left\langle |e\rangle\langle g|e^{-i\omega t}\right\rangle \nabla\left[\Omega(\mathbf{r})\right] + c.c.$$

where we have used

$$\frac{d\hat{\mathbf{p}}}{dt} = \frac{i}{\hbar}[H,\hat{\mathbf{p}}]$$

and

$$[f(\mathbf{r}),\hat{\mathbf{p}}] = i\hbar\nabla f(\mathbf{r})$$

Now $\left\langle |e\rangle\langle g|e^{-i\omega t}\right\rangle = \langle\tilde{\sigma}_{eg}\rangle$. Generally, the characteristic time scale for the atomic internal dynamics is of the order of Γ^{-1}, which is much faster than the corresponding time scale for the center-of-mass dynamics.

If this is the case, the internal state of the atoms can be assumed to be in a quasi-steady state relative to that of the center of mass. So we can replace $\langle\tilde{\sigma}_{eg}\rangle$ by its steady state value

$$\tilde{\sigma}_{eg,st} = \frac{\Omega^*(\mathbf{r})}{2\Delta - i\Gamma}\frac{1}{1+s}$$

So the force acting on the atom becomes

$$\mathbf{F}(\mathbf{r}) = -\frac{\hbar}{2}\tilde{\sigma}_{eg,st}\nabla\Omega(\mathbf{r}) + c.c.$$

Using

$$\nabla\Omega(\mathbf{r}) = \nabla\left(\tilde{\Omega}(\mathbf{r})e^{-i\phi(\mathbf{r})}\right) = \Omega(\mathbf{r})\left(\frac{\nabla\tilde{\Omega}}{\tilde{\Omega}} - i\nabla\phi\right)$$

we have

$$\begin{aligned}
\mathbf{F}(\mathbf{r}) &= \mathbf{F}_{\text{dissipative}}(\mathbf{r}) + \mathbf{F}_{\text{reactive}}(\mathbf{r}) && (3.2)\\
\mathbf{F}_{\text{dissipative}}(\mathbf{r}) &= -\frac{\hbar\Gamma}{2}\frac{s}{1+s}\nabla\phi(\mathbf{r}) && (3.3)\\
\mathbf{F}_{\text{reactive}}(\mathbf{r}) &= -\frac{\hbar\Delta}{\tilde{\Omega}(\mathbf{r})}\frac{s}{1+s}\nabla\tilde{\Omega}(\mathbf{r}) && (3.4)
\end{aligned}$$

where $s(\mathbf{r}) = 2\tilde{\Omega}^2(\mathbf{r})/(4\Delta^2 + \Gamma^2)$.

Example 1: travelling wave with wave vector $\mathbf{k} = k\hat{k}$

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0\left(e^{-i\omega t + i\mathbf{k}\cdot\mathbf{r}} + c.c.\right)$$

therefore,

$$\tilde{\Omega}(\mathbf{r}) = \text{const}, \quad \phi(\mathbf{r}) = -\mathbf{k}\cdot\mathbf{r}$$

Using Eqs. (5.11) and (5.12), we have,

$$\mathbf{F}_{\text{dissipative}}(\mathbf{r}) = \frac{\hbar k\Gamma}{2}\frac{s}{1+s}\hat{k}, \quad \mathbf{F}_{\text{reactive}}(\mathbf{r}) = 0$$

Example 2: standing wave

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}_0\cos(\mathbf{k}\cdot\mathbf{r})\left(e^{-i\omega t} + c.c.\right)$$

therefore,

$$\tilde{\Omega}(\mathbf{r}) = -(2\mathbf{d}\cdot\mathbf{E}_0/\hbar)\cos(\mathbf{k}\cdot\mathbf{r}), \quad \phi(\mathbf{r}) = 0$$

Using Eqs. (5.11) and (5.12), we have,

$$\mathbf{F}_{\text{dissipative}}(\mathbf{r}) = 0, \quad \mathbf{F}_{\text{reactive}}(\mathbf{r}) = \frac{\hbar k\Delta}{1+s(\mathbf{r})}\frac{\sin(2\mathbf{k}\cdot\mathbf{r})}{4\Delta^2+\Gamma^2}\hat{k}$$

3.2 Nature of the force

In general, an arbitrary light field consists of a multiple of plane wave components.

Dissipative force, $\mathbf{F}_{\text{dissipative}}$ is also called *radiation pressure force* or *spontaneous force.* It arises from the momentum kick received from the photon absorbed out of one plane wave component interacting with the *dissipative* component of the dipole moment induced by the light. Its direction is determined by the phase gradient of the light, and the strength increases with light intensity but will saturate. For a travelling wave, as the intensity tends to infinity, $F_{\text{dissipative}}$ reaches its maximum value $\hbar k\Gamma/2$.

Reactive force, $\mathbf{F}_{\text{reactive}}$ is also called the *dipole force* or *stimulated force.* It arises from the momentum kick received from the photon absorbed out of one plane wave component interacting with the *reactive* component of the dipole moment induced by the light. Reactive interaction is a stimulated effect, involving absorbing one photon from one plane wave component then stimulated emission into another component. Obviously, reactive effects requires more than one plane wave components. From Eq. (5.12), one can see that $\mathbf{F}_{\text{reactive}}$ can be written as the gradient of a "optical dipole potential"

$$U_{\text{opt}} = \frac{\hbar\Delta}{2}\ln(1+s) = \frac{\hbar\Delta}{2}\ln\left(1+\frac{2\tilde{\Omega}^2(\mathbf{r})}{4\Delta^2+\Gamma^2}\right)$$

and $\mathbf{F}_{\text{reactive}} = -\nabla U_{\text{opt}}$. U_{opt} can therefore regarded as the interaction potential between the light and the induce atomic dipole moment. Note that $\mathbf{F}_{\text{reactive}}$ is sensitive to the sign of Δ. For red detuning ($\Delta < 0$), the induced dipole moment and the light field are in-phase, and the minima of U_{opt} coincide with the maxima of light intensity, the atom is thus "strong field seeking"; for blue detuning ($\Delta > 0$), the atom is "weak field seeking".

For far off resonance light, $|\Delta| \gg \Gamma, \tilde{\Omega}$,

$$U_{\text{opt}} \approx \frac{\hbar\tilde{\Omega}^2(\mathbf{r})}{4\Delta}$$

The spontaneous emission rate, given by $\sigma_{ee,st}\Gamma \approx s\Gamma/2$, in the mean time, is proportional to $\tilde{\Omega}^2/\Delta^2$. So it is always possible to increase both the laser intensity and detuning such that the spontaneous emission is minimized while the dipole potential depth is kept fixed.

3.3 Doppler Cooling

For simplicity, we confine our discussion in 1D.

Consider two counter-propagating travelling light fields with wave vector $\pm k$ and Rabi frequency $\tilde{\Omega}$. Neglect the interference between them (e.g., they have orthogonal polarizations). We will also assume low intensity, i.e., $\tilde{\Omega} \ll \Delta, \Gamma$. An two-level atom at rest will feel no force since the radiation pressure force from the two beams cancel each other. Now consider the atom has a small velocity, v. What will happen then?

We can calculate the forces each light field exerted onto the atom. Due to the doppler effect, the effective detuning of the beam co-propagating with the atom will become $\Delta_1 = \Delta - kv$, while that of the beam counter-propagating with the atom will be $\Delta_2 = \Delta + kv$. Other than that, the force still has the same expression as $F_{\text{dissipative}}$ in **Example 1**. So we have

$$F_1 = \frac{\hbar k\Gamma}{2}\frac{\tilde{\Omega}^2/2}{\Delta_1^2+\Gamma^2/4+\tilde{\Omega}^2/2} \tag{3.5}$$

$$F_2 = -\frac{\hbar k\Gamma}{2}\frac{\tilde{\Omega}^2/2}{\Delta_2^2+\Gamma^2/4+\tilde{\Omega}^2/2} \tag{3.6}$$

The total force is then $F = F_1 + F_2$. For small velocity such that $kv \ll \Delta$, we can expand the force as power series of v. Keep only the linear term, we have:

$$F = \frac{\hbar k^2 \Gamma \tilde{\Omega}^2 \Delta}{(\Delta^2 + \Gamma^2/4)^2}\, v \tag{3.7}$$

Therefore, we have a damping or cooling force for red detuning $\Delta < 0$.

From Eq. (3.7), we know the cooling rate (when $\Delta < 0$) is given by

$$(dE/dt)_{\text{cool}} = Fv$$

However, at each moment, the atom can absorb a photon from either beam with equal probability (neglecting the small Doppler effect). For the low intensity limit we are considering here, each absorption event is independent from each other. Following each absorption, there is a spontaneous emission which is also random in nature. If we neglect spontaneous emission pattern, and assume that the ith emitted photon has momentum k_i which can take values k or $-k$ with equal probability, then the momentum change for the atom after an N absorption-emission cycle is

$$\Delta p = (N_1 - N_2)\hbar k - \sum_{i=1}^{N} \hbar k_i$$

or

$$(\Delta p)^2 = (N_1^2 + N_2^2 - 2N_1 N_2)\hbar^2 k^2 - 2(N_1 - N_2)\hbar^2 k \sum_{i=1}^{N} k_i + \hbar^2 k^2 N + \hbar^2 \sum_{i \neq j} k_i k_j$$

where N_1 and N_2 are number of photons absorbed from beam 1 and 2 respectively. Now $N_{1,2}$ obey Poisson statistics since the absorption events are independent:

$$\langle N_1 \rangle = \langle N_2 \rangle = N/2, \quad \langle N_1 N_2 \rangle = \langle N_1 \rangle \langle N_2 \rangle = N^2/4, \quad \langle N_1^2 \rangle = \langle N_1 \rangle^2 + \langle N_1 \rangle = N^2/4 + N/2 = \langle N_2^2 \rangle$$

For the spontaneously emitted photon, we have

$$\langle \sum_i k_i \rangle = 0$$

Therefore, the total kinetic energy change due to the random nature of light absorption and emission is

$$(\Delta E)_{\text{heat}} = \langle (\Delta p)^2 \rangle / (2m) = 2N\hbar^2 k^2/(2m)$$

So the corresponding heating rate is

$$(dE/dt)_{\text{heat}} = (\hbar^2 k^2/m) dN/dt$$

Here dN/dt is the absorption rate and is give by $\Gamma \sigma_{ee,st} \approx \Gamma s/2 = \Gamma \tilde{\Omega}^2/(4\Delta^2 + \Gamma^2)$. So the heating rate (under the small velocity, low intensity limit) is

$$(dE/dt)_{\text{heat}} = \frac{\hbar^2 k^2 \Gamma}{4m} \frac{\tilde{\Omega}^2}{\Delta^2 + \Gamma^2/4}$$

In the steady state, cooling and heating reaches an equilibrium. so $(dE/dt)_{\text{cool}} + (dE/dt)_{\text{heat}} = 0$, or

$$\frac{\hbar k^2 \Gamma \tilde{\Omega}^2 \Delta}{(\Delta^2 + \Gamma^2/4)^2}\, v^2 + \frac{\hbar^2 k^2 \Gamma}{4m} \frac{\tilde{\Omega}^2}{\Delta^2 + \Gamma^2/4} = 0$$

or

$$k_B T = mv^2 = -\frac{\hbar}{4}\frac{\Delta^2 + \Gamma^2/4}{\Delta}$$

The minimum temperature is obtained when $\Delta = -\Gamma/2$,

$$k_B T_{\text{Doppler}} = \hbar\Gamma/4$$

This temperature is called the Doppler limit. A more sophisticated calculation including higher dimensionality and spontaneous emission pattern shows that the Doppler limit is a factor of 2 higher than the above expression, i.e. $k_B T_{\text{Doppler}} = \hbar\Gamma/2$.

Chapter 4

Density Matrix

4.1 A state vector is not enough

A quantum state can be described by a state vector. However, in many situations, we don't have a full knowledge about the state of the system. Such situations arise, for example, when the system is coupled to a reservoir and we can no longer keep track of all the degrees of freedom.

Let us try to gain some insight from the following example. Given a particle with a state described by state vector $|\psi\rangle$. The probability density to find the particle at x is

$$P(x) = |\langle x|\psi\rangle|^2 = \langle x|\psi\rangle\langle\psi|x\rangle = \langle x|\hat{\rho}|x\rangle$$

where we have introduced the hermitian operator

$$\hat{\rho} \equiv |\psi\rangle\langle\psi|$$

This operator is called the **density operator** since we can use it to calculate probability densities.

Suppose the state $|\psi\rangle$ is expanded onto a complete basis $\{|m\rangle\}$ as

$$|\psi\rangle = \sum_m c_m |m\rangle$$

then the density operator reads:

$$\hat{\rho} = \sum_{m,n} c_m c_n^* |m\rangle\langle n| = \sum_{m,n} \rho_{mn} |m\rangle\langle n|$$

The complex-valued numbers $\rho_{mn} = c_m c_n^*$ form a matrix consisting of products made out of the expansion coefficients c_m. The matrix formed by ρ_{mn} is called the **density matrix**.

Now suppose we don't have good knowledge about the state. We only know that the system has probability $P_m = |c_m|^2$ to be in state $|m\rangle$, but no information on phase is gained. In other words, we have

$$c_m = \sqrt{P_m}\, e^{i\phi_m}$$

where ϕ_m is a random phase. Then we need to average over these phases in order to calculate any expectation values. The density matrix element ρ_{mn} averaged over the phase becomes

$$\rho_{mn} = \overline{c_m c_n^*} = \overline{\sqrt{P_m P_n} e^{i(\phi_m - \phi_n)}} = P_m \delta_{mn}$$

and the density operator becomes

$$\hat{\rho} = \sum_m P_m |m\rangle\langle m|$$

In conclusion, we have two kinds of averages: The first one results from quantum mechanics and the fact that a quantum state can only provide a statistical description. The second average is a classical one. It reflects the fact that we don not have complete information about the system (in the example above, we don't know the phases of the probability amplitudes): We do not know in which quantum state the system is.

4.2 Definition and properties

For a set of states $|\psi_m\rangle$ ($m = 0, 1, 2, ...$), the density operator is defined as

$$\hat{\rho} = \sum_m P_m |\psi_m\rangle\langle\psi_m|$$

where P_m is the classical probability with which state $|\psi_m\rangle$ appears. Note that in the definition, the states $|\psi_m\rangle$ don't have to form an orthonormal set, but the density operator is most conveniently defined if they do. So we'll take such an assumption. Under this condition, we have

$$\langle\psi_m|\hat{\rho}|\psi_m\rangle = P_m$$

Since P_m are probabilities, they have to add up to unity, hence

$$\text{Tr}\hat{\rho} \equiv \sum_m \langle\psi_m|\hat{\rho}|\psi_m\rangle = \sum_m P_m = 1$$

Let us take this opportunity to say a few words about the trace of operator.

- The definition of the trace of the operator $\hat{O}$ reads

  $$\text{Tr}\hat{O} \equiv \sum_m \langle\psi_m|\hat{O}|\psi_m\rangle$$

  where $|\psi_m\rangle$ is a complete set of states. Hence

  $$\mathbf{1} = \sum_m |\psi_m\rangle\langle\psi_m|$$

  Therefore,

  $$\hat{O} = \mathbf{1}\hat{O}\mathbf{1} = \sum_{mn} |\psi_m\rangle\langle\psi_m|\hat{O}|\psi_n\rangle\langle\psi_n| = \sum_{mn} O_{mn} |\psi_m\rangle\langle\psi_n|$$

  with $O_{mn} = \langle\psi_m|\hat{O}|\psi_n\rangle$. And the trace of $\hat{O}$ is indeed the sum over the diagonal elements O_{mm}.

- **Trace is independent of representation** To show this, let us consider a different complete set of orthonormal states $|\phi_n\rangle$ and $\mathbf{1} = \sum_n |\phi_n\rangle\langle\phi_n|$. Then

$$\begin{aligned}
\mathrm{Tr}\hat{O} &= \sum_m \langle\psi_m|\mathbf{1}\hat{O}\mathbf{1}|\psi_m\rangle = \sum_{m,n,l} \langle\psi_m|\phi_n\rangle\langle\phi_n|\hat{O}|\phi_l\rangle\langle\phi_l|\psi_m\rangle \\
&= \sum_{n,l} \langle\phi_l \left(\sum_m |\psi_m\rangle\langle\psi_m| \right) \phi_n\rangle\langle\phi_n|\hat{O}|\phi_l\rangle \\
&= \sum_{n,l} \delta_{nl}\langle\phi_n|\hat{O}|\phi_l\rangle \\
&= \sum_n \langle\phi_n|\hat{O}|\phi_n\rangle
\end{aligned}$$

- $\mathrm{Tr}[\hat{A}\hat{B}] = \mathrm{Tr}[\hat{B}\hat{A}]$

- **Expectation value is the Trace** The trace operation allows us to calculate expectation values of operators. First, the expectation value of operator $\hat{O}$ is defined as

$$\langle\hat{O}\rangle = \sum_m P_m \langle\psi_m|\hat{O}|\psi_m\rangle$$

It can be easily shown that

$$\langle\hat{O}\rangle = \mathrm{Tr}[\hat{O}\hat{\rho}]$$

Using the above property, we have the following properties for density operator:

- $\langle\hat{\rho}\rangle \le 1$ since $\langle\hat{\rho}\rangle = \mathrm{Tr}[\hat{\rho}\hat{\rho}] = \sum_m P_m^2 \le \sum_m P_m = 1$. The equal sign occurs if and only if there is one single state $|\psi_l\rangle$ contributing to the sum, i.e., $P_m = \delta_{lm}$. In this case, the quantum system is described by a single state, and is therefore a **pure state**. Otherwise, the state is call a **mixed state**.

- The matrix elements of the density matrix in any basis $\{|\psi_n\rangle\}$ is given by

$$\rho_{nm} = \langle\psi_n|\hat{\rho}|\psi_m\rangle = \rho^*_{mn}$$

and are constrained by the inequality

$$\rho_{nm}\rho_{mn} \le \rho_{nn}\rho_{mm} \tag{4.1}$$

where the equal sign holds for pure state.

The proof of the inequality goes as follows: Define two states as

$$|\phi_1\rangle = \hat{\rho}^{1/2}|\psi_n\rangle, \quad |\phi\rangle = \hat{\rho}^{1/2}|\psi_m\rangle$$

then we have

$$\langle\phi_1|\phi_2\rangle = \rho_{nm}, \quad \langle\phi_1|\phi_1\rangle = \rho_{nn}, \quad \langle\phi_2|\phi_2\rangle = \rho_{mm}$$

and the inequality (4.1) follows from the Cauchy-Schwarz inequality

$$|\langle\phi_1|\phi_2\rangle|^2 \le \langle\phi_1|\phi_1\rangle\langle\phi_2|\phi_2\rangle$$

To show that the equal sign holds in (4.1) for a pure state, we realize that the operator $\hat{\rho}^{1/2}$ can be written as

$$\hat{\rho}^{1/2} = \sum_n \sqrt{\sigma_n} |\lambda_n\rangle\langle\lambda_n|$$

where $\{|\lambda_n\rangle\}$ is a set of basis states where the density matrix is diagonal, i.e., $\hat{\rho} = \sum_n \sigma_n |\lambda_n\rangle\langle\lambda_n|$. For a pure state, one and only one of the σ_n's will be equal to 1 and all the other will be zero. Let's say $\sigma_n = \delta_{n1}$, then we have

$$|\phi_1\rangle = \langle\lambda_1|\psi_n\rangle|\lambda_1\rangle, \quad |\phi_2\rangle = \langle\lambda_1|\psi_m\rangle|\lambda_1\rangle$$

i.e., $|\phi_1\rangle$ and $|\phi_2\rangle$ correspond to the same state with a *c*-number constant factor. Thus, the equal sign holds for the Cauchy-Schwarz inequality, hence also for (4.1).

4.3 Time evolution of the density operator

The density matrix operator, introduced as a device to represent our knowledge of the initial state of the quantum system under study, is frequently employed for time-dependent purposes. How can a bookkeeping statement about the system at $t = 0$ acquire dynamic properties? The answer is, by switching from the Heisenberg picture to the Schrödinger picture. To see this, consider the expectation value of $\hat{O}$:

$$\langle\hat{O}(t)\rangle = \mathrm{Tr}[\hat{\rho}\hat{O}] = \mathrm{Tr}[\hat{\rho}U^{-1}(t,0)\hat{O}(0)U(t,0)] = \mathrm{Tr}[U(t,0)\hat{\rho}U^{-1}(t,0)\hat{O}(0)] = \mathrm{Tr}[\hat{\rho}(t)\hat{O}(0)]$$

where

$$\hat{\rho}(t) \equiv U(t,0)\hat{\rho}U^{-1}(t,0)$$

and $U(t,0)$ is the time evolution operator which satisfies

$$i\hbar\frac{\partial}{\partial t}U(t,0) = HU(t,0)$$

Note that $\hat{\rho}(t)$ and $\hat{\rho}$ are **not** related in the same way as any Heisenberg operators $\hat{O}(t)$ and $\hat{O}(0)$ are related, since

$$\hat{O}(t) = U^{-1}(t,0)\hat{O}(0)U(t,0)$$

The consequence of this difference is that $\hat{\rho}(t)$ obeys an equation of motion:

$$i\hbar\dot{\hat{\rho}}(t) = [H, \hat{\rho}]$$

which is sometimes called the quantum Liouville equation.

4.4 Application to two-level atom

The Hilbert space is spanned by states $|g\rangle$ and $|e\rangle$. So the density operator can be represented by a 2×2 matrix whose elements are given by $\rho_{ij} = \langle i|\hat{\rho}|j\rangle$ $(i, j = g, e)$. Let us find the relationship between ρ_{ij} and $\hat{\sigma}_{ij}$ we encountered earlier. To do so, let us check that

$$\sigma_{ij}(t) = \langle\hat{\sigma}_{ij}(t)\rangle = \mathrm{Tr}[\hat{\rho}(t)\hat{\sigma}_{ij}(0)] = \mathrm{Tr}[\hat{\rho}(t)|i\rangle\langle j|] = \sum_{k=g,e}\langle k|\hat{\rho}(t)|i\rangle\langle j|k\rangle = \langle j|\hat{\rho}(t)|i\rangle = \rho_{ji}(t)$$

The optical Bloch equations can be also written in terms of ρ_{ij}.

Chapter 5

Sisyphus cooling

5.1 OBEs for Arbitrary $J_g \leftrightarrow J_e$ dipole transition

A dipole allowed transition requires $J_g - J_e = 0, \pm 1$. The ground state has $N_g = 2J_g + 1$ magnetic sublevels with $m_g = -J_g, -J_g + 1, ..., J_g$, similarly, the excited manifold has $N_e = 2J_e + 1$ sublevels with $m_e = -J_e, -J_e + 1, ..., J_e$. Define projection operators

$$\begin{aligned} P_g &= \sum_{m_g=-J_g}^{J_g} |J_g, m_g\rangle\langle J_g, m_g| \\ P_e &= \sum_{m_e=-J_e}^{J_e} |J_e, m_e\rangle\langle J_e, m_e| \end{aligned}$$

which satisfy:

$$\mathbf{1} = P_g + P_e, \quad P_i P_j = P_i \delta_{ij}$$

The density operator can be decomposed as

$$\hat{\rho} = \rho_{gg} + \rho_{ge} + \rho_{eg} + \rho_{ee}$$

Note that ρ_{ij} is an operator itself, not a density matrix element.

An arbitrary light field is given by

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}^{(+)}(\mathbf{r}) e^{-i\omega t} + \mathbf{E}^{(-)}(\mathbf{r}) e^{i\omega t}$$

with $\mathbf{E}^{(+)} = [\mathbf{E}^{(-)}]^*$. We can further decompose $\mathbf{E}^{(+)}$ into a spherical basis of olarization vectors

$$\hat{\varepsilon}_{\pm 1} = \mp \frac{1}{\sqrt{2}}(\hat{x} \pm i\hat{y}), \quad \hat{\varepsilon}_0 = \hat{z}$$

corresponding, respectively, to the $\sigma^{\pm}$ and π polarizations, such that $\mathbf{E}^{(+)} = \sum_{q=-1,0,1} E_q \hat{\varepsilon}_q$.

The atomic dipole operator is given by $\hat{\mathbf{D}} = \mathcal{D}\hat{\mathbf{d}} = \mathcal{D}\hat{\mathbf{d}}^{(+)} + \mathcal{D}\hat{\mathbf{d}}^{(-)}$ where $\mathcal{D}$ is the reduced dipole matrix and is assumed to be real, the dimensionless operators

$$\hat{\mathbf{d}}^{(+)} = P_e \, \hat{\mathbf{d}} \, P_g \tag{5.1}$$

$$\hat{\mathbf{d}}^{(-)} = P_g \, \hat{\mathbf{d}} \, P_e \tag{5.2}$$

The Wigner-Echart theorem applied to the dipole operator gives

$$\langle J_e m_e|\hat{\varepsilon}_q \cdot \hat{\mathbf{d}}^{(+)}|J_g m_g\rangle = \langle J_e m_e|J_g 1 m_g q\rangle$$

where the right hand side is nothing but the Clebsch-Gordon coefficient.

The interaction Hamiltonian under the RWA is

$$H_{AF} = -\hat{\mathbf{D}} \cdot \mathbf{E} = -\mathcal{D}\hat{\mathbf{d}}^{(+)} \cdot \mathbf{E}^{(+)} e^{-i\omega t} + h.c. \tag{5.3}$$

Now we can derive the equations of motion as before:

$$\begin{aligned}
i\dot{\tilde{\rho}}_{eg} &= (-\Delta - i\Gamma/2)\tilde{\rho}_{eg} - \hat{\Omega}^{(+)}\rho_{gg} + \rho_{ee}\hat{\Omega}^{(+)} && (5.4)\\
i\dot{\tilde{\rho}}_{ge} &= (\Delta - i\Gamma/2)\tilde{\rho}_{ge} + \rho_{gg}\hat{\Omega}^{(-)} - \hat{\Omega}^{(+)}\rho_{ee} && (5.5)\\
i\dot{\rho}_{ee} &= -i\Gamma\rho_{ee} + \tilde{\rho}_{eg}\hat{\Omega}^{(-)} - \hat{\Omega}^{(+)}\tilde{\rho}_{ge} && (5.6)\\
i\dot{\rho}_{gg} &= i(\dot{\rho}_{gg})_{\text{sp}} + \tilde{\rho}_{ge}\hat{\Omega}^{(+)} - \hat{\Omega}^{(-)}\tilde{\rho}_{eg} && (5.7)
\end{aligned}$$

where we have defined as before the slowly varying operators

$$\tilde{\rho}_{eg} = \rho_{eg}\, e^{i\omega t}, \quad \tilde{\rho}_{ge} = \rho_{ge}\, e^{-i\omega t}$$

and

$$\hat{\Omega}^{(+)} = \mathcal{D}\hat{\mathbf{d}}^{(+)} \cdot \mathbf{E}^{(+)}/\hbar, \quad \hat{\Omega}^{(-)} = \mathcal{D}\hat{\mathbf{d}}^{(-)} \cdot \mathbf{E}^{(-)}/\hbar$$

and

$$(\dot{\rho}_{gg})_{\text{sp}} = \Gamma \sum_{q=-1,0,1} \left(\hat{\varepsilon}_q^* \cdot \hat{\mathbf{d}}^{(-)}\right) \rho_{ee} \left(\hat{\varepsilon}_q \cdot \hat{\mathbf{d}}^{(+)}\right) \tag{5.8}$$

represents the effect of spontaneous emission on the ground manifold.

5.2 Force under the low intensity low velocity limit

Under the low velocity limit, the atomic center-of-mass motion follows its internal dynamics. So to calculate the light pressure force, we can first calculate the steady state solutions of OBEs.

Under the low intensity limit, we can adiabatically eliminate the excited state population ρ_{ee} and the ground-excited coherence $\tilde{\rho}_{eg}$ and $\tilde{\rho}_{ge}$. This is because in such a limit, the characteristic times for the evolution of the ground state become much longer than those of the excited state. Hence ρ_{gg} is a slow variable compared to ρ_{ee}, $\tilde{\rho}_{eg}$ and $\tilde{\rho}_{ge}$. After a short transient regime, last for a time on the order of $1/\Gamma$, ρ_{ee} "slaves" the other variables by imposing its slow rate of variation, so that one can write

$$|\dot{\rho}_{ee}| \ll \Gamma\rho_{ee}, \quad |\dot{\tilde{\rho}}_{ge,ge}| \ll \Gamma|\tilde{\rho}_{ge,ge}| \tag{5.9}$$

It is then possible to put the left hand side of Eqs. (5.5), (5.4) and (5.6) into zero in comparison with the damping terms at the right hand side. Remark: For a moving atom with velocity $\mathbf{v}$, one must not forget that the time derivative $\dot{\rho}_{ij}$ are actually total time derivatives $d/dt = \partial/\partial t + \mathbf{v}\cdot\nabla$, so that one must also consider the order of magnitude of the term $\mathbf{v}\cdot\nabla\rho_{ij} \approx kv\rho_{ij}$. For the ultracold system we are interested in, the velocity is very small such that $kv \ll \Gamma$, so that condition (10.14) is satisfied.

After this procedure, Eqs. (5.5) and (5.4) yield

$$\tilde{\rho}_{ge} = -\frac{\rho_{gg}\hat{\Omega}^{(-)}}{\Delta - i\Gamma/2}, \quad \tilde{\rho}_{eg} = -\frac{\hat{\Omega}^{(+)}\rho_{gg}}{\Delta + i\Gamma/2} \tag{5.10}$$

where we have neglected the contribution of ρ_{ee} which is small.

Now let us obtain the expression for the force

$$\begin{aligned} \mathbf{F} &= -\langle \nabla H_{AF} \rangle \\ &= \mathcal{D} \sum_{i=x,y,z} \langle \hat{d}_i^{(+)} \rangle \nabla E_i^{(+)} \, e^{-i\omega t} + c.c. \end{aligned}$$

and

$$\langle \hat{d}_i^{(+)} \rangle = \mathrm{Tr}[P_e \hat{d}_i P_g \hat{\rho}] = \mathrm{Tr}[\hat{d}_i \rho_{ge}]$$

Therefore,

$$\mathbf{F} = \sum_{i=x,y,z} \mathrm{Tr}[\hat{d}_i \tilde{\rho}_{ge}] \nabla E_i^{(+)} + c.c.$$

Using (5.10), we have

$$\mathbf{F} = -\frac{1}{\Delta - i\Gamma/2} \mathrm{Tr}[\hat{d}_i \rho_{gg} \hat{\Omega}^{(-)}] \nabla E_i^{(+)}$$

Now let us take a look at the trace

$$\mathrm{Tr}[\hat{d}_i \rho_{gg} \hat{\Omega}^{(-)}] = \mathrm{Tr}[\hat{\Omega}^{(-)} \hat{d}_i \rho_{gg}] = \mathrm{Tr}[\hat{\Omega}^{(-)} (P_e + P_g) \hat{d}_i P_g P_g \hat{\rho} P_g] = \mathrm{Tr}[\hat{\Omega}^{(-)} \hat{d}_i^{(+)} \rho_{gg}] = \langle \hat{\Omega}^{(-)} \hat{d}_i^{(+)} \rangle$$

where we have used $\langle X \rangle = \mathrm{Tr}[X \rho_{gg}]$. Hence

$$\mathbf{F} = -\frac{\hbar}{\Delta - i\Gamma/2} \langle \hat{\Omega}^{(-)} \nabla \hat{\Omega}^{(+)} \rangle + c.c.$$

Decompose the force into the dissipative part and the reactive part, we have

$$F_{\text{dissipative}} = -\frac{i\hbar\Gamma/2}{\Delta^2 + \Gamma^2/4} \left[\langle \hat{\Omega}^{(-)} \nabla \hat{\Omega}^{(+)} \rangle - \langle (\nabla \hat{\Omega}^{(-)}) \hat{\Omega}^{(+)} \rangle \right] \tag{5.11}$$

$$F_{\text{reactive}} = -\frac{\hbar\Delta}{\Delta^2 + \Gamma^2/4} \left\langle \nabla (\hat{\Omega}^{(-)} \hat{\Omega}^{(+)}) \right\rangle \tag{5.12}$$

5.3 Equation of motion of the ground state density matrix

From Eqs. (5.6) and (5.10), we have

$$\rho_{ee} = \frac{1}{\Delta^2 + \Gamma^2/4} \hat{\Omega}^{(+)} \rho_{gg} \hat{\Omega}^{(-)}$$

So we have

$$\begin{aligned} \dot{\rho}_{gg} &= \left[\frac{-i}{\Delta + i\Gamma/2} \hat{\Omega}^{(-)} \hat{\Omega}^{(+)} \rho_{gg} + h.c. \right] + \frac{\Gamma}{\Delta^2 + \Gamma^2/4} \sum_{q=-1,0,1} \left(\hat{\varepsilon}_q^* \cdot \hat{\mathbf{d}}^{(-)} \right) \hat{\Omega}^{(+)} \rho_{gg} \hat{\Omega}^{(-)} \left(\hat{\varepsilon}_q \cdot \hat{\mathbf{d}}^{(+)} \right) \\ &= \frac{-i\Delta}{\Delta^2 + \Gamma^2/4} \left[\hat{\Omega}^{(-)} \hat{\Omega}^{(+)}, \rho_{gg} \right] - \frac{\Gamma/2}{\Delta^2 + \Gamma^2/4} \left(\hat{\Omega}^{(-)} \hat{\Omega}^{(+)} \rho_{gg} + \rho_{gg} \hat{\Omega}^{(-)} \hat{\Omega}^{(+)} \right) \\ &\quad + \frac{\Gamma}{\Delta^2 + \Gamma^2/4} \sum_{q=-1,0,1} \left(\hat{\varepsilon}_q^* \cdot \hat{\mathbf{d}}^{(-)} \right) \hat{\Omega}^{(+)} \rho_{gg} \hat{\Omega}^{(-)} \left(\hat{\varepsilon}_q \cdot \hat{\mathbf{d}}^{(+)} \right) \end{aligned}$$

Let $\mathbf{E}^{(+)}(\mathbf{r}) = \sum_q E_q \hat{\varepsilon}_q = \frac{1}{2}\mathcal{E}_0(\mathbf{r})\hat{\varepsilon}(\mathbf{r})$, where $\hat{\varepsilon}(\mathbf{r})$ is the unit polarization vector which satisfies

$$\hat{\varepsilon}^*(\mathbf{r}) \cdot \hat{\varepsilon}(\mathbf{r}) = 1$$

Then we have

$$\hat{\Omega}^{(+)} = \frac{\Omega_0}{2}\left(\hat{\varepsilon}(\mathbf{r}) \cdot \hat{\mathbf{d}}^{(+)}\right), \quad \hat{\Omega}^{(-)} = \frac{\Omega_0}{2}\left(\hat{\varepsilon}^*(\mathbf{r}) \cdot \hat{\mathbf{d}}^{(-)}\right)$$

with $\Omega_0(\mathbf{r}) = \mathcal{D}\mathcal{E}_0(\mathbf{r})/\hbar$. Further define the Hermitian, semi-positive and dimensionless operator

$$\Lambda(\mathbf{r}) = \left(\hat{\varepsilon}^*(\mathbf{r}) \cdot \hat{\mathbf{d}}^{(-)}\right)\left(\hat{\varepsilon}(\mathbf{r}) \cdot \hat{\mathbf{d}}^{(+)}\right)$$

Then the equation for ρ_{gg} can be written as

$$\begin{aligned}\dot{\rho}_{gg} &= -i\Delta'(\mathbf{r})[\Lambda(\mathbf{r}), \rho_{gg}] - \frac{\Gamma'(\mathbf{r})}{2}[\Lambda(\mathbf{r})\rho_{gg} + \rho_{gg}\Lambda(\mathbf{r})] \\ &\quad +\Gamma'(\mathbf{r}) \sum_{q=-1,0,1} \left(\hat{\varepsilon}_q^* \cdot \hat{\mathbf{d}}^{(-)}\right)\left(\hat{\varepsilon}(\mathbf{r}) \cdot \hat{\mathbf{d}}^{(+)}\right)\rho_{gg}\left(\hat{\varepsilon}^*(\mathbf{r}) \cdot \hat{\mathbf{d}}^{(-)}\right)\left(\hat{\varepsilon}_q \cdot \hat{\mathbf{d}}^{(+)}\right) \end{aligned} \tag{5.13}$$

where

$$\Delta'(\mathbf{r}) = \Delta\frac{\Omega_0^2(\mathbf{r})/4}{\Delta^2 + \Gamma^2/4}, \quad \Gamma'(\mathbf{r}) = \Gamma\frac{\Omega_0^2(\mathbf{r})/4}{\Delta^2 + \Gamma^2/4}$$

Let us take a closer look at the three terms at the right hand side of Eq. (5.13).

The first term can be written as $(-i/\hbar)[H_{\text{eff}}, \rho_{gg}]$, with the effective Hamiltonian $H_{\text{eff}} = \hbar\Delta'(\mathbf{r})\Lambda(\mathbf{r})$. Denote $|g_\alpha(\mathbf{r})\rangle$ and $\lambda_\alpha(\mathbf{r})$ to be the eigenstates and corresponding eigenvalues of $\Lambda(\mathbf{r})$. Since $\Lambda(\mathbf{r})$ is Hermitian and semi-positive, then we have

$$\Lambda(\mathbf{r})|g_\alpha(\mathbf{r})\rangle = \lambda_\alpha(\mathbf{r})|g_\alpha(\mathbf{r})\rangle, \quad \lambda_\alpha(\mathbf{r}) \geq 0$$

Each eigenstate $|g_\alpha(\mathbf{r})\rangle$ gets a well-defined energy shift $\delta E_\alpha = \hbar\Delta'\lambda_\alpha$ which is called the **light shift** or **AC Stark Shift**. δE_α is proportional to Ω_0^2, hence the light intensity. All the δE_α have the same sign, which is the sign of laser detuning Δ. The light shift can be considered as the polarization energy of the induced atomic dipole moment in the driving laser field.

The second term of (5.13) represents a loss term for the ground state atom and describes how the atomic ground state is emptied by the absorption process. The contribution of this term to the rate of variation of the population in eigenstate $|g_\alpha\rangle$ of Λ can be easily calculated as

$$-\Gamma'\lambda_\alpha\langle\rho_{gg}\rangle$$

Note that $\lambda_\alpha \geq 0$, so the above term indeed represents a loss. When $\lambda_\alpha = 0$, then the corresponding state is a trap state of dark state.

The atoms which have left the ground state by photon absorption fall back in the ground state by spontaneous emission. Such an effect is described by the last term of (5.13). Now let us show that the trace of the second term cancels exactly that of the third term, a fact means that there are as many atoms leaving the ground state per unit time as atoms falling back in it, i.e., the population of the ground state is conserved. The proof goes like this:

Let's find out the trace of the third term (neglecting the factor Γ').

$$
\begin{aligned}
& \mathrm{Tr}\left[\sum_{q=-1,0,1}\left(\hat{\varepsilon}_q^*\cdot\hat{\mathbf{d}}^{(-)}\right)\left(\hat{\varepsilon}(\mathbf{r})\cdot\hat{\mathbf{d}}^{(+)}\right)\rho_{gg}\left(\hat{\varepsilon}^*(\mathbf{r})\cdot\hat{\mathbf{d}}^{(-)}\right)\left(\hat{\varepsilon}_q\cdot\hat{\mathbf{d}}^{(+)}\right)\right] \\
= & \sum_{m_g}\sum_{q}\langle m_g|\left(\hat{\varepsilon}_q^*\cdot\hat{\mathbf{d}}^{(-)}\right)|\sum_{m_e}m_e\rangle\langle m_e|\left(\hat{\varepsilon}(\mathbf{r})\cdot\hat{\mathbf{d}}^{(+)}\right)|\sum_{m_g'}m_g'\rangle\langle m_g'|\rho_{gg}|\sum_{m_g''}m_g''\rangle \\
& \langle m_g''|\left(\hat{\varepsilon}^*(\mathbf{r})\cdot\hat{\mathbf{d}}^{(-)}\right)|\sum_{m_e'}m_e'\rangle\langle m_e'|\left(\hat{\varepsilon}_q\cdot\hat{\mathbf{d}}^{(+)}\right)|m_g\rangle \\
= & \sum_{m_e}\sum_{m_e'}\left[\sum_{m_g}\sum_{q}\langle m_g|\left(\hat{\varepsilon}_q^*\cdot\hat{\mathbf{d}}^{(-)}\right)|m_e\rangle\langle m_e'|\left(\hat{\varepsilon}_q\cdot\hat{\mathbf{d}}^{(+)}\right)|m_g\rangle\right]\sum_{m_g'}\sum_{m_g''}\langle m_e|\left(\hat{\varepsilon}(\mathbf{r})\cdot\hat{\mathbf{d}}^{(+)}\right)|m_g'\rangle \\
& \langle m_g'|\rho_{gg}|m_g''\rangle\langle m_g''|\left(\hat{\varepsilon}^*(\mathbf{r})\cdot\hat{\mathbf{d}}^{(-)}\right)|m_e'\rangle \\
= & \sum_{m_e}\sum_{m_g'}\sum_{m"_g}\langle m_e|\left(\hat{\varepsilon}(\mathbf{r})\cdot\hat{\mathbf{d}}^{(+)}\right)|m_g'\rangle\langle m_g'|\rho_{gg}|m"_g\rangle\langle m"_g|\left(\hat{\varepsilon}^*(\mathbf{r})\cdot\hat{\mathbf{d}}^{(-)}\right)|m_e\rangle
\end{aligned}
$$

where we have used the orthomormality condition for C-G coefficient: The quantity in the square bracket of the second to last equality gives $\delta_{m_e,m_e'}$. And finally we can easily identify the last equality is just opposite of the trace of the second term in (5.13).

5.4 application to a $1/2 \leftrightarrow 3/2$ transition

The ground manifold has two sublevels with $m_g = -1/2$ and $1/2$. Take the light field to be the so-called 1D Lin⊥Lin configuration:

$$\mathbf{E}^{(+)}(z) = \frac{1}{2}E_0\left(\hat{x}e^{ikz} - i\hat{y}e^{-ikz}\right)$$

Decompose it into the spherical basis, we have $\mathbf{E}^{(+)}(z) = \frac{1}{2}\mathcal{E}_0\hat{\varepsilon}(z)$ where $\mathcal{E}_0 = \sqrt{2}E_0$ and

$$\hat{\varepsilon}(z) = \hat{\varepsilon}_{-1}\cos kz - i\hat{\varepsilon}_{+1}\sin kz$$

Then the matrix for $\left(\hat{\varepsilon}^*(\mathbf{r})\cdot\hat{\mathbf{d}}^{(-)}\right)$ and $\left(\hat{\varepsilon}(\mathbf{r})\cdot\hat{\mathbf{d}}^{(+)}\right)$ are given by

$$
\begin{aligned}
\left(\hat{\varepsilon}^*(\mathbf{r})\cdot\hat{\mathbf{d}}^{(-)}\right) &= \begin{pmatrix} \cos kz & 0 & -i\sqrt{\frac{1}{3}}\sin kz & 0 \\ 0 & \sqrt{\frac{1}{3}}\cos kz & 0 & -i\sin kz \end{pmatrix} \\
\left(\hat{\varepsilon}(\mathbf{r})\cdot\hat{\mathbf{d}}^{(+)}\right) &= \begin{pmatrix} \cos kz & 0 \\ 0 & \sqrt{\frac{1}{3}}\cos kz \\ i\sqrt{\frac{1}{3}}\sin kz & 0 \\ 0 & i\sin kz \end{pmatrix}
\end{aligned}
$$

Therefore, $\Lambda(z) = \left(\hat{\varepsilon}^*(\mathbf{r})\cdot\hat{\mathbf{d}}^{(-)}\right)\left(\hat{\varepsilon}(\mathbf{r})\cdot\hat{\mathbf{d}}^{(+)}\right)$ takes a diagonal form

$$\Lambda(z) = \begin{pmatrix} \cos^2 kz + \frac{1}{3}\sin^2 kz & 0 \\ 0 & \frac{1}{3}\cos^2 kz + \sin^2 kz \end{pmatrix} = \begin{pmatrix} 1 - \frac{2}{3}\sin^2 kz & 0 \\ 0 & 1 - \frac{2}{3}\cos^2 kz \end{pmatrix}$$

This means that the bare atomic ground state $m_g = \pm 1/2$ are the eigenstates of H_{eff}, with lights shifts given by

$$E_{-1/2}(z) = -\frac{3U_0}{2} + U_0\sin^2 kz, \quad E_{1/2}(z) = -\frac{3U_0}{2} + U_0\cos^2 kz \tag{5.14}$$

with $U_0 = -\frac{2}{3}\hbar\Delta'$.

From Eq. (5.11) we immediately see that $F_{\text{dissipative}} = 0$. Now let us calculate F_{reactive}. From Eq. (5.12) we have

$$F_{\text{reactive}} = -\langle \nabla H_{\text{eff}} \rangle = -\Pi_{-1/2}\nabla E_{-1/2} - \Pi_{1/2}\nabla E_{1/2}$$

where $\Pi_{\pm 1/2}$ is the population for ground state sublevel $m_g = \pm 1/2$, and it's easy to see that

$$F_{\text{reactive}}(z) = F(z) = kU_0 \sin(2kz)\, \mathcal{M}(z)\, \hat{z}$$

where

$$\mathcal{M}(z) = \Pi_{1/2}(z) - \Pi_{-1/2}(z)$$

is the steady state population difference between the two ground state sublevels, which is z-dependent.

Now we need to obtain $\Pi_{\pm 1/2}$.

5.5 Optical pumping rates

Using Eq. (5.13), we can easily obtain the equations of motion for ground state populations. The first term of (5.13) gives rise to an energy shift and hence does not contribute to the population dynamics. Also, due to the lack of π-polarized light, population only couples to populations, not to ground state coherence. After some algebra, we may obtain

$$\dot{\Pi}_{-1/2} = -\Gamma_{-\to+}\Pi_{-1/2} + \Gamma_{+\to-}\Pi_{1/2} \tag{5.15}$$

$$\dot{\Pi}_{1/2} = \Gamma_{-\to+}\Pi_{-1/2} - \Gamma_{+\to-}\Pi_{1/2} = -\dot{\Pi}_{-1/2} \tag{5.16}$$

where the pumping rates are given by

$$\Gamma_{-\to+} = \frac{2}{9}\Gamma' \sin^2 kz, \quad \Gamma_{+\to-} = \frac{2}{9}\Gamma' \cos^2 kz \tag{5.17}$$

According to Eqs. (5.14) and (5.17), the maxima pumping rate out of state $m_g = -1/2\rangle$ $(\Gamma_{-\to+})$ coincides with those of the light shift for the state $(E_{-1/2})$, provided that $\Delta < 0$, i.e., $U_0 > 0$. And the same is true for state $|m_g = 1/2\rangle$.

5.6 sisyphus cooling mechanism

Consider an atom moving with velocity v along z-axis in the bi-potential $E_{\pm 1/2}$. Suppose initially the kinetic energy of the atom is larger than U_0 so that the atom is not trapped in one of the potential wells. Also assume that

$$\Gamma' \ll kv \ll \Gamma$$

so that, on the one hand, the atom travels over several wavelengths before being optically pumped from one sublevel to the other; on the other hand, the atom travels over a distance very small compared to the wavelength during the duration $1/\Gamma$ of a fluorescence cycle, hence each optical-pumping cycle can be considered as occurring instantaneously in a given spatial point. $kv \ll \Gamma$ is also required for the adiabatic elimination of fast variables.

Suppose that initially the atom is in the sublevel $|m_g = -1/2\rangle$. As long as it remains in this sublevel, its total energy is conserved. We neglect for the moment the recoil due to the absorbed and re-emitted photons in the fluorescence cycles. Because of the spatial dependence of the optical pumping rate, the transfer by optical pumping from $|m_g = -1/2\rangle$ to $|m_g = 1/2\rangle$ will occur preferentially near the maxima of $E_{-1/2}$, and the atom will jump suddenly from a point near the top of one hill of $E_{-1/2}$ to a point near the bottom of one valley of $E_{1/2}$. The corresponding change of its potential energy δU will, therefore, be negative and on the order of U_0. If we neglect photon recoil, then the total energy of atom will decrease by δU.

From there, the same sequence can be repeated. On the average, the atom is running up the hills more than down (hence the name "Sisyphus") and its total energy decreases by a series of discontinuous steps until its kinetic energy becomes on the order of or smaller than U_0. So the cooling limit of this mechanism (for $|\Delta| \gg \Gamma$) is

$$k_B T \sim U_0 \sim \frac{\hbar\tilde{\Omega}^2}{|\Delta|}$$

It seems from above that one can cool down the atom indefinitely by decreasing U_0. However, the above discussion neglects photon recoil. When U_0 becomes a few $E_R = \hbar^2 k^2/(2m)$, the Sisyphus effect is no longer sufficient to overcome the heating due to the recoil. So Sisyphus cooling is "recoil-limited".

Chapter 6

Subrecoil Cooling

6.1 Single-photon recoil limit

All cooling mechanisms described so far (Doppler and Sisyphus) are based on a friction force which damps the atomic velocity. Spontaneous emission processes play a basic role for dissipating the energy removed from the external degrees of freedom of the atom. Therefore, it is impossible to avoid the random recoil due to spontaneously emitted photons and the corresponding single-photon recoil energy

$$E_R = \frac{\hbar^2 k^2}{2m} = k_B T_R$$

The temperature T_R is called the recoil limit and appears as a fundamental limit for any cooling process using spontaneous emission. The corresponding velocity

$$v_R = \hbar k/m$$

and frequency $\omega_R = E_R/\hbar$ are the recoil velocity and recoil frequency, respectively.

In order to get temperatures lower than T_R, we must somehow stop the spontaneous emission precesses for those atoms we want to cool down. For this purpose, we just need to select those cold atoms and put them into the ground state and somehow persuade them not to absorb photon anymore. How can we achieve this?

6.2 Velocity-Selective Coherent Population Trapping

So here is our goal: We want to construct a “trap” in velocity space with width δv. Because of the momentum transferred to the atom by absorbed photon and the momentum carried away by the fluorescence photon, there a random change of atomic momentum after each fluorescence cycle. We want an atom with $v > \delta v$ to undergo such a cycle and end up with $v < \delta v$. Once this is done, the atom falls into the trap and stops interacting with light. The cooling mechanism radically differs from the other ones since it is not based on a friction force but on a combination of momentum diffusion and VSCPT.

To anticipate the ultra-low velocity this can achieve, we don't want to use the semi-classical treatment used earlier where we treat the atom as a point particle which valid when the atomic de Broglie wavelength $\ll$ laser wavelength. But for atomic velocities lower than the recoil velocity, this assumption is no longer valid. Hence, a fully quantum treatment of all degrees of freedom is required.

6.3 VSCPT for a $1 \leftrightarrow 1$ transition

We consider a $J_g = 1 \leftrightarrow J_e = 1$ atomic dipole transition with a $\sigma^+ - \sigma^-$ laser field configuration (we again restrict our discussion in 1D z-direction and the two laser fields have equal detuning Δ):

$$\mathbf{E}(\mathbf{r}, t) = \mathbf{E}^{(+)}(z)\, e^{-i\omega t} + \mathbf{E}^{(-)}(z)\, e^{i\omega t}$$

and

$$\mathbf{E}^{(+)}(z) = \frac{1}{2} E_0 \left(\hat{\varepsilon}_{+1} e^{ikz} + \hat{\varepsilon}_{-1} e^{-ikz}\right)$$

Such a field decouples the atomic system into two uncoupled sub-systems: a V-type composed of $|e_{-1}\rangle$, $|e_{+1}\rangle$ and $|g_0\rangle$ and a Λ-type composed of $|g_{-1}\rangle$, $|g_{+1}\rangle$ and $|e_0\rangle$. Due to zero C-G coefficient between transition e_0 and g_0, spontaneous emission will optically pump the population out of V-system into Λ. Therefore, we can neglect the V altogether and the atomic system reduces to a Λ-type three-level transition.

In the rotating frame, the interaction Hamiltonian under RWA can then be written as

$$H_{AF} = -\frac{\hbar\Omega}{2\sqrt{2}} \left(e^{ikz} |e_0\rangle\langle g_{-1}| + e^{-ikz} |e_0\rangle\langle g_1|\right) + h.c.$$

with $\Omega = -\mathcal{D} E_0/\hbar$. Since $e^{\pm ikz}$ are translation operators in momentum space, we have

$$\begin{aligned} H_{AF}|g_{-1}, p\rangle &= -\frac{\hbar\Omega}{2\sqrt{2}} |e_0, p + \hbar k\rangle \\ H_{AF}|g_{+1}, p\rangle &= \frac{\hbar\Omega}{2\sqrt{2}} |e_0, p - \hbar k\rangle \end{aligned}$$

where we have labelled the atomic states by its internal state and the momentum. This suggests to introduce the states

$$|\psi_{\mathrm{NC}}(p)\rangle = \frac{1}{\sqrt{2}} \left(|g_{-1}, p - \hbar k\rangle + |g_{+1}, p + \hbar k\rangle\right)$$

which are not coupled to the laser light since

$$H_{AF}|\psi_{\mathrm{NC}}(p)\rangle = \frac{\hbar\Omega}{4} \left(-|e_0, p\rangle + |e_0, p\rangle\right) = 0$$

In other words, the two absorption amplitudes starting respectively from states $|g_{-1}, p - \hbar k\rangle$ and $|g_{+1}, p + \hbar k\rangle$, and ending both in the same final state $|e_0, p\rangle$, interfere destructively.

The state

$$|\psi_{\mathrm{C}}(p)\rangle = \frac{1}{\sqrt{2}} \left(-|g_{-1}, p - \hbar k\rangle + |g_{+1}, p + \hbar k\rangle\right)$$

is orthogonal to $|\psi_{\mathrm{NC}}\rangle$ and coupled to $|e_0, p\rangle$:

$$H_{AF}|\psi_{\mathrm{C}}(p)\rangle = \frac{\hbar\Omega}{2} |e_0, p\rangle$$

Therefore the three states

$$\mathcal{F}(p) = \{|e_0, p\rangle,\ |g_{-1}, p - \hbar k\rangle,\ |g_{+1}, p + \hbar k\rangle\} = \{|e_0, p\rangle,\ |\psi_{\rm C}(p)\rangle,\ |\psi_{\rm NC}(p)\rangle\}$$

form a closed family when spontaneous emission is ignored. This fact does not change when the bare Hamiltonian considered below is taken into account.

Now we need to consider the bare atomic Hamiltonian

$$H_A = \frac{P^2}{2m} - \hbar\Delta|e_0\rangle\langle e_0|$$

Using

$$H_A|g_{\pm1}, p \pm \hbar k\rangle = \frac{(p \pm \hbar k)^2}{2m}|g_{\pm1}, p \pm \hbar k\rangle$$

we have

$$\begin{aligned} H_A|\psi_{\rm NC}(p)\rangle &= \left(\frac{p^2}{2m} + E_R\right)|\psi_{\rm NC}(p)\rangle + \frac{\hbar kp}{m}|\psi_{\rm C}(p)\rangle \\ H_A|\psi_{\rm C}(p)\rangle &= \left(\frac{p^2}{2m} + E_R\right)|\psi_{\rm C}(p)\rangle + \frac{\hbar kp}{m}|\psi_{\rm NC}(p)\rangle \end{aligned}$$

Such a result shows that H_A shifts the two states $|\psi_{\rm C}(p)\rangle$ and $|\psi_{\rm NC}(p)\rangle$ by the same amount $p^2/(2m) + E_R$ and introduces a *motional coupling* between these two states

$$\langle\psi_{\rm C}(p)|H_A|\psi_{\rm NC}(p)\rangle = \frac{\hbar kp}{m}$$

Therefore, the non-coupling state $|\psi_{\rm NC}(p)\rangle$ is not truly "dark" unless $p = 0$.

6.4 Effect of spontaneous emission

When spontaneous emission is ignored, an atomic state which initially belongs to $\mathcal{F}(p)$, cannot leave $\mathcal{F}(p)$. Spontaneous emission gives a width Γ to the excited state. To account for this effect, we can add an imaginary part $-i\hbar\Gamma/2$ to the energy of $|e_0, p\rangle$. The effective Hamiltonian matrix, written in the rotating frame and under the basis of $|e_0, p\rangle$, $|\psi_{\rm C}(p)\rangle$ and $|\psi_{\rm NC}(p)\rangle$, reads

$$H_{\rm eff} = \hbar\begin{pmatrix} -\Delta - i\Gamma/2 & \Omega/2 & 0 \\ \Omega/2 & 0 & kp/m \\ 0 & kp/m & 0 \end{pmatrix}$$

where $\Delta = \omega - \omega_0 + \omega_R$. As a result of coupling, the three basis states are not the eigenstates of $H_{\rm eff}$. However, under the limit of low light intensity ($\Omega \ll \sqrt{\Delta^2 + \Gamma^2/4}$) and low velocity (specified later), these three states are still *approximately* eigenstates of $H_{\rm eff}$.

Consider first the case $p = 0$. In this case $|\psi_{\rm NC}(p = 0)\rangle$ is completely isolated from the other two states which are described by Hamiltonian matrix

$$\hbar\begin{pmatrix} -\Delta - i\Gamma/2 & \Omega/2 \\ \Omega/2 & 0 \end{pmatrix}$$

Under the low light intensity limit, a second order perturbation calculation gives that the energy of $|\psi_{\mathrm{C}}(p = 0)\rangle$ is

$$E_{\mathrm{C}} = \frac{(\hbar\Omega/2)^2}{\hbar(\Delta + i\Gamma/2)} = \hbar(\Delta_{\mathrm{C}} - i\Gamma_{\mathrm{C}}/2)$$

with

$$\Delta_{\mathrm{C}} = \frac{s}{2}\Delta = \frac{\Omega^2}{4\Delta^2 + \Gamma^2}\,\Delta, \quad \Gamma_{\mathrm{C}} = \frac{s}{2}\Gamma = \frac{\Omega^2}{4\Delta^2 + \Gamma^2}\,\Gamma$$

which means that under the effect of laser light, the state $|\psi_{\mathrm{C}}(p = 0)\rangle$ is light shifted by $\hbar\Delta_{\mathrm{C}}$ and gets a finite width Γ_{C}.

Now suppose p is nonzero but sufficiently small, such that

$$k|p|/m \ll \sqrt{\Delta_C^2 + \Gamma_C^2/4}$$

then we can treat the motional coupling between $|\psi_{\mathrm{C}}(p)\rangle$ and $|\psi_{\mathrm{NC}}(p)\rangle$ as a small perturbation. The results obtained above for $|\psi_{\mathrm{C}}(p)\rangle$ are still valid, but the state $|\psi_{\mathrm{NC}}(p)\rangle$ has an energy under the second order calculation:

$$E_{\mathrm{NC}} = \frac{(\hbar kp/m)^2}{-E_{\mathrm{C}}} = \hbar(\Delta_{\mathrm{NC}} - i\Gamma_{\mathrm{NC}}/2)$$

with

$$\Delta_{\mathrm{NC}} = \frac{4k^2p^2}{m^2\Omega^2}\,\Delta, \quad \Gamma_{\mathrm{NC}} = \frac{4k^2p^2}{m^2\Omega^2}\,\Gamma$$

Therefore, the departure rate Γ_{NC} out of the dark state is very small when p is small, and vanishes for $p = 0$. An atom put in the dark state at $t = 0$ can remain there for a time on the order of $1/\Gamma_{\mathrm{NC}}(p)$. Conversely, for a given interaction time Θ, we can find a range of δp of values of p around $p = 0$ such that, if $|p| < \delta p$, an atom in dark state $|\psi_{\mathrm{NC}}(p)\rangle$ will have a high probability to remain trapped in that state during the whole interaction time Θ. The corresponding value of δp is given by the condition $\Gamma_{\mathrm{NC}}(\delta p)\Theta < 1$ or

$$\delta p < \frac{m}{2k\sqrt{\Gamma}}\frac{\Omega}{\sqrt{\Theta}}$$

which can be as small as we want.

6.5 spontaneous transfers between different families

After a spontaneous emission process, the atom can move into a new family. This diffusion in momentum space is essential for transferring atoms into the trapping states with $|p| < \delta p$.

Let us again stick to the 1D situation. A spontaneous emission process give the atom a momentum kick $\hbar k$ along a random direction. Its projection along the z-axis, $u = \hbar k_z$, takes a value anywhere between $-\hbar k$ and $\hbar k$. Assume just before the spontaneous emission, the atom is in state $|e_0, p\rangle$ which belongs to the family $\mathcal{F}(p)$. Just after the spontaneous emission, the atom is in a linear superposition of $|g_{+1}, p + u\rangle$ and $|g_{-1}, p + u\rangle$ (i.e., an entangled state with photon polarization). If we do not care about the polarization of the emitted photon, we can trace over that degree of freedom. This yields the atom to be in a statistical mixture of $|g_{+1}, p + u\rangle$ and $|g_{-1}, p + u\rangle$, which belongs to the families $\mathcal{F}(p - \hbar k + u)$ and $\mathcal{F}(p + \hbar k + u)$, respectively. Since $-\hbar k \leq u \leq \hbar k$, the spontaneous process can transfer atoms between families $\mathcal{F}(p)$ and $\mathcal{F}(p')$ with $p - 2\hbar k \leq p' \leq p + 2\hbar k$.

Chapter 7

Second Quantization

7.1 Fock state and Fock space

Second quantization is just a clever way of bookkeeping. Single particle quantum formalism is powerful in study of a single particle. But often times, we need to deal with a system consisted of a macroscopic number of particles. To write explicitly the wave function for such a many-body system, is as impossible as to determine the momentary position and velocity of each particle in its classical counterpart. In classical statistical mechanics, the problem is avoided by introducing *distribution functions*, giving *probabilities* of, e.g., finding a particle with velocity $\mathbf{v}_1$ at point $\mathbf{r}_1$, and another with velocity $\mathbf{v}_2$ at point $\mathbf{r}_2$, and so on. The distribution functions give information on how many particles occupy each unit of phase space.

There is of course a whole hierarchy of them, including one-, two-, ... N-particle distribution functions, and together they contain exactly the same amount of information as the record of velocities and positions of all particles in the system. The enormous advantage is that we usually need only the few first functions of this hierarchy.

In quantum statistics, we have to operate with the wave function of the N-body system as a whole, $\Phi(\xi_1, \xi_2, ..., \xi_N)$, with ξ_i denoting the parameter(s) characterizing the ith particle. In quantum mechanics, identical particles cannot be distinguished in principle. This indistinguishability requires that if we exchange two particles, the wave function can only acquire an overall phase factor:

$$\Phi(\xi_1, \xi_2, ..., \xi_i, ...\xi_j, ..., \xi_N) = e^{i\chi}\Phi(\xi_1, \xi_2, ..., \xi_j, ...\xi_i, ..., \xi_N)$$

After making the second permutation of the same pair of particles, we have

$$\Phi(\xi_1, \xi_2, ..., \xi_i, ...\xi_j, ..., \xi_N) = e^{i2\chi}\Phi(\xi_1, \xi_2, ..., \xi_i, ...\xi_j, ..., \xi_N)$$

so that $e^{i2\chi} = 1$ or $e^{i\chi} = \pm 1$, and we are left with two choices:

$$\Phi(\xi_1, \xi_2, ..., \xi_i, ...\xi_j, ..., \xi_N) = \begin{cases} +\Phi(\xi_1, \xi_2, ..., \xi_j, ...\xi_i, ..., \xi_N) & \mathrm{Bose-Einstein\ \ statistics} \\ -\Phi(\xi_1, \xi_2, ..., \xi_j, ...\xi_i, ..., \xi_N) & \mathrm{Fermi-Dirac\ \ statistics} \end{cases} \tag{7.1}$$

The N-particle wave function can be expanded over a complete set of functions, which are provided by the eigenfunctions of some one-particle Hamiltonian $\mathcal{H}_1$:

$$\Phi(\xi_1, \xi_2, ..., \xi_N) = \sum_{\{p_i\}} C_{p_1,p_2,...,p_N}\, \phi_{p_1}(\xi_1)\phi_{p_2}(\xi_2)\cdots\phi_{p_N}(\xi_N)$$

where $\mathcal{H}_1\phi_j(\xi) = \varepsilon_j\phi_j(\xi)$, p_j labels the one-particle state and the summation is performed over all possible permutations. For homogeneous systems, we often choose for $\phi_j(\xi)$ plane waves.

The condition of (7.1) means that we can use only properly symmetrized products of one-particle functions. For bosons, we have

$$\Phi_B^{N_1,N_2,\cdots}(\xi_1, \xi_2, ..., \xi_N) = |N_1, N_2, ...\rangle_B = \sqrt{\frac{N_1!N_2!\cdots}{N!}} \sum_{\{p_i\}} \phi_{p_1}(\xi_1)\phi_{p_2}(\xi_2)\cdots\phi_{p_N}(\xi_N)$$

Here the non-negative integer number N_i shows how many times the ith one-particle eigenfunction ϕ_i enters the product and is called the **occupation number** of state ϕ_i. The occupation number are subject to the condition

$$\sum N_i = N$$

For fermions, we use Slater's determinants

$$\Phi_F^{N_1,N_2,\cdots}(\xi_1, \xi_2, ..., \xi_N) = |N_1, N_2, ...\rangle_F = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{p_1}(\xi_1) & \phi_{p_1}(\xi_2) & \cdots & \phi_{p_1}(\xi_N) \\ \phi_{p_2}(\xi_1) & \phi_{p_2}(\xi_2) & \cdots & \phi_{p_2}(\xi_N) \\ \cdots & \cdots & \cdots & \cdots \\ \phi_{p_N}(\xi_1) & \phi_{p_N}(\xi_2) & \cdots & \phi_{p_N}(\xi_N) \end{vmatrix}$$

The properties of determinants guarantee the necessary antisymmetry of the wave function. Indeed, a transmutation of two particles in this case corresponds to transmutation of two rows in the determinant, which by definition changes its sign. Then, if two rows are equivalent (e.g., $p_i = p_j$), the determinant equals zero. Physically this means that two fermions cannot occupy the same quantum state (Pauli Principle).

The states $|N_1, N_2, ...\rangle_{B,F}$ have definite numbers in each single particle state and are called the **Fock states**. The Hilbert space spanned by the Fock states is called **Fock space**, and it is in Fock space that second-quantized operators act. The state vectors here are defined by the corresponding set of occupation numbers, and the second-quantized operators change these numbers. Thus, any operator can be represented by some combination of basic **creation** and **annihilation** operators, which act as follows:

$$\begin{aligned} c_j|..., N_j, ...\rangle &\propto |..., N_j - 1, ...\rangle \\ c_j^\dagger|..., N_j, ...\rangle &\propto |..., N_j + 1, ...\rangle \end{aligned}$$

Evidently, any Fock state can be obtained by the repeated action of creation operators on the **vacuum state** $|0\rangle = |0, 0, 0, ...\rangle$:

$$|N_1, N_2, ...\rangle \propto \left(c_1^\dagger\right)^{N_1} \left(c_2^\dagger\right)^{N_2} \cdots |0\rangle$$

and the vacuum state is annihilated by any annihilation operator

$$c_j|0\rangle = 0$$

We have to keep in mind that while in the representation of second quantization we explicitly deal with occupation numbers only, our calculations make sense only as long as we can point out the correct one-particle basis functions.

7.2 bosons

Let us first focus on the bosons.

7.2.1 one-particle operators

Consider a one-particle operator

$$\mathcal{O}_1 = \sum_j o_1(\xi_j)$$

, where $o_1(\xi_j)$ is an operator acting on a one-particle state $\phi(\xi_j)$ and the summation is over all N particles. [Example: kinetic energy operator $K = -\sum_j (\hbar^2 \nabla_j^2)/(2m)$]

Let us take a matrix element of $\mathcal{O}_1$ between two N-particle boson states, $\langle \Phi_{B'} | \mathcal{O}_1 | \Phi_B \rangle$. Since $\mathcal{O}_1$ is a one-particle operator, after its action, there two possibilities: 1) It does not change the state of particle it acted on. Then the only non-zero elements are diagonal ones with $|\Phi_B\rangle = |\Phi_{B'}\rangle$. 2) It transfers the particle from its initial state $|i\rangle = \phi_i(\xi)$ to some final state $|f\rangle = \phi_f(\xi)$. Then the non-zero elements are off-diagonal ones between the states $|\Phi_B\rangle = |..., N_i, ..., N_f, ...\rangle$ and $|\Phi_{B'}\rangle = |..., N_i - 1, ..., N_f + 1, ...\rangle$.

Let us now calculate the matrix elements. First we notice that since the system consists of N identical particles, we have

$$\langle \Phi_{B'} | \mathcal{O}_1 | \Phi_B \rangle = \langle \Phi_{B'} | \sum_j o_1(\xi_j) | \Phi_B \rangle = N \langle \Phi_{B'} | o_1(\xi_1) | \Phi_B \rangle$$

that is, we can just pick an arbitrary particle (say particle 1), calculate its matrix element and times N.

For the diagonal matrix, we have

$$\begin{aligned} \langle \Phi_B | o_1(\xi_1) | \Phi_B \rangle &= \left(\frac{N_1! N_2! \cdots}{N!} \right) \int \int \cdots \int d\xi_1 d\xi_2 \cdots d\xi_N \\ &\quad \times \sum_{\{p_i\},\{p'_i\}} \phi^*_{p'_1}(\xi_1) \phi^*_{p'_2}(\xi_2) \cdots \phi^*_{p'_N}(\xi_N)\, o_1(\xi_1)\, \phi_{p_1}(\xi_1) \phi_{p_2}(\xi_2) \cdots \phi_{p_N}(\xi_N) \end{aligned}$$

and $p'_i = p_i$. Suppose now particle 1 occupy state $|k\rangle$ (k will be summed over at the end), we can take the diagonal matrix element of $o_1(\xi_1)$ as

$$\langle k | o_1 | k \rangle = \int d\xi_1\, \phi^*_k(\xi_1) o_1(\xi_1) \phi_k(\xi_1)$$

The other integrals over the remain $N-1$ particles (which are equal to one due to orthonormality) can be symmetrically rearranged in $(N-1)!/[N_1! N_2! \cdots (N_k - 1)! \cdots]$ ways. Therefore

$$\langle \Phi_B | o_1(\xi_1) | \Phi_B \rangle = \sum_k \left(\frac{N_1! N_2! \cdots}{N!} \right) \left(\frac{(N-1)!}{N_1! N_2! \cdots (N_k - 1)! \cdots} \right) \langle k | o_1 | k \rangle = \sum_k \frac{N_k}{N} \langle k | o_1 | k \rangle$$

Therefore

$$\langle \Phi_B | \mathcal{O}_1 | \Phi_B \rangle = \sum_k N_k \langle k | o_1 | k \rangle$$

For the off-diagonal matrix, there will be one extra $\phi_f^*(\xi)$ on the left side and one extra $\phi_i(\xi)$ on the right side of o_1, we have

$$\begin{aligned}\langle\Phi_{B'}|o_1(\xi_1)|\Phi_B\rangle &= \left(\frac{N_1!\cdots(N_i-1)!\cdots(N_f+1)!\cdots}{N!}\right)^{1/2}\left(\frac{N_1!\cdots N_i!\cdots N_f!\cdots}{N!}\right)^{1/2}\\ \int\!\!\int\cdots\int \quad d\xi_1 \quad d\xi_2\cdots d\xi_N & \sum_{\{p_i\},\{p'_i\}}\phi^*_{p'_1}(\xi_1)\phi^*_{p'_2}(\xi_2)\cdots\phi^*_{p'_N}(\xi_N)\,o_1(\xi_1)\,\phi_{p_1}(\xi_1)\phi_{p_2}(\xi_2)\cdots\phi_{p_N}(\xi_N)\end{aligned}$$

These unmatched functions must be integrated with the operator to yield

$$\langle f|o_1|i\rangle = \int d\xi_1\, \phi_f^*(\xi_1)o_1(\xi_1)\phi_i(\xi_1)$$

while the rest can be rearranged in $(N-1)!/[N_1!N_2!\cdots(N_i-1)!\cdots N_f!\cdots]$ Putting all these together, we have

$$\begin{aligned}\langle\Phi_{B'}|\mathcal{O}_1|\Phi_B\rangle &= N\langle\Phi_{B'}|o_1(\xi_1)|\Phi_B\rangle\\ &= N\sum_{i,f}\left(\frac{N_1!\cdots(N_i-1)!\cdots(N_f+1)!\cdots}{N!}\right)^{1/2}\\ &\quad\times\left(\frac{N_1!\cdots N_i!\cdots N_f!\cdots}{N!}\right)^{1/2}\frac{(N-1)!}{N_1!\cdots(N_i-1)!\cdots N_f!\cdots}\langle f|o_1|i\rangle\\ &= \sum_{i,f}\sqrt{N_i(N_f+1)}\langle f|o_1|i\rangle\end{aligned}$$

Now we are in a position to employ the creation/annihilation operators introduced earlier which we will denote as $a^\dagger$ and a here. We define them with the following:

$$\begin{aligned}a_j\,|...,N_j,...\rangle &= \sqrt{N_j}\,|...,N_j,...\rangle\\ a_j^\dagger\,|...,N_j,...\rangle &= \sqrt{N_j+1}\,|...,N_j,...\rangle\end{aligned}$$

Since $a_j^\dagger a_j|N_j\rangle = N_j|N_j\rangle$, $\hat{N}_j = a_j^\dagger a_j$ is called the **number operator** for particle j. The creation/annihilation operators thus defined obey the boson commutation relations

$$[a_j, a_k^\dagger] = \delta_{jk}, \quad [a_j^\dagger, a_k^\dagger] = [a_j, a_k] = 0$$

Returning to the one-particle operator $\mathcal{O}_1 = \sum o_1$, we see that it can be expressed as

$$\mathcal{O}_1 = \sum_{i,f}\langle f|o_1|i\rangle\, a_f^\dagger a_i \tag{7.2}$$

Intuitively, this expression looks evident: a particle is being “scattered” from state i to f (note that i and f can be the same).

7.2.2 boson field operators

Equation (7.2) suggests that we rewrite it as

$$\mathcal{O}_1 = \int d\xi\, \hat{\phi}^\dagger(\xi)\, o_1\, \hat{\phi}(\xi)$$

where

$$\hat{\phi}(\xi) = \sum_k \phi_k(\xi)\, a_k, \quad \hat{\phi}^\dagger(\xi) = \sum_k \phi^*_k(\xi)\, a^\dagger_k$$

are the so-called **field operators**. The operator $a^\dagger_k$ creates a particle with a wave function $\phi_k(\xi')$, the field operator $\hat{\phi}^\dagger(\xi)$ therefore creates a particle with wave function

$$\sum_k \phi^*_k(\xi)\phi_k(\xi') = \delta(\xi - \xi')$$

where we have used the completeness of the basis of one-particle states. That is, the field operator creates (or annihilates) a particle at a given point. The operator

$$\rho(\xi) = \hat{\phi}^\dagger(\xi)\hat{\phi}(\xi) = \sum_k |\phi_k(\xi)|^2 a^\dagger_k a_k = \sum_k |\phi_k(\xi)|^2 \hat{N}_k$$

evidently gives the density of particles at point ξ, and therefore is called the **density operator**.

The commutation relations for field operators follow those for creation/annihilation operators:

$$[\hat{\phi}(\xi,t), \hat{\phi}^\dagger(\xi',t)] = \delta(\xi - \xi'), \quad [\hat{\phi}(\xi,t), \hat{\phi}(\xi',t)] = [\hat{\phi}^\dagger(\xi,t), \hat{\phi}^\dagger(\xi',t)] = 0$$

Note that time dependence of the field operators arise through the operators $a^\dagger$, a (Heisenberg picture), or through the basis functions $\phi_k(\xi)$ (Schrödinger picture), or both (interaction picture). What is important is that *definite commutation relations exist only between field operators taken at the same moment of time.*

The definition of the field operators is reminiscent of the expansion of an arbitrary single-particle wave function under some basis states $\psi(\xi) = \sum_k \phi_k(\xi)c_k$. That is why the method is called **second quantization**: It looks as if we quantize the quantum wave function one more time, transforming it into an operator!

7.2.3 two-particle operators

Consider now a two-particle operator

$$\mathcal{O}_2 = \frac{1}{2}\sum_{i\neq j} o_2(\xi_i, \xi_j)$$

(Example: scalar two-body collision interaction potential) The non-zero matrix elements occurs between two N-body states that differ at most in two single-particle states. So the non-zero elements are:

$$\langle \quad ..., N_i, ...|\mathcal{O}_2|..., N_i, ...\rangle, \quad \text{(affecting no particle)}$$

$$\langle \quad ..., N_i - 1, ..., N_f + 1, ...|\mathcal{O}_2|..., N_i, ..., N_f, ...\rangle, \quad \text{(affecting only one particle)}$$

$$\langle \quad ..., N_i - 2, ..., N_f + 2, ...|\mathcal{O}_2|..., N_i, ..., N_f, ...\rangle$$

$$\langle \quad ..., N_i - 2, ..., N_f + 1, ..., N_g + 1, ...|\mathcal{O}_2|..., N_i, ..., N_f, ..., N_g, ...\rangle$$

$$\langle \quad ..., N_i - 1, ..., N_f - 1, ..., N_g + 2|\mathcal{O}_2|..., N_i, ..., N_f, ..., N_g, ...\rangle$$

$$\langle \quad ..., N_i - 1, ..., N_j - 1, ..., N_f + 1, ..., N_g + 1|\mathcal{O}_2|..., N_i, ..., N_j, ..., N_f, ..., N_g, ...\rangle$$

Let us consider the last one as an example. Follow a similar procedure as in one-particle operator case, first we notice that

$$\langle\mathcal{O}_2\rangle = \frac{1}{2}\sum_{i\neq j}\langle o_2(\xi_i, \xi_j)\rangle = \frac{N(N-1)}{2}\langle o_2(\xi_1, \xi_2)\rangle$$

then

$$\begin{aligned}
& \langle ..., N_i - 1, ..., N_j - 1, ..., N_f + 1, ..., N_g + 1 | o_2 | ..., N_i, ..., N_j, ..., N_f, ..., N_g, ... \rangle \\
= & \left(\frac{\cdots (N_i - 1)! \cdots (N_j - 1)! \cdots (N_f + 1)! \cdots (N_g + 1)! \cdots}{N!} \right)^{(1/2)} \\
& \times \left(\frac{\cdots N_i! \cdots N_j! \cdots N_f! \cdots N_g! \cdots}{N!} \right)^{(1/2)} \frac{(N-2)!}{\cdots (N_i - 1)! \cdots (N_j - 1)! \cdots N_f! \cdots N_g! \cdots} \overline{o_2} \\
= & \frac{\sqrt{N_i N_j (N_f + 1)(N_g + 1)}}{N(N-1)} \overline{o_2}
\end{aligned}$$

where

$$\overline{o_2} = \langle fg | o_2 | ij \rangle + \langle gf | o_2 | ij \rangle + \langle fg | o_2 | ji \rangle + \langle gf | o_2 | ji \rangle$$

We have in the above written explicitly all terms following from symmetrization and

$$\langle fg | o_2 | ij \rangle = \int d\xi_1 \int d\xi_2 \, \phi_f^*(\xi_1) \phi_g^*(\xi_2) \, o_2(\xi_1, \xi_2) \, \phi_i(\xi_2) \phi_j(\xi_1)$$

Finally we have

$$\langle ..., N_i - 1, ..., N_j - 1, ..., N_f + 1, ..., N_g + 1 | \mathcal{O}_2 | ..., N_i, ..., N_j, ..., N_f, ..., N_g, ... \rangle = \frac{\sqrt{N_i N_j (N_f + 1)(N_g + 1)}}{2} \overline{o_2}$$

It is quite obvious that the operator must be of the form

$$\mathcal{O}_2 = \sum_{m,n,p,q} C_{mnpq} \, a_m^\dagger a_n^\dagger a_p a_q \tag{7.3}$$

Using

$$\begin{aligned}
& \langle ..., N_i - 1, ..., N_j - 1, ..., N_f + 1, ..., N_g + 1 | a_m^\dagger a_n^\dagger a_p a_q | ..., N_i, ..., N_j, ..., N_f, ..., N_g, ... \rangle \\
= & \sqrt{N_i N_j (N_f + 1)(N_g + 1)} (\delta_{mf} \delta_{ng} \delta_{pi} \delta_{qj} + \delta_{mg} \delta_{nf} \delta_{pi} \delta_{qj} + \delta_{mf} \delta_{ng} \delta_{pj} \delta_{qi} + \delta_{mg} \delta_{nf} \delta_{pj} \delta_{qi})
\end{aligned}$$

we have

$$C_{mnpq} = \frac{1}{2} \langle mn | o_2 | pq \rangle$$

One can check that this is also the case for the rest of the matrix elements as well. Therefore, we have

$$\mathcal{O}_2 = \frac{1}{2} \sum_{m,n,p,q} \langle mn | o_2 | pq \rangle \, a_m^\dagger a_n^\dagger a_p a_q = \frac{1}{2} \int d\xi_1 \int d\xi_2 \, \hat{\phi}^\dagger(\xi_1) \hat{\phi}^\dagger(\xi_2) \, o_2(\xi_1, \xi_2) \, \hat{\phi}(\xi_2) \hat{\phi}(\xi_1)$$

In general, an n-particle operator can be written as

$$\begin{aligned}
\mathcal{O}_n = & \frac{1}{n!} \sum_{j_1 \neq j_2 \neq \cdots \neq j_n} o_n(\xi_{j_1}, \xi_{j_2}, ..., \xi_{j_n}) \\
= & \frac{1}{n!} \int d\xi_1 \int d\xi_2 \cdots \int d\xi_n \, \hat{\phi}^\dagger(\xi_1) \hat{\phi}^\dagger(\xi_2) \cdots \hat{\phi}^\dagger(\xi_n) \, o_n(\xi_1, \xi_2, ..., \xi_n) \, \hat{\phi}(\xi_n) \cdots \hat{\phi}(\xi_2) \hat{\phi}(\xi_1)
\end{aligned}$$

Notice the ordering of the field operators in the integral.

7.3 fermions

From previous discussion, we know that no more than 1 fermion can occupy the same one-particle state. Therefore, in state

$$\Phi_F^{N_1,N_2,\cdots}(\xi_1,\xi_2,...,\xi_N) = |N_1,N_2,...\rangle_F = \frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_{p_1}(\xi_1) & \phi_{p_1}(\xi_2) & \cdots & \phi_{p_1}(\xi_N) \\ \phi_{p_2}(\xi_1) & \phi_{p_2}(\xi_2) & \cdots & \phi_{p_2}(\xi_N) \\ \cdots & \cdots & \cdots & \cdots \\ \phi_{p_N}(\xi_1) & \phi_{p_N}(\xi_2) & \cdots & \phi_{p_N}(\xi_N) \end{vmatrix}$$

N_i's can only take values of 0 and 1. For any one-particle state k, $c_k^\dagger c_k^\dagger|\Phi\rangle_F = c_k c_k|\Phi\rangle_F = 0$, i.e.,

$$\left(c_k^\dagger\right)^2 = (c_k)^2 = 0$$

Let us try first to find out the matrix elements for creation and annihilation operators. Evidently,

$$c_j^\dagger|N_1,N_2,...,N_{j-1},1_j,N_{j+1},...\rangle = 0$$

Let us calculate $c_j^\dagger|N_1,N_2,...,N_{j-1},0_j,N_{j+1}...\rangle$ (naively, one would think the obvious answer is $|N_1,N_2,...,N_{j-1},1_j,N_{j+1}.$ but ...):

$$\begin{aligned} c_j^\dagger|N_1,N_2,...,N_{j-1},0_j,N_{j+1},...\rangle &= c_j^\dagger\left[\left(c_1^\dagger\right)^{N_1}\left(c_2^\dagger\right)^{N_2}\cdots\left(c_{j-1}^\dagger\right)^{N_{j-1}}\left(c_{j+1}^\dagger\right)^{N_{j+1}}\cdots\right]|0\rangle \\ &= |1_j,N_1,N_2,...,N_{j-1},N_{j+1},...\rangle \\ &= (-1)^{\sum_{i=1}^{j-1}N_i}|N_1,N_2,...,N_{j-1},1_j,N_{j+1},...\rangle \end{aligned}$$

The factor of $(-1)^{\sum_{i=1}^{j-1}N_i}$ arises because we want to put the particle at j into the right order. So we have the following matrix elements:

$$\langle 0_j|c_j|1_j\rangle = \langle 1_j|c_j^\dagger|0_j\rangle = (-1)^{\sum_{i=1}^{j-1}N_i}$$

where, for brevity, $|N_j\rangle = |N_1,N_2,...,N_{j-1},N_j,N_{j+1},...\rangle$. Obviously, the number operator is still defined as

$$\hat{N}_j = c_j^\dagger c_j$$

as one can check that

$$\hat{N}_j|N_j\rangle = N_j|N_j\rangle$$

Another important operator for fermions is the transmission operator or the particle-hole operator $c_f^\dagger c_i$ (assume $i < f$). The only nonzero matrix element is given by

$$\begin{aligned} \langle 1_f,0_i|c_f^\dagger c_i|1_i,0_f\rangle &= \langle 1_f,0_i|c_f^\dagger|0_i,0_f\rangle\langle 0_f,0_i|c_i|1_i,0_f\rangle \\ &= (-1)^{\sum_{s=1}^{f-1}N_s-N_i}(-1)^{\sum_{z=1}^{i-1}N_z} \\ &= (-1)^{Q_{if}} \end{aligned}$$

where $Q_{if} = \sum_{s=i+1}^{f-1}N_s$ is the number of occupied state between i and f. On the other hand, for the operator $c_i c_f^\dagger$, we have

$$\begin{aligned} \langle 1_f,0_i|c_i c_f^\dagger|1_i,0_f\rangle &= \langle 1_f,0_i|c_i|1_i,1_f\rangle\langle 1_f,1_i|c_f^\dagger|1_i,0_f\rangle \\ &= (-1)^{\sum_{z=1}^{i-1}N_z}(-1)^{\sum_{s=1}^{f-1}N_s-N_i+1} \\ &= (-1)^{Q_{if}+1} \end{aligned}$$

These results give us the **Fermi anticommutation relations**:

$$\{c_i, c_j^\dagger\} = \delta_{ij}, \quad \{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0$$

Despite the different commutation relations obeyed by boson and fermion operators, the operators in the second quantization representation have exactly same form. In particular, the one- and two-particle operators are given by:

$$\begin{aligned} \mathcal{O}_1 &= \sum_{i,f} \langle f|o_1|i\rangle c_f^\dagger c_i \\ \mathcal{O}_2 &= \frac{1}{2} \sum_{m,n,p,q} \langle mn|o_2|pq\rangle c_m^\dagger c_n^\dagger c_p c_q \end{aligned}$$

Remember that the order of the creation/annihilation operators in above expressions are important. Written in terms of fermion field operators, we again have

$$\begin{aligned} \mathcal{O}_n &= \frac{1}{n!} \sum_{j_1 \neq j_2 \neq \cdots \neq j_n} o_n(\xi_{j_1}, \xi_{j_2}, ..., \xi_{j_n}) \\ &= \frac{1}{n!} \int d\xi_1 \int d\xi_2 \cdots \int d\xi_n \, \hat{\psi}^\dagger(\xi_1)\hat{\psi}^\dagger(\xi_2) \cdots \hat{\psi}^\dagger(\xi_n) \, o_n(\xi_1, \xi_2, ..., \xi_n) \, \hat{\psi}(\xi_n) \cdots \hat{\psi}(\xi_2)\hat{\psi}(\xi_1) \end{aligned}$$

where the field operators have a similar definition as in bosonic case, but they obey the equal-time *anticommutation* relations:

$$\{\hat{\psi}(\xi, t), \hat{\psi}^\dagger(\xi', t)\} = \delta(\xi - \xi'), \quad \{\hat{\psi}(\xi, t), \hat{\psi}(\xi', t)\} = \{\hat{\psi}^\dagger(\xi, t), \hat{\psi}^\dagger(\xi', t)\} = 0$$

7.4 Example: expectation value of a two-body operator

Let us calculate the expectation value of a two-body interaction operator $U = (1/2)\sum_{i \neq j} u(\xi_i, \xi_j)$ with a many-body state with definite number of particles $|\Phi\rangle = |N_1, N_2, ...\rangle$.

First we realize that

$$U = \frac{1}{2} \sum_{m,n,p,q} \langle mn|u|pq\rangle a_m^\dagger a_n^\dagger a_p a_q$$

for both bosons and fermions. So we need to evaluate the expectation value of $a_m^\dagger a_n^\dagger a_p a_q$. Since the single-particle states we work with are orthogonal, the expectation value of this operator vanishes unless the two orbitals in which particles are annihilated are identical with those in which they are created. Let us discuss the bosonic and fermionic case separately.

Bosons In this case, we have two possibilities:

Case 1: $p = q$. Then we must have $m = n = p = q$. And its contribution to $\langle U\rangle$ is

$$\frac{1}{2} \sum_m \langle mm|u|mm\rangle N_m(N_m - 1)$$

Case 2: $p \neq q$. There are two more situations. 1) $m = q$ and $n = p$. We have

$$\frac{1}{2} \sum_{m \neq n} \langle mn|u|nm\rangle N_m N_n$$

This is called the **direct** or **Hartree** term. 2) $m = p$ and $n = q$. We have

$$\frac{1}{2}\sum_{m\neq n}\langle mn|u|mn\rangle N_m N_n$$

This is called the **exchange** or **Fock** term.

If the interaction has a contact potential, i.e., $u(\xi_i, \xi_j) \propto \delta(\xi_i - \xi_j)$, then the direct term has the same value as the exchange term since $\langle mn|u|nm\rangle = \langle mn|u|mn\rangle$. So for this case

$$\langle U\rangle = \frac{1}{2}\sum_{m}\langle mm|u|mm\rangle N_m(N_m - 1) + \sum_{m\neq n}\langle mn|u|nm\rangle N_m N_n$$

Fermions Obviously, for fermions, $p \neq q$. The direct term gives

$$\frac{1}{2}\sum_{m\neq n}\langle mn|u|nm\rangle N_m N_n$$

But the requirement of anticommutation requires the exchange term has a minus sign:

$$-\frac{1}{2}\sum_{m\neq n}\langle mn|u|mn\rangle N_m N_n$$

For contact interaction, these two terms cancel each other.

7.5 summary

- You can find discussions on Second Quantization in many books on quantum field theory. My notes follow closely with the discussion on the book *Quantum Theory of Many-Body Systems*, by A. Z. Zagoskin. You may also refer to the following books: *Quantum Theory of Many-Particle Systems* by Fetter and Walecka; *Quantum Many-Particle Systems* by Negele and Orland; *Many-Particle Physics* by G. D. Mahan.

- Quantum N-body wavefunction is symmetrized (boson) or anti-symmetrized (fermion).

- Fock states $|N_1, N_2, ...\rangle$ and the associated creation/annihilation operators ($a_k^\dagger$, a_k) only make sense when you can identify the corresponding single-particle states $\varphi_k(\xi)$, which you specify at the beginning. E.g., N_i is the occupation number at single-particle state k with wavefunction $\varphi_k(\xi)$, $a_k^\dagger$ creates a particle in state k. The Fock state $|N_1, N_2, ...\rangle$ can be created from the vacuum state as (notice the ordering)
$$|N_1, N_2, ...\rangle = \sqrt{\frac{1}{N_1!N_2!\cdots}} \left(a_1^\dagger\right)^{N_1} \left(a_2^\dagger\right)^{N_2} \cdots |0\rangle$$

- Single-particle operator $\hat{\mathcal{O}}_1 = \sum_j o_1(\xi_j)$, and two-particle operator $\hat{\mathcal{O}}_2 = (1/2)\sum_{i\neq j} o_2(\xi_i, \xi_j)$ can be expressed using the creation/annihilation operators as
$$\hat{\mathcal{O}}_1 = \sum_{i,f} \langle f|o_1|i\rangle a_f^\dagger a_i, \quad \hat{\mathcal{O}}_2 = \frac{1}{2} \sum_{m,n,p,q} \langle mn|o_2|pq\rangle a_m^\dagger a_n^\dagger a_p a_q$$

- Field operator $\hat{\phi}^\dagger(\xi) = \sum_k \varphi_k(\xi) a_k^\dagger$ creates a particle at a given point ξ, in other words, it creates a particle with wavefunction $\delta(\xi - \xi')$. In terms of the field operators, an n-particle operator can be expressed as
$$\begin{aligned}\mathcal{O}_n &= \frac{1}{n!} \sum_{j_1\neq j_2\neq\cdots\neq j_n} o_n(\xi_{j_1}, \xi_{j_2}, ..., \xi_{j_n}) \\ &= \frac{1}{n!} \int d\xi_1 \int d\xi_2 \cdots \int d\xi_n\, \hat{\phi}^\dagger(\xi_1)\hat{\phi}^\dagger(\xi_2)\cdots\hat{\phi}^\dagger(\xi_n)\, o_n(\xi_1, \xi_2, ..., \xi_n)\, \hat{\phi}(\xi_n)\cdots\hat{\phi}(\xi_2)\hat{\phi}(\xi_1)\end{aligned}$$
Notice the ordering of the field operators in the integral. The ordering doesn't make any difference for bosons, but they are important for fermions.

- The field operators are time dependent through the time-dependence of the creation/annihilation operators $a_k^\dagger(t)$, $a_k(t)$ (Heisenberg picture) or the time-dependence of the single-particle wavefunctions $\varphi_k(\xi, t)$ (Schrödigner picture). Definite commutation relations exist *only* between field operators taken at the same moment of time:
$$[\hat{\phi}(\xi, t), \hat{\phi}^\dagger(\xi', t)] = \delta(\xi - \xi')), \quad [\hat{\phi}(\xi, t), \hat{\phi}(\xi', t)] = [\hat{\phi}^\dagger(\xi, t), \hat{\phi}^\dagger(\xi', t)] = 0$$

Chapter 8

BEC: mean-field theory

8.1 Hamiltonian

The Hamiltonian of a Bose-Einstein condensate is given by

$$H = H_0 + \frac{1}{2}\sum_{i\neq j} U(\mathbf{r}_i, \mathbf{r}_j)$$

where

$$H_0 = \sum_i \left[\frac{\hat{\mathbf{p}}_i^2}{2m} + V(\mathbf{r}_i)\right]$$

is the single-particle Hamiltonian and $U(\mathbf{r}_i, \mathbf{r}_j)$ represents the two-body interaction potential. We can write the above Hamiltonian in the second quantized form using the boson field operator $\hat{\Psi}$ as:

$$H = \int d\mathbf{r}\, \hat{\Psi}^\dagger(\mathbf{r}) \left[\frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r})\right] \hat{\Psi}(\mathbf{r}) + \frac{1}{2}\int d\mathbf{r} \int d\mathbf{r}'\, \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r}')U(\mathbf{r}, \mathbf{r}')\hat{\Psi}(\mathbf{r}')\hat{\Psi}(\mathbf{r}) \tag{8.1}$$

We assume a contact two-body interaction such that

$$U(\mathbf{r}_i, \mathbf{r}_j) = g\delta(\mathbf{r}_i - \mathbf{r}_j), \quad g = \frac{4\pi\hbar^2 a}{m}$$

so that the Hamiltonian becomes

$$H = \int d\mathbf{r}\, \hat{\Psi}^\dagger(\mathbf{r}) \left[\frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r})\right] \hat{\Psi}(\mathbf{r}) + \frac{g}{2}\int d\mathbf{r}\, \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})\hat{\Psi}(\mathbf{r}) \tag{8.2}$$

Since the *average* number of particles is conserved, then the number operator

$$N = \int d\mathbf{r}\, \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})$$

is a constant of motion. For generalization of variational method of finding the ground state we need to minimize not the Hamiltonian (14.1), but the quantity

$$\begin{aligned} K &= H - \mu\left(\int d\mathbf{r}\, \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r}) - N\right) \\ &= \int d\mathbf{r}\, \hat{\Psi}^\dagger(\mathbf{r}) \left[\frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r}) - \mu\right] \hat{\Psi}(\mathbf{r}) + \frac{g}{2}\int d\mathbf{r}\, \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})\hat{\Psi}(\mathbf{r}) \end{aligned} \tag{8.3}$$

where the Lagrange multiplier μ is also called the **chemical potential** of the condensate. In the second line of K, we have dropped the constant μN. K is also called the *grand canonical Hamiltonian.*

8.2 Hartree mean-field approximation

In the fully condensed state, all bosons occupy the *same* single-particle state $\phi(\mathbf{r})$, i.e., the many-body wave function is given by

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = \Pi_{i=1}^{N} \, \phi(\mathbf{r}_i)$$

In the Hartree mean-field approximation, the single particle wave function $\phi\mathbf{r}$ is identified as the expectation value of the boson field operator

$$\langle \hat{\Psi}(\mathbf{r}) \rangle = \sqrt{N}\phi(\mathbf{r})$$

the factor of $\sqrt{N}$ is included so that $\phi(\mathbf{r})$ is normalized to unity. The mean-field energy functional (divided by total number N) is obtained from Eq. (9.1) by replacing field operators with c-number wave function

$$E(\phi)/N = \int d\mathbf{r} \, \left[\frac{\hbar^2}{2m} |\nabla \phi(\mathbf{r})|^2 + V(\mathbf{r}) |\phi(\mathbf{r})|^2 + \frac{Ng}{2} |\phi(\mathbf{r})|^4 \right]$$

From the discussion above, we need to minimize not the energy functional directly, but the quantity $K(\phi) = E(\phi) - N\mu \int d\mathbf{r} \, |\phi(\mathbf{r})|^2$. Variations of ϕ and ϕ^* yield the equation satisfied by the ground state wave function. From $\delta K(\phi)/\delta\phi^* = 0$, we have

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) + Ng|\phi(\mathbf{r})|^2 \right] \phi(\mathbf{r}) = \mu\phi(\mathbf{r}) \tag{8.4}$$

This equation is called the **Gross-Pitaevskii Equation** (GPE). Note that energy per particle is related to the chemical potential by

$$E/N = \mu - E_{\text{int}}/N$$

where $E_{\text{int}}/N = (Ng/2) \int d\mathbf{r} \, |\phi(\mathbf{r})|^4$ is the interaction energy per particle (in other words, the interaction energy is double counted in μ). The time-dependent version of the GPE is obtained by replacing μ at the right hand side by $i\hbar\partial/\partial t$.

The mean-field GPE neglects quantum fluctuations and correlations. More specifically, the derivation of the equation implicitly makes the factorization ansatz

$$\langle \hat{\Psi}^\dagger \hat{\Psi} \hat{\Psi} \rangle = \langle \hat{\Psi}^\dagger \rangle \langle \hat{\Psi} \rangle \langle \hat{\Psi} \rangle$$

This is equivalent to say that the condensate is in a density-coherent state which is an eigenstate of the annihilation field operator

$$\hat{\Psi} \, |\phi\rangle = \sqrt{N}\phi \, |\phi\rangle$$

8.3 Bogoliubov treatment of fluctuations

To account for the quantum fluctuations above the mean field, we can decompose the field operator as

$$\hat{\Psi} = \langle \hat{\Psi} \rangle + \hat{\psi} = \sqrt{N}\phi + \hat{\psi}$$

where the *operator* $\hat{\psi}$ represents the fluctuations. Note that both $\hat{\Psi}$ and $\hat{\psi}$ obey the boson commutation relations.

We now put this decomposition back into the grand canonical Hamiltonian and keep terms up to second order in $\hat{\psi}$ and $\hat{\psi}^\dagger$. The zeroth order term is nothing but the energy function $E(\phi)$; the first order terms vanishes identically if ϕ satisfies the GPE; the second order terms are:

$$K_2 = \int d\mathbf{r}\, \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + 2Ng|\phi(\mathbf{r})|^2 - \mu \right] \hat{\psi}(\mathbf{r}) + \frac{Ng}{2} \int d\mathbf{r}\, \left[\phi^2(\mathbf{r}) \hat{\psi}^\dagger \hat{\psi}^\dagger + (\phi^*(\mathbf{r}))^2 \hat{\psi}\hat{\psi} \right] \qquad (8.5)$$

from which we can derive the equation of motion for $\hat{\psi}$.

Chapter 9

BEC in a uniform gas

9.1 Hamiltonian

Consider a uniform gas of interacting bosons contained in a box of volume V with periodic boundary condition. The Hamiltonian of the system is

$$H = \sum_i \frac{\hat{\mathbf{p}}_i^2}{2m} + \frac{g}{2}\sum_{i\neq j}\delta(\mathbf{r}_i - \mathbf{r}_j)$$

Obviously it is most convenient to choose plane waves as our basis single-particle orbitals and we label these plane waves by their momentum $\mathbf{k}$:

$$\phi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}}\, e^{i\mathbf{k}\cdot\mathbf{r}}$$

Now we can write the Hamiltonian in second quantized form as:

$$H = \sum_{\mathbf{k},\mathbf{k}'}\langle\mathbf{k}'|(\hat{\mathbf{p}}^2/2m)|\mathbf{k}\rangle a^\dagger_{\mathbf{k}'}a_{\mathbf{k}} + \frac{g}{2}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'}\langle\mathbf{q}\mathbf{q}'|\delta(\mathbf{r}_i-\mathbf{r}_j)|\mathbf{k}\mathbf{k}'\rangle a^\dagger_{\mathbf{q}}a^\dagger_{\mathbf{q}'}a_{\mathbf{k}}a_{\mathbf{k}'}$$

It is easy to see that $\langle\mathbf{k}'|(\hat{\mathbf{p}}^2/2m)|\mathbf{k}\rangle = \epsilon_k^0\delta_{\mathbf{k},\mathbf{k}'}$ with $\epsilon_k^0 = \hbar^2k^2/(2m)$, and

$$\begin{aligned}\langle\mathbf{q}\mathbf{q}'|U(\mathbf{r}_i,\mathbf{r}_j)|\mathbf{k}\mathbf{k}'\rangle &= \frac{g}{V^2}\int d\mathbf{r}_i\int d\mathbf{r}_j\, e^{-i\mathbf{q}\cdot\mathbf{r_i}}e^{-i\mathbf{q}'\cdot\mathbf{r_j}}\,\delta(\mathbf{r}_i-\mathbf{r}_j)\, e^{i\mathbf{k}\cdot\mathbf{r_j}}e^{i\mathbf{k}'\cdot\mathbf{r_i}} \\ &= \frac{g}{V}\delta_{\mathbf{q}+\mathbf{q}',\mathbf{k}+\mathbf{k}'}\end{aligned}$$

Therefore, we can write the second quantized Hamiltonian as

$$H = \sum_{\mathbf{k}}\epsilon_p^0\, a^\dagger_{\mathbf{k}}a_{\mathbf{k}} + \frac{g}{2V}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} a^\dagger_{\mathbf{k}+\mathbf{q}}a^\dagger_{\mathbf{k}'-\mathbf{q}}a_{\mathbf{k}}a_{\mathbf{k}'} \tag{9.1}$$

Alternatively, we can derive the above Hamiltonian from

$$H = \int d\mathbf{r}\,\hat{\Psi}^\dagger(\mathbf{r})\left[\frac{\hat{\mathbf{p}}^2}{2m}+V(\mathbf{r})\right]\hat{\Psi}(\mathbf{r}) + \frac{1}{2}\int d\mathbf{r}\int d\mathbf{r}'\,\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r}')U(\mathbf{r},\mathbf{r}')\hat{\Psi}(\mathbf{r}')\hat{\Psi}(\mathbf{r}) \tag{9.2}$$

and using the definition of the field operator as

$$\hat{\Psi}(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}\, a_{\mathbf{k}}$$

For a condensate, the lowest lying state, here it is the zero-momentum state $\mathbf{k} = 0$, is macroscopically occupied. The condensate wave function is therefore

$$\phi(\mathbf{r}) = \phi_{\mathbf{k}=0}(\mathbf{r}) = \frac{1}{\sqrt{V}}$$

and is spatially uniform. According to the Gross-Pitaevskii equation (with vanishing trapping term), the chemical potential is thus given by

$$\mu = Ng/V = n_0 g$$

where $n = N/V$ is condensate density.

The second order quadratic grand canonical Hamiltonian

$$K_2 = \int d\mathbf{r}\, \hat{\psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + 2Ng|\phi(\mathbf{r})|^2 - \mu \right] \hat{\psi}(\mathbf{r}) + \frac{Ng}{2} \int d\mathbf{r} \left[\phi^2(\mathbf{r}) \hat{\psi}^\dagger \hat{\psi}^\dagger + (\phi^*(\mathbf{r}))^2 \hat{\psi}\hat{\psi} \right] \tag{9.3}$$

therefore takes the form

$$K_2 = \sum_{\mathbf{k}\neq 0} (\epsilon_k^0 + n_0 g)\, a_\mathbf{k}^\dagger a_\mathbf{k} + \frac{n_0 g}{2} \sum_{\mathbf{k}\neq 0} (a_\mathbf{k}^\dagger a_{-\mathbf{k}}^\dagger + a_\mathbf{k}\, a_{-\mathbf{k}}) \tag{9.4}$$

where we have used

$$\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}\neq 0} e^{i\mathbf{k}\cdot\mathbf{r}} a_\mathbf{k}$$

The first term in Hamiltonian (9.4) is the energy of N_0 particles in the condensate. The second term describes the independent excitations with energy $\epsilon_k^0 + 2n_0 g$, in which ϵ_k^0 is the free energy of the excitation with momentum $\mathbf{k}$ and $2n_0 g$ is the Hartree-Fock mean field energy produced by interactions with condensate atoms. One half of this interaction comes from the direct term where a particle $\mathbf{k}$ is scattered off the condensate; the other half of this interaction comes from the exchange term where the particle $\mathbf{k}$ is scattered into the condensate, while a condensate atom is simultaneously scattered into $\mathbf{k}$. For contact interaction, the direct (Hartree) energy is equal to the exchange (Fock) energy. The last term in the Hamiltonian represents pair process in which two condensate atoms are scattered into $\pm\mathbf{k}$ and vice versa.

9.2 Bogoliubov transformation

Hamiltonian (9.4) is not diagonalized. So we need to find a transformation that transforms ($a_\mathbf{k}$'s) into some other boson operators ($b_\mathbf{k}$'s) such that

$$K_2 = \sum_\mathbf{k} \epsilon_k b_\mathbf{k}^\dagger b_\mathbf{k} + \Delta$$

where Δ is some c-number constant.

Observation: K_2 mixes only $a_\mathbf{k}$ with $a_{-\mathbf{k}}^\dagger$. This suggests the following transformation:

$$b_\mathbf{k} = u_k a_\mathbf{k} + v_k^* a_{-\mathbf{k}}^\dagger, \quad b_\mathbf{k}^\dagger = u_k^* a_\mathbf{k}^\dagger + v_k a_{-\mathbf{k}} \tag{9.5}$$

From the symmetry of the system, the coefficients u and v shouldn't depend on the direction of $\mathbf{k}$, that's why we use u_k and v_k, instead of $u_\mathbf{k}$ and $v_\mathbf{k}$. And now we need to find out the expressions of these coefficients.

Now we require that $b_{\mathbf{k}}$'s also obey boson commutation relations. Since

$$[b_{\mathbf{k}}, b^\dagger_{\mathbf{k}'}] = \delta_{\mathbf{k},\mathbf{k}'} \left[|u_k|^2 - |v_k|^2\right]$$

we have

$$|u_k|^2 - |v_k|^2 = 1 \tag{9.6}$$

We can also check that the transformation automatically satisfies $[b^\dagger_{\mathbf{k}}, b^\dagger_{\mathbf{k}'}] = [b_{\mathbf{k}}, b_{\mathbf{k}'}] = 0$.

It is also instructive to write down the reverse transformation:

$$a_{\mathbf{k}} = u^*_k b_{\mathbf{k}} - v^*_k b^\dagger_{-\mathbf{k}}, \quad a^\dagger_{\mathbf{k}} = u_k b^\dagger_{\mathbf{k}} - v_k b_{-\mathbf{k}} \tag{9.7}$$

Using this transformation, we can calculate

$$\begin{aligned}
K_2 &= \sum_{\mathbf{k}} \epsilon_k b^\dagger_{\mathbf{k}} b_{\mathbf{k}} + \Delta \\
&= \sum_{\mathbf{k}} \epsilon_k (a^*_k a^\dagger_{\mathbf{k}} + v_k a_{-\mathbf{k}})(u_k a_{\mathbf{k}} + v^*_k a^\dagger_{-\mathbf{k}}) + \Delta \\
&= \sum_{\mathbf{k}} \epsilon_k \left[(|u_k|^2 + |v_k|^2) a^\dagger_{\mathbf{k}} a_{\mathbf{k}} + u^*_k v^*_k a^\dagger_{\mathbf{k}} a^\dagger_{-\mathbf{k}} + u_k v_k a_{\mathbf{k}} a_{-\mathbf{k}} + |v_k|^2\right] + \Delta
\end{aligned}$$

Equating this with (9.4), we have

$$\Delta = -\sum_{\mathbf{k}} \epsilon_k |v_k|^2$$

and

$$\begin{aligned}
\epsilon_k(|u_k|^2 + |v_k|^2) &= \epsilon^0_k + n_0 g \\
\epsilon_k u_k v_k &= \epsilon_k u^*_k v^*_k = n_0 g/2
\end{aligned}$$

This set of equations have real solutions. Using Eq. (9.6), we have

$$\begin{aligned}
\epsilon^2_k &= \epsilon^2_k (u^2_k - v^2_k)^2 \\
&= \epsilon^2_k \left[(u^2_k + v^2_k)^2 - 4u^2_k v^2_k\right] \\
&= (\epsilon^0_k + n_0 g)^2 - (n_0 g)^2 \\
&= \epsilon^0_k(\epsilon^0_k + 2n_0 g)
\end{aligned}$$

Therefore we obtain the Bogoliubov excitation spectrum as

$$\epsilon_k = \sqrt{\epsilon^0_k(\epsilon^0_k + 2n_0 g)}$$

And the coefficients u_k and v_k are given by

$$u_k = \sqrt{\frac{1}{2}\left(\frac{\epsilon^0_k + n_0 g}{\epsilon_k} + 1\right)}, \quad v_k = \sqrt{\frac{1}{2}\left(\frac{\epsilon^0_k + n_0 g}{\epsilon_k} - 1\right)}$$

9.3 Discussion

We have now succeeded in diagonalize the second quantized Hamiltonian for a uniform interacting bosons. We see that the diagonalized Hamiltonian looks like a summation of that for an ensemble of non-interacting particles. These non-interacting particles are annihilated and created by operators $b_{\mathbf{k}}$ and $b_{\mathbf{k}}^{\dagger}$, respectively. From the Bogoliubov transformation, we know that $b_{\mathbf{k}}$ does not really annihilate a particle unless the coefficient $v_k = 0$. On the other hand, $b_{\mathbf{k}}$ behaves every way like an annihilation operator. So we call the particle annihilated by $b_{\mathbf{k}}$ is a **quasiparticle** or **elementary excitation**. The basic idea of the many-body approach is that instead of following a large number of interacting real particles, we should try to get away with considering a relatively small number of non-interacting (or weakly-interacting) quasiparticles.

- For a non-interacting system, i.e., $g = 0$, we see that $u_k = 1$, $v_k = 0$. Hence the quasiparticle corresponds to the real one, which is rather intuitive.
- For attractive interaction, i.e., $g < 0$, we see that ϵ_k becomes imaginary at long wavelength when $\epsilon_k^0 < 2n_0|g|$. This signals a dynamical instability of the system.
- For repulsive interaction, ϵ_k is always positive. In the long wavelength limit, i.e., when $\epsilon_k^0 \ll 2n_0 g$, we have
$$\epsilon_k \approx c_s \hbar k$$
Hence the quasiparticle energy becomes linear to its momentum (such excitations are called *phonons*), and
$$c_s = \sqrt{n_0 g/m}$$
is called the *Bogoliubov sound velocity*. In the short wavelength limit, when $\epsilon_k^0 \gg 2n_0 g$, we have $\epsilon_k \approx \epsilon_k^0 + n_0 g$ and $v_k \approx 0$, i.e., the quasiparticles become real ones (free particles).
- Each phonon excitation of a repulsive condensate involves an ensemble of atoms moving with opposite momenta. This is confirmed in the experiment [Vogels *et al.*, PRL **88**, 060402 (2002)].

9.4 Depletion of the condensate

For a fully condensed system, i.e., a zero-temperature “pure” condensate, there is no excitation. So the state, denoted by $|G\rangle$, must correspond to the **quasiparticle vacuum state**:

$$b_{\mathbf{k}} |G\rangle = 0$$

But are there excited *real* particles?

For this purpose, let us calculate the number density for the excited atoms

$$n_{\text{ex}} = \frac{N_{\mathbf{ex}}}{V} = \frac{\sum_{\mathbf{k}\neq 0} \langle a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} \rangle}{V}$$

with the expectation value calculated with respect to state $|G\rangle$. Using the inverse transformation (9.7), we have

$$\langle G|a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}|G\rangle = \langle G|(u_k b_{\mathbf{k}}^{\dagger} - v_k b_{-\mathbf{k}})(a_{\mathbf{k}} = u_k^* b_{\mathbf{k}} - v_k^* b_{-\mathbf{k}}^{\dagger})|G\rangle = |v_k|^2$$

Therefore,

$$n_{\text{ex}} = \frac{\sum_{\mathbf{k}\neq 0}|v_k|^2}{V} = \frac{1}{(2\pi)^3}\int d\mathbf{k}|v_k|^2 = \frac{1}{3\pi^2}\left(\frac{mc_s}{\hbar}\right)^3$$

which can also be written as (using $g = 4\pi\hbar^2 a/m$):

$$\frac{n_{\text{ex}}}{n_0} = \frac{8}{3\sqrt{\pi}}\sqrt{na^3}$$

Here we encounter an important parameter na^3. The decomposition of boson field operators into a mean-field part and small fluctuations won't work unless the excitation above the mean field is small, which means our theory is only valid under the condition

$$na^3 \ll 1$$

When this is satisfied, we can call our system *weakly-interacting.*

This calculation also shows that a "pure" condensate is not really pure as long as there is interactions between atoms. The nonvanishing excitation density n_{ex} at zero-temperature is a result of **quantum depletion** induced by interactions. At finite temperatures, besides this quantum depletion, there is also thermal depletion resulted from quasiparticle excitations. In the framework of Bogoliubov treatment, the quasiparticles form a non-interacting ideal Bose gas, so there numbers obey Bose statistics, i.e.,

$$\langle b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}\rangle = \frac{1}{e^{\epsilon_k/(k_B T)} - 1}$$

9.5 Healing of condensate wave function

Consider the condensate is confined in a box with volume V. The boundary of the box represents an infinite potential. Far away from the wall, the condensate is uniform and the discussions above apply. Obviously, the wave function of the condensate must vanish at the wall. So in a region near the wall, the density of the condensate drops from its bulk value n_0 to zero. Let us find out the wave function near the wall.

The equation we need to solve is (consider 1D only, and the wall is located at $x = 0$)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + Ng|\psi(x)|^2\psi(x) = \mu\psi(x)$$

and the boundary conditions are

$$\psi(0) = 0, \quad \psi(\infty) = 1/\sqrt{V}$$

The presence of the wall won't change the chemical potential significantly, we can still use $\mu = Ng/V$. And we rewrite the nonlinear Schrödinger equation as

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2mNg}{\hbar^2}\left[\frac{1}{V} - |\psi(x)|^2\right]\psi(x)$$

This equation can be solved analytically and the solution satisfying the boundary conditions above is

$$\psi(x) = \frac{1}{\sqrt{V}} \tanh\left(\frac{x}{\sqrt{2}\xi}\right)$$

where

$$\xi = \sqrt{\frac{\hbar^2}{2mn_0 g}} = \frac{1}{\sqrt{8\pi n_0 a}}$$

is the **healing length** or **coherence length** which is sometimes called. Therefore, the presence of the wall suppress the condensate density, but the density recovers or "heals" to its bulk value over a length scale $\sim \xi$.

The healing length can also be understood as follows: The shape of the condensate wave function results from the competition between the kinetic energy and the nonlinear interaction energy. For a wave function varies spatially over a length scale ξ, the associating kinetic energy is $\sim \hbar^2/(2m\xi^2)$. The mean-field interaction energy is $n_0 g$. So the healing length is defined as when these two energies are equal.

The healing length sets the length scale over which the bulk density recovers in the presence of a localized perturbation.

Chapter 10

Static properties of trapped BEC

10.1 Gross-Pitaevskii Equation

We have learned that the ground state function satisfies the GPE:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + Ng|\phi(\mathbf{r})|^2\right]\phi(\mathbf{r}) = \mu\phi(\mathbf{r}) \tag{10.1}$$

where $V(\mathbf{r})$ represents the external trapping potential. Usually it is in the form of a harmonic potential, and the most common ones uses in experiments have cylindrical symmetry.

For vanishing interaction, $g \to 0$, the condensate ground state is just the ground state of the trapping potential. But generally, the GPE has to be solved numerically to obtain the exact solution. Approximate solution, however, can be obtained using, for example, variational method. When the interaction dominates ($g > 0$), we can use the Thomas-Fermi approximation to obtain the ground state wave function.

10.2 Thomas-Fermi Approximation

Repulsive interaction between atoms tends to spread out the wave function, this has the effect of decreasing kinetic energy. We can see this using the variational method.

Let the trapping potential have the form

$$V(x, y, z) = \frac{1}{2}m(\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2)$$

For a non-interacting system, the ground state is given by a Gaussian with width $a_i = \sqrt{\hbar/(m\omega_i)}$ along i-direction. So we adopt the following as our trial wave function:

$$\phi(x, y, z) = \frac{1}{\pi^{3/4}(b_1 b_2 b_3)^{1/2}} e^{-x^2/(2b_1^2) - y^2/(2b_2^2) - z^2/(2b_3^2)} \tag{10.2}$$

with b_i's being the variational parameters. The energy functional per particle is

$$e(\phi) = E(\phi)/N = \int d\mathbf{r}\, \left[\frac{\hbar^2}{2m}|\nabla\phi(\mathbf{r})|^2 + V(\mathbf{r})|\phi(\mathbf{r})|^2 + \frac{Ng}{2}|\phi(\mathbf{r})|^4\right]$$

Putting in the trial wave function, we have

$$\begin{aligned} e(b_1, b_2, b_3) &= e_{\text{kin}} + e_{\text{trap}} + e_{\text{int}} \\ e_{\text{kin}} &= \frac{1}{4} \sum_{i=x,y,z} \hbar\omega_i \frac{1}{x_i^2} \\ e_{\text{trap}} &= \frac{1}{4} \sum_{i=x,y,z} \hbar\omega_i x_i^2 \\ e_{\text{int}} &= \frac{Ng}{2(2\pi)^{3/2} b_1 b_2 b_3} \end{aligned}$$

with $x_i = b_i/a_i$. Minimizing $E(b_1, b_2, b_3)$ with respect to b_i yields three coupled equations:

$$\hbar\omega_i(x_i^2 - 1/x_i^2) - \frac{Ng}{(2\pi)^{3/2}\bar{a}^3} \frac{1}{x_1 x_2 x_3} = 0$$

where we have introduced $\bar{a} = \sqrt{\hbar/(m\bar{\omega})}$ and $\bar{\omega} = (\omega_1\omega_2\omega_3)^{1/3}$ is the geometric mean of the trapping frequency.

Under the condition that $x_i \gg 1$, we can neglect $1/x_i^2$ terms in the above equations. This makes the equations analytically solvable with solutions

$$x_i = \left(\frac{2}{\pi}\right)^{1/10} \left(\frac{Na}{\bar{a}}\right)^{1/5} \left(\frac{\bar{\omega}}{\omega_i}\right)^{1/2}$$

So the condition $x_i \gg 1$ can be satisfied as long as Na is sufficiently large. And the various energies scale as

$$e_{\text{kin}} \sim (Na)^{-2/5}, \quad e_{\text{trap}} \sim (Na)^{2/5}, \quad e_{\text{int}} \sim (Na)^{2/5}$$

So the kinetic energy can be neglected when Na becomes large.

If we neglect the kinetic energy term from the GPE, the equation becomes an algebraic one

$$\left[V(\mathbf{r}) + Ng|\phi(\mathbf{r})|^2\right] \phi(\mathbf{r}) = \mu\phi(\mathbf{r})$$

and can be solved by

$$n(\mathbf{r}) = |\phi(\mathbf{r})|^2 = \frac{\mu - V(\mathbf{r})}{Ng}$$

in the region where the right hand side is positive and $n(\mathbf{r}) = 0$ outside this region. The boundary of the cloud is given by

$$V(\mathbf{r}) = \mu$$

For the harmonic potential given above, the radius of the cloud is therefore:

$$R_i = \sqrt{\frac{2\mu}{m\omega_i^2}}, \quad i = 1, 2, 3$$

The value of μ is set by the normalization $\int d\mathbf{r} n(\mathbf{r}) = 1$ which yields:

$$\mu = \frac{15^{2/5}}{2} \left(\frac{Na}{\bar{a}}\right)^{2/5} \hbar\bar{\omega}$$

Since $\mu = \partial E/\partial N = \partial(Ne)/\partial N$, we have

$$\frac{E}{N} = \frac{5}{7}\mu$$

Remark: under the Thomas-Fermi limit, the density profile is completely determined by the trapping potential. For a axial-symmetric harmonic trap, the density has an inverted parabolic profile and the same aspect ratio as the trap. By contrast, for a non-interaction system, the density has a Gaussian shape and the aspect ratio is the square root of that for the trap.

10.3 Virial theorem for GPE

Let $\phi(\mathbf{r})$ be the ground state solution of the GPE. Define wave function

$$\phi_\lambda(\mathbf{r}) = \lambda^{3/2}\,\phi(\lambda\mathbf{r})$$

(The factor $\lambda^{3/2}$ is necessary so that $\phi_\lambda(\mathbf{r})$ is also normalized bo unity, i.e., $\int d\mathbf{r}|\phi_\lambda(\mathbf{r})|^2 = 1$.) So the ground state wave function corresponds to $\phi_{\lambda=1}(\mathbf{r})$.

The energies associated with $\phi_\lambda(\mathbf{r})$ are

$$\begin{aligned} E_{\rm kin}(\lambda)/N &= -\frac{\hbar^2}{2m}\langle\phi_\lambda|\nabla^2|\phi_\lambda\rangle = -\frac{\hbar^2}{2m}\lambda^3\int d\mathbf{r}\,\phi^*(\lambda\mathbf{r})\nabla^2\phi(\lambda\mathbf{r}) = \lambda^2 E_{\rm kin}/N \\ E_{\rm trap}(\lambda)/N &= \frac{1}{2}m\omega^2\lambda^3\int d\mathbf{r}\,\phi^*(\lambda\mathbf{r})r^2\phi(\lambda\mathbf{r}) = \frac{1}{\lambda^2}E_{\rm trap}/N \\ E_{\rm int}(\lambda)/N &= = Ng\lambda^6\int d\mathbf{r}\,|\phi(\lambda\mathbf{r})|^4 = \lambda^3 E_{\rm int}/N \end{aligned}$$

where $E_{\rm kin}$, $E_{\rm trap}$ and $E_{\rm int}$ are energies associated with the ground state.

Since the ground state corresponds to $\lambda = 1$, we must have

$$\left.\frac{d}{d\lambda}E(\lambda)\right|_{\lambda=1} = 0$$

where $E(\lambda) = E_{\rm kin}(\lambda) + E_{\rm trap}(\lambda) + E_{\rm int}(\lambda)$. This yields

$$2E_{\rm kin} - 2E_{\rm trap} + 3E_{\rm int} = 0$$

For a gas in the Thomas-Fermi limit, $E_{\rm kin}$ is negligible. So we have

$$\frac{E_{\rm int}}{N} = \frac{2}{7}\mu, \quad \frac{E_{\rm trap}}{N} = \frac{3}{7}\mu$$

In a time of flight experiment, the trap is turned off, the cloud expands. Then the interaction energy is converted into kinetic energy. The release energy per particle is then just $2\mu/7$.

10.4 Bogoliubov Equations

The condensate wave function satisfies the time-dependent GPE:

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + g|\Psi(\mathbf{r},t)|^2\right]\Psi(\mathbf{r},t) \tag{10.3}$$

Just as in the uniform case, we can calculate the excitation spectrum of a trapped condensate using a Bogoliubov procedure: decompose the condensate wave function into the dominant mean-field part (which is nothing but the ground state wave function) plus small fluctuations:

$$\Psi(\mathbf{r},t) = e^{-i\mu t/\hbar}\sqrt{N}\phi(\mathbf{r}) + \psi(\mathbf{r},t)$$

where the ground state wave function $\phi(\mathbf{r})$ satisfies the time-independent GPE (10.1).

Putting the above decomposition into (11.1), the linearized equation reads (only the first order terms in ψ are kept):

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + 2Ng|\phi(\mathbf{r})|^2\right]\psi(\mathbf{r},t) + e^{-2i\mu t/\hbar}\,\phi^2(\mathbf{r})\psi^*(\mathbf{r},t) \tag{10.4}$$

The excitation frequencies of the condensate are just the normal modes of ψ. To calculate the mode frequencies, we want to find solutions of the form

$$\psi(\mathbf{r},t) = e^{-i\mu t/\hbar}\left[u(\mathbf{r})e^{-i\omega t} - v^*(\mathbf{r})e^{i\omega t}\right]$$

The reason we need both positive and negative components is that in Eq. (10.4), ψ is coupled to ψ^*. Putting the above equation in to Eq. (10.4), we obtain a set of two coupled equations for u and v:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + 2Ng|\phi(\mathbf{r})|^2 - \mu\right]u_i(\mathbf{r}) - Ng\phi^2(\mathbf{r})v_i(\mathbf{r}) = \hbar\omega_i\,u_i(\mathbf{r}) \tag{10.5}$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + 2Ng|\phi(\mathbf{r})|^2 - \mu\right]v_i(\mathbf{r}) - Ng[\phi^*(\mathbf{r})]^2u_i(\mathbf{r}) = -\hbar\omega_i\,v_i(\mathbf{r}) \tag{10.6}$$

where the index i labels different modes. These two equations are called the Bogoliubov Equations.

Now we want to derive certain properties of u_i and v_i. Multiplying both sides of (10.5) by u_k^*, we have

$$u_k^*\mathcal{L}u_i - Ng\phi^2u_k^*v_i = \hbar\omega_iu_iu_k^* \tag{10.7}$$

where

$$\mathcal{L} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + 2Ng|\phi(\mathbf{r})|^2 - \mu$$

is a Hermitian operator. Exchanging the indices i and k in (10.7), we have

$$u_i^*\mathcal{L}u_k - Ng\phi^2u_i^*v_k = \hbar\omega_ku_ku_i^* \tag{10.8}$$

The phase conjugate of (10.8) reads

$$u_i\mathcal{L}u_k^* - Ng(\phi^*)^2u_iv_k^* = \hbar\omega_ku_k^*u_i \tag{10.9}$$

Subtracting (10.9) from (10.7) then integrating both sides of the resultant equation yields:

$$\hbar(\omega_i-\omega_k)\int d\mathbf{r}\,u_k^*u_i = Ng\int d\mathbf{r}\,\left[(\phi^*)^2u_iv_k^* - \phi^2u_k^*v_i\right] \tag{10.10}$$

where we have used

$$\int d\mathbf{r}\,u_k^*\mathcal{L}u_i = \int d\mathbf{r}\,u_i\mathcal{L}u_k^*$$

a property of the Hermitian operator (alternatively, this can be easily approved using integral by parts).

Multiplying both sides of (10.6) by v_k^* and following a similar procedure, we have

$$\hbar(\omega_i-\omega_k)\int d\mathbf{r}\,v_k^*v_i = Ng\int d\mathbf{r}\,\left[(\phi^*)^2u_iv_k^* - \phi^2u_k^*v_i\right] \tag{10.11}$$

As we see that the right hand sides of (10.10) and (10.11) are identical, so we have

$$\hbar(\omega_i-\omega_k)\int d\mathbf{r}\,(u_k^*u_i - v_k^*v_i)$$

which shows that u_i and v_i obey the following orthonormal condition:

$$\int d\mathbf{r}\,(u_k^* u_i - v_k^* v_i) = \delta_{ik}$$

Multiplying Eq. (10.5), (10.6) by v_k and u_k, respectively, following the same procedure, we have

$$\int d\mathbf{r}\,(u_i v_k - u_k v_i) = 0$$

Remark: We have assumed in the above derivation that the excitation frequencies ω_i are real. If ω_i becomes complex with finite imaginary part, then the system is dynamically unstable. For these modes, the mode functions satisfy

$$\int d\mathbf{r}\,(u_i^* u_i - v_i^* v_i) = 0$$

10.5 attractive condensate

The Thomas-Fermi approximation is valid only for repulsive interaction. For attractive interaction, i.e., $g < 0$, things are completely different. Due to the attraction, the condensate tends to shrink in size. In a homogeneous system, an attractive condensate is unstable against collapse. This also shows in the existence of imaginary excitation modes we encountered earlier. For a trapped condensate, a metastable state can be achieved as long as the attractive interaction (as measured by $|Ng|$) is not sufficiently strong, such that its effect can be balanced by the kinetic energy. For large $|Ng|$, the kinetic energy is not able to hold the attraction, so the condensate will collapse. This means there exists a critical value of $|Ng|$, below which an attractive condensate exists in a trap. We want to find out what this critical value is.

We will achieve this using the variational method. For simplicity, let us consider an isotropic harmonic potential:

$$V(r) = \frac{1}{2} m\omega_0^2 r^2$$

The harmonic oscillator length is given by $a_0 = \sqrt{\hbar/(m\omega_0)}$. The trial wave function has the same form as in (10.2), but now with $b_1 = b_2 = b_3 = b$. The total energy is given by

$$E(x) = \frac{3}{4}\hbar\omega_0 \left(\frac{1}{x^2} + x^2\right) + \frac{Ng}{2(2\pi)^{3/2} a_o^3}\frac{1}{x^3}$$

where $x = b/a_0$ and the three terms at the right hand side correspond to kinetic, trapping and interaction energy, respectively.

It is obvious that $E(x)$ is not bound below since $E(x) \to -\infty$ as $x \to 0$. But it might happen that a local minimum exists at a certain x_0 which is finite, i.e., $x_0 > 0$. The condition for this to happen is

$$\left.\frac{\partial E(x)}{\partial x}\right|_{x=x_0} = 0, \quad \left.\frac{\partial^2 E(x)}{\partial x^2}\right|_{x=x_0} > 0$$

which yields

$$f(x_0) = x_0^5 - x_0 + \beta = 0 \tag{10.12}$$

$$x_0^5 + 3x_0 - 4\beta > 0 \tag{10.13}$$

where

$$\beta = -\frac{Ng}{2(2\pi)^{3/2}a_o^3\hbar\omega_0} > 0$$

$f(x)$ has a single minimum which occurs at $x_{\text{min}} = (1/5)^{1/4}$ and the minimum value is $f_{\text{min}} = \beta - 4/5^{5/4}$. In order for function $f(x)$ has a root at positive x, f_{min} must be negative, which yields

$$\beta < \frac{4}{5^{5/4}} \tag{10.14}$$

When this is satisfied, there must exist a root $x_0 > x_{\text{min}}$ for $f(x_0) = 0$, and the $f(x)$ is an increasing function at $x = x_0$, hence the inequality (10.13) is automatically satisfied at that point. Therefore we obtain the condition when an attractive condensate exists in a harmonic trap. Condition (10.14) can be rewritten as

$$\frac{N|a|}{a_0} < \frac{2\sqrt{2\pi}}{5^{5/4}} \approx 0.67$$

Chapter 11

Hydrodynamic approach and self-similar solutions

The dynamical equations of a weakly-interacting condensate generally have to be solved numerically. But under certain situations, (approximate) analytical solutions can be found. One example is certain excitation modes under Thomas-Fermi limit, using a hydrodynamic approach. Another example is the so-called self-similar solution where the spatial density of the condensate can be characterized by three scling factors which allow a classical interpretation of the dynamics.

11.1 Hydrodynamic equations

The hydrodynamic equations are completely equivalent to the ordinary (nonlinear) Schrödinger equations. But under certain situations, the hydrodynamic equations may be easier to solve, and/or give a more intuitive physical picture.

Once again, let us start with the time-dependent GPE:

$$i\hbar \frac{\partial \Psi(\mathbf{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + Ng|\Psi(\mathbf{r},t)|^2 \right] \Psi(\mathbf{r},t) \tag{11.1}$$

Writing Ψ in terms of its amplitude f and phase ϕ (both of these quantities are real):

$$\Psi = f e^{i\phi} \tag{11.2}$$

The density and velocity field associated with the wave function Ψ is defined as

$$n = N|\Psi|^2, \quad \mathbf{v} = \frac{N\hbar}{2mni}\left(\Psi^* \nabla \Psi - \Psi \nabla \Psi^*\right)$$

which can be related to f and ϕ as

$$n = Nf^2, \quad \mathbf{v} = \frac{\hbar}{m}\nabla\phi$$

Provided that the condensate phase ϕ is not singular, we have

$$\nabla \times \mathbf{v} = \frac{\hbar}{m}\nabla \times \nabla\phi = 0$$

which means that condensate is *irrotational.*

Putting (11.2) into the GPE, and separating the real and imaginary parts, we obtain two equations, called the continuity and Euler equation, respectively,

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0 \tag{11.3}$$

$$m\frac{\partial \mathbf{v}}{\partial t} = -\nabla \left(\tilde{\mu} + \frac{1}{2}mv^2 \right) \tag{11.4}$$

where

$$\tilde{\mu} = V + ng - \frac{\hbar^2}{2m\sqrt{n}} \nabla^2 \sqrt{n} \tag{11.5}$$

Eq. (11.3) is the continuity equation for particle density. The last term at the right hand side of (11.5) is the so-called *quantum pressure* term. It arises from the kinetic energy term in the GPE.

For a condensate in ground state, the phase is a constant, so we have

$$n = n_0, \quad \mathbf{v} = \mathbf{v}_0 = 0$$

If the system is perturbed slightly, i.e.,

$$n = n_0 + \delta n, \quad \mathbf{v} = \mathbf{v}_0 + \delta \mathbf{v} = \delta \mathbf{v}$$

We can linearize Eqs. (11.3) and (11.4) by treating δn and $\delta \mathbf{v}$ as small quantities. The linearized equations are given by:

$$\frac{\partial}{\partial t}\delta n = -\nabla \cdot (n_0 \delta \mathbf{v}) \tag{11.6}$$

$$m\frac{\partial \delta \mathbf{v}}{\partial t} = -\nabla \delta \tilde{\mu} \tag{11.7}$$

where

$$\delta \tilde{\mu} = \delta n\, g + \frac{\hbar^2}{4m\sqrt{n_0}} \left(\frac{\delta n}{n_0} \nabla^2 \sqrt{n_0} - \nabla^2 \frac{\delta n}{\sqrt{n_0}} \right)$$

Combining (11.6) and (11.7) we have

$$m\frac{\partial^2}{\partial t^2}\delta n = \nabla \cdot (n_0 \nabla \delta \tilde{\mu}) \tag{11.8}$$

11.2 Uniform case

For a uniform condensate, n_0 is spatial independent. Looking for travelling wave solutions $\delta n \sim \exp(i\mathbf{k}\cdot\mathbf{r} - i\omega_k t)$, we have

$$\delta \tilde{\mu} = \left(g + \frac{\hbar^2 k^2}{4mn_0} \right) \delta n$$

then Eq. (11.8) becomes

$$m\omega_k^2 \delta n = \left(n_0 g k^2 + \frac{\hbar^2 k^4}{4m} \right) \delta n$$

which gives rise to the Bogoliubov spectrum

$$\hbar\omega_k = \sqrt{\epsilon_k^0(\epsilon_k^0 + 2n_0 g)}$$

with $\epsilon_k^0 = \hbar^2 k^2/(2m)$.

11.3 Trapped case under Thomas-Fermi limit

Under the Thomas-Fermi limit, the kinetic or quantum pressure term is neglected. Hence

$$\delta\tilde{\mu} = g\delta n$$

and

$$m\frac{\partial^2}{\partial t^2}\delta n = g\nabla\cdot(n_0\nabla\delta n)$$

To find the excitation frequency, we look for solutions with time dependence $\delta n \propto e^{-i\omega t}$, then

$$-\omega^2\delta n = \frac{g}{m}(\nabla n_0\cdot\nabla\delta n + n_0\nabla^2\delta n) \tag{11.9}$$

The density under the Thomas-Fermi limit is given by

$$n_0 = [\mu - V(\mathbf{r})]/g$$

therefore, we have

$$m\omega^2\delta n = \nabla V\cdot\nabla\delta n - (\mu - V)\nabla^2\delta n \tag{11.10}$$

11.3.1 spherical trap

For a isotropic harmonic trap

$$V(\mathbf{r}) = \frac{1}{2}m\omega_0^2 r^2$$

Working in spherical coordinate system (r, θ, φ), we have

$$\omega^2\delta n = \omega_0^2 r\frac{\partial}{\partial r}\delta n - \frac{1}{2}\omega_0^2(R^2 - r^2)\nabla^2\delta n \tag{11.11}$$

where R is the Thomas-Fermi radius of the condensate which is given by

$$\mu = \frac{1}{2}m\omega_0^2 R^2$$

Due to the symmetry, Eq. (11.11) has solutions with a form

$$\delta n = D(r)Y_{lm}(\theta, \varphi)$$

and the radial funciton $D(r)$ can be solved using hypergeometric functions. And the excitation frequencies are given by

$$\omega = \omega_0\sqrt{l + 3n + 2nl + 2n^2}$$

where $n, l = 0, 1, 2, 3, ...$ This should be compared to the excitation frequencies of a non-interacting system

$$\omega = \omega_0(2n + l)$$

The $n = 0$ modes are the surface modes since they don't have radial nodes. Their spectrum is given by $\omega = \sqrt{l}\omega_0$. For $l = 1$, we have the *dipole modes* where the condensate's center of mass oscillates in the trap as a whole, hence the interactions do not play a role, and $\omega = \omega_0$.

The monopole or *breathing mode* is given by $n = 1$ and $l = 0$ which has frequency $\sqrt{5}\omega_0$. This mode is spherically symmetric ($l = 0$) and the radial velocity has the same sign everywhere.

11.3.2 cylindrical trap

In a cylindrical trap, things become a little more complicated. Now the third component of the angular momentum, m, is still a good quantum number, and the mode frequencies in general depends on m also.

11.4 Self-similar behavior

Suppose we have a time-dependent harmonic trapping potential

$$V(\mathbf{r},t) = \frac{1}{2}m\sum_{j=1}^{3}\omega_j^2(t)r_j^2 \tag{11.12}$$

with $r_{1,2,3} = x, y, z$. At $t = 0$, the condensate is in its ground state whose wave function satisfies the GPE

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},0) + Ng|\phi(\mathbf{r})|^2\right]\phi(\mathbf{r}) = \mu\phi(\mathbf{r})$$

At $t = 0$, we start to modulate the trapping potential. The condensate wave function from there on obey the time-dependent GPE

$$i\hbar\frac{\partial}{\partial t}\phi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r},t) + Ng|\phi(\mathbf{r},t)|^2\right]\phi(\mathbf{r},t)$$

To cast the problem into a classical from, the condensate can be treated as a classical gas in which each particle moves in an effective potential

$$V_{\text{eff}}(\mathbf{r},t) = V(\mathbf{r},t) + g\rho(\mathbf{r},t)$$

where $\rho(\mathbf{r},t) = N|\phi(\mathbf{r},t)|^2$ is the condensate density. The force exerted on the condensate is then

$$F(\mathbf{r},t) = -\nabla V_{\text{eff}}(\mathbf{r},t)$$

At $t = 0$, the condensate is in equilibrium and we assume the Thomas-Fermi limit is reached, thus

$$\rho(\mathbf{r},0) = \frac{\mu - V(\mathbf{r},0)}{g}, \quad F(\mathbf{r},0) = 0$$

For $t > 0$, the exact solution for the classical model can be obtained for the class of potentials (11.12): In this case, the gas merely experiences a dilatation, any infinitesimally small fraction of the expanding cloud mocing along a trajectory

$$R_j(t) = \lambda_j(t)R_j(0) \tag{11.13}$$

from which we obtain the spatial density as

$$\rho(\mathbf{r},t) = \frac{1}{\lambda_1(t)\lambda_2(t)\lambda_3(t)}\,\rho(\{r_j/\lambda_j(t)\},0)$$

From Newton's law $m\ddot{R}_j(t) = F_j(\mathbf{R}(t),t)$, we have

$$m\ddot{\lambda}_j(t)R_j(0) = -\left.\partial_{r_j}V(\mathbf{r},t)\right|_{\mathbf{R}(t)} + \frac{1}{\lambda_1\lambda_2\lambda_3}\left.\partial_{r_j}V(\{r_j/\lambda_j(t)\},0)\right|_{\mathbf{R}(t)} \tag{11.14}$$

where we have used

$$g\nabla\rho(\{r_j/\lambda_j(t)\},0) = -\nabla V(\{r_j/\lambda_j(t)\},0)$$

Using potential (11.12), we have

$$\begin{aligned} \partial_{r_j} V(\mathbf{r},t)\big|_{\mathbf{R}(t)} &= m\omega_j^2(t)R_j(t) = m\omega_j^2(t)\lambda_j(t)R_j(0) \\ \partial_{r_j} V(\{r_j/\lambda_j(t)\},0)\big|_{\mathbf{R}(t)} &= \frac{m\omega_j^2(0)}{\lambda_j^2(t)}R_j(t) = \frac{m\omega_j^2(0)}{\lambda_j(t)}R_j(0) \end{aligned}$$

Therefore, we obtain equations of motion for the scaling parameters λ_j as

$$\ddot{\lambda}_j = \frac{\omega_j^2(0)}{\lambda_j\lambda_1\lambda_2\lambda_3} - \omega_j^2(t)\lambda_j \tag{11.15}$$

The initial conditions for the λ_j are

$$\lambda_j(0) = 1, \quad \dot{\lambda}_j(0) = 0 \tag{11.16}$$

Below, let us apply this theory to two specific examples.

11.4.1 free expansion

Consider the situation of free expansion: at $t = 0$, the trap is turned off, i.e., $\omega_j(t > 0) = 0$. Let us consider an axial symmetric trap:

$$\omega_1(0) = \omega_2(0) = \omega_\perp, \quad \omega_3(0) = \omega_z = \epsilon\omega_\perp$$

In this case, the condensate remains axially symmetric:

$$\lambda_1(t) = \lambda_2(t) = \lambda_\perp(t), \quad \lambda_3(t) = \lambda_z(t)$$

According to (11.15), we have

$$\frac{d^2}{d\tau^2}\lambda_\perp = \frac{1}{\lambda_\perp^3\lambda_z}, \quad \frac{d^2}{d\tau^2}\lambda_z = \frac{\epsilon^2}{\lambda_\perp^2\lambda_z^2} \tag{11.17}$$

where $\tau = \omega_\perp t$. If initially the condensate has a cigar shape, i.e., $\epsilon \ll 1$, to the zeroth order in ϵ, we have

$$\lambda_z(\tau) = 1, \quad \lambda_\perp(\tau) = \sqrt{1+\tau^2}$$

This means that to zeroth order in ϵ, the condensate expands along the radial direction, but the width in z remains the same. Eventually a cigar-shaped condensate becomes pancake-shaped. If we go beyond the zeroth order, generally we have to solve Eqs. (11.17) numerically. The condensate will also expand along z-direction. But still the condensate aspect ratio will cross 1. By contrast, due to the anisotropic momentum distribution, the aspect ratio of a free-expanding cloud of thermal atoms will approach 1, but never cross it.

11.4.2 breathing oscillation

Consider a spatially isotropic condensate, i.e.,

$$\omega_j(0) = \omega_0, \quad \lambda_j(t) = \lambda(t)$$

Consider we disturb the trap (changing trapping frequency) briefly, but then return back to the original trap, i.e., $\omega(t > T) = \omega_0$. The condensate will then *breathe*. The scaling parameter satisfies:

$$\ddot{\lambda} = \frac{\omega_0^2}{\lambda^4} - \omega_0^2\lambda \tag{11.18}$$

If we regard λ as a spatial coordinate, then Eq. (11.18) describes a particle with mass m moving in a potential

$$V(\lambda) = \frac{1}{2} m\omega_0^2 \lambda^2 + \frac{m}{3}\frac{\omega_0^2}{\lambda^3} \tag{11.19}$$

which has a minimum at $\lambda_0 = 1$. For small oscillations, we can expand λ around this minimum, i.e., $\lambda = 1+\epsilon$. Then keeping terms up to second order in ϵ, we have

$$\lambda^2 = 1 + 2\epsilon + \epsilon^2, \quad \lambda^{-3} = 1 - 3\epsilon + 6\epsilon^2$$

And

$$V(\lambda) = \frac{5}{6} m\omega_0^2 + \frac{1}{2} m(5\omega_0^2)\epsilon^2$$

So the particle is like moving in a harmonic potential with trapping frequency $\omega = \sqrt{5}\omega_0$, in agreement with the hydrodynamic result.

Chapter 12

Quantum Vortices

Quantum vortices is an important concept for superfluid. The special properties of quantum vortices are a consequence of their motions being constrained by the fact that the velocity of the condensate is proportional to the gradient of the phase of the wave function.

12.1 potential flow and quantized circulation

We have seen that the velocity of the condensate is directly related to the phase of the condensate wave function $fe^{i\phi}$:

$$\mathbf{v} = \frac{\hbar}{m}\nabla\phi$$

Thus, as long as the phase ϕ is not singular, the condensate is irrotational, i.e.,

$$\nabla \times \mathbf{v} = 0$$

Since the wave function is single-valued, the change of the phase $\Delta\phi$ around any closed contour must be a multiple of 2π, i.e.,

$$\Delta\phi = \oint \nabla\phi \cdot d\mathbf{l} = 2\pi\ell$$

where ℓ is an integer and is called the **winding number**. Thus the **circulation** Γ around the same contour is given by

$$\Gamma = \oint \mathbf{v} \cdot d\mathbf{l} = \frac{\hbar}{m}2\pi\ell = \ell\frac{h}{m}$$

12.2 a single vortex in a uniform condensate

An example: consider purely azimuthal flow in a trap invariant under rotation about the z-axis. The single-valuedness of the condensate wave function requires that the wave function varies as $e^{i\ell\varphi}$ [we use cylindrical coordinates: (z, ρ, φ)]. Then the velocity is along φ-direction with a magnitude

$$v_\varphi = \ell\frac{\hbar}{m\rho}$$

The circulation is thus $\ell\hbar/m$ if the contour encloses the axis, and zero otherwise.

Let us take this simple example a step further. We write the wave function as

$$\psi(\mathbf{r}) = f(\rho, z)e^{i\ell\varphi}$$

the mean-field energy functional is then

$$E = \int d\mathbf{r}\left\{\frac{\hbar^2}{2m}\left[\left(\frac{\partial f}{\partial\rho}\right)^2 + \left(\frac{\partial f}{\partial z}\right)^2\right] + \frac{\hbar^2}{2m}\ell^2\frac{f^2}{\rho^2} + V(\rho, z)f^2 + \frac{1}{2}Ngf^4\right\}$$

from which we can derive the GPE satisfied by f as

$$-\frac{\hbar^2}{2m}\left[\frac{1}{\rho}\frac{d}{d\rho}\left(\rho\frac{df}{d\rho}\right) + \frac{d^2f}{dz^2}\right] + \frac{\hbar^2}{2m\rho^2}\ell^2 f + V(\rho, z)f^2 + Ngf^3 = \mu f$$

It therefore seems that the only effect of the circulation is the addition of the $1/\rho^2$ term, which is called the *centrifugal* barrier term.

For a uniform condensate, we take $V(\rho, z) = 0$. The ground state of the condensate must be z-independent. Away from the circulation axis (or vortex core) $\rho = 0$, the centrifugal is unimportant. Hence f takes its bulk value $f = f_0$. Near the region of the core, the centrifugal term is balanced by the kinetic energy term. The solution regular on the axis varies as $\rho^{|\ell|}$. The crossover between the two regions occurs at the length scale determined by the healing length $\xi = \hbar/\sqrt{2mn_0g}$ where $n_0 = Nf_0^2$ is the bulk density of the condensate.

Now consider the case $\ell = 1$. Suppose the condensate is confined radially in a cylinder with radius R ($R \gg \xi$). Then the energy per unit length (along z) of the vortex is

$$\epsilon = N\int_0^R 2\pi\rho d\rho\left[\frac{\hbar^2}{2m}\left(\frac{df}{d\rho}\right)^2 + \frac{\hbar^2}{2m}\frac{f^2}{\rho^2} + \frac{1}{2}Ngf^4\right]$$

We want to compare this with the energy per unit length of a uniform condensate, ϵ_0, for the same number of particles per unit length, which is given by

$$\epsilon_0 = \frac{1}{2}g\frac{\nu^2}{\pi R^2}$$

where $\nu = N\int_0^R 2\pi\rho d\rho\, f^2$ is the number of particles per unit length. The difference between these two, $\epsilon_{\mathrm{v}} = \epsilon - \epsilon_0$ is therefore the excitation energy per unit length associated with a single vortex. Numerical results give

$$\epsilon_{\mathrm{v}} = \pi n_0\frac{\hbar^2}{m}\ln\left(1.464\frac{R}{\xi}\right)$$

This result can also be derived in the following. The wave function of the condensate with a vortex can be thought of homogeneous everywhere (with a value of $\sqrt{n_0/N}$) except for the core region which is given by $\rho \le \xi$. Therefore the kinetic energy associated with the vortex is

$$\epsilon_{\mathrm{v}} = \frac{1}{2}mn_0\int_\xi^R 2\pi\rho d\rho\, v^2$$

with $v = \hbar/(m\rho)$, we have

$$\epsilon_{\mathrm{v}} = \pi n_0\frac{\hbar^2}{m}\ln\left(\frac{R}{\xi}\right)$$

which agrees with the numerical results with logarithmic accuracy.

Generalize to a vortex with arbitrary winding number ℓ, the core size becomes $|\ell|\xi$ and we have $\epsilon_{\rm v}(\ell) = \ell^2\epsilon_{\rm v}(1)$. Now let us calculate the interaction energy between two vortices with winding numbers ℓ_1 and ℓ_2, respectively. Suppose the first vortex is located at the origin and the second one at x-axis with $x = d$ ($\xi \ll d \ll R$). The total velocity field is the superposition of the two fields produced by the two vortices individually: $\mathbf{v} = \mathbf{v}_1 + \mathbf{v}_2$, where

$$\mathbf{v}_1 = \ell_1 \frac{\hbar}{m\rho}\hat{\varphi} = \ell_1 \frac{\hbar}{m}\frac{-y\hat{x} + x\hat{y}}{x^2+y^2}, \quad \mathbf{v}_2 = \ell_2 \frac{\hbar}{m}\frac{-y\hat{x} + (x-d)\hat{y}}{(x-d)^2+y^2}$$

The total energy for these two vortices is

$$\epsilon_{\rm v} = \frac{1}{2}mn_0 \int\int dxdy\, |\mathbf{v}_1 + \mathbf{v}_2|^2 = \epsilon_{\rm v}(\ell_1) + \epsilon_{\rm v}(\ell_2) + \epsilon_{\rm int}(\ell_1,\ell_2)$$

where $\epsilon_{\rm int}(\ell_1,\ell_2) = mn_0 \int\int dxdy\, \mathbf{v}_1\cdot\mathbf{v}_2$ can be identified as the interaction energy between the two vortices and it can calculated explicitly if we go back to the polar coordinate:

$$\begin{aligned}
\epsilon_{\rm int}(\ell_1,\ell_2) &= mn_0 \int\int dxdy\, \mathbf{v}_1\cdot\mathbf{v}_2 \\
&= \ell_1\ell_2 n_0 \frac{\hbar^2}{m}\int_0^R \rho d\rho \int_0^{2\pi} d\varphi\, \frac{\rho^2 - d\rho\cos\varphi}{\rho^2(\rho^2 + d^2 - 2d\rho\cos\varphi)} \\
&= \ell_1\ell_2 n_0 \frac{\hbar^2}{m}\int_0^{R/d} dr \int_0^{2\pi} d\varphi\, \frac{r - \cos\varphi}{r^2 - 2r\cos\varphi + 1}, \quad (r = \rho/d)
\end{aligned}$$

Do the angle integral first

$$\int_0^{2\pi} d\varphi\, \frac{r-\cos\varphi}{r^2-2r\cos\varphi+1} = \int_0^{2\pi} d\varphi\, \frac{r}{r^2-2r\cos\varphi+1} - \int_0^{2\pi} d\varphi\, \frac{\cos\varphi}{r^2-2r\cos\varphi+1}$$

Using integral tables, the two integrals are

$$\int_0^{2\pi} d\varphi\, \frac{r}{r^2-2r\cos\varphi+1} = \begin{cases} \frac{2\pi r}{1-r^2}, & (r<1) \\ \frac{2\pi r}{r^2-1}, & (r>1) \end{cases}, \quad \int_0^{2\pi} d\varphi\, \frac{\cos\varphi}{r^2-2r\cos\varphi+1} = \begin{cases} \frac{2\pi r}{1-r^2}, & (r<1) \\ \frac{2\pi}{r(r^2-1)}, & (r>1) \end{cases}$$

Therefore we have

$$\int_0^{2\pi} d\varphi\, \frac{r-\cos\varphi}{r^2-2r\cos\varphi+1} = \begin{cases} 0, & (r<1) \\ \frac{2\pi}{r}, & (r>1) \end{cases}$$

Finally we have

$$\epsilon_{\rm int}(\ell_1,\ell_2) = 2\pi\ell_1\ell_2 n_0 \frac{\hbar^2}{m}\ln\left(\frac{R}{d}\right)$$

Two observations: 1) If the two vortices rotate along the same direction (i.e., ℓ_1 and ℓ_2 have the same sign), then the interaction energy between them is positive, signalling a repulsive interaction; vice versa. 2) Since $\xi \ll d$, we see that the total energy for the two vortices is less than the energy for one vortex with winding number $\ell_1 + \ell_2$ when ℓ_1 and ℓ_2 have the same sign. This means that a multiply-quantized vortex tends to disintegrate into several singly-quantized vortices.

12.3 a vortex in a trap

Consider a axial symmetric harmonic trap, with z-axis being the symmetry axis. There is a vortex whose core is situated along z. Assume we are under the Thomas-Fermi limit.

Consider a 2D problem first, i.e., the z-dimension is infinite. The radius of the condensate is R and the density of the condensate varies radially as $n(\rho) = n(0)(1 - \rho^2/R^2)$ where $n(0)$ is the density at the trap center. The vortex energy can be decomposed into two parts: the first part is the energy out to a radius ρ_1 intermediate between the core size and R (i.e., $\xi \ll \rho_1 \ll R$), and the second part is the rest. The first part can be approximated with the energy calculated for a uniform system since the condensate wave function does not vary significantly for $\rho \ll R$. Then the total energy per unit length is

$$\begin{aligned}
\epsilon_{\rm v} &= \pi n_0 \frac{\hbar^2}{m} \ln\left(1.464\frac{\rho_1}{\xi}\right) + \frac{1}{2}\int_{\rho_1}^{R} 2\pi\rho d\rho\, mn(\rho)v^2(\rho) \\
&= \pi n_0 \frac{\hbar^2}{m}\left[\ln\left(1.464\frac{\rho_1}{\xi}\right) + \int_{\rho_1}^{R}\frac{\rho d\rho}{\rho^2}\left(1 - \frac{\rho^2}{R^2}\right)\right] \\
&\approx \pi n_0 \frac{\hbar^2}{m}\left[\ln\left(1.464\frac{R}{\xi}\right) - \frac{1}{2}\right] = \pi n_0 \frac{\hbar^2}{m}\ln\left(0.888\frac{R}{\xi}\right)
\end{aligned}$$

The total angular momentum per unit length $\mathcal{L}$ is $\hbar$ times the total number of particles per unit length

$$\mathcal{L} = n_0\hbar\int_0^R 2\pi\rho d\rho\left(1 - \frac{\rho^2}{R^2}\right) = \frac{1}{2}n_0\pi R^2\hbar$$

For the 3D case under Thomas-Fermi limit, we just need to integrate the above results along z to obtain the total vortex excitation energy and total angular momentum, using

$$n_0(z) = n_0(1 - z^2/Z^2), \quad R(z) = R(1 - z^2/Z^2)^{1/2}, \quad \xi(z) = \xi[n_0/n_0(z)]^{1/2}$$

Here R and Z are the radial and axial width, respectively, n_0 and ξ are density and healing length at the trap center without vortex. Finally we get

$$\begin{aligned}
E_{\rm v} &= \frac{\pi\hbar^2}{m}\int_{-Z}^{Z} dz\, n_0(z)\ln\left[0.888\frac{R(z)}{\xi(z)}\right] = \frac{4\pi n_0 Z}{3}\frac{\hbar^2}{m}\ln\left(0.671\frac{R}{\xi}\right) && (12.1) \\
L_z &= \hbar N = \hbar\frac{8\pi}{15}n_0 R^2 Z && (12.2)
\end{aligned}$$

I write L_z instead of L, because the angular momentum is along z.

12.4 rotating trap

From Eq. (12.1) we see that it takes energy to create a vortex. So the ground state can not have vortex in it. But this is only true for a non-rotating trap.

Suppose the trap is rotated along z-axis with angular frequency Ω. It will be convenient to work in the rotating frame so that the trapping potential is time-independent. The energy functional E' in the rotating frame is related to that in the lab frame E by

$$E' = E - \langle \mathbf{L} \cdot \mathbf{\Omega} \rangle = E - \Omega L_z$$

Therefore a state with finite L_z and energy E_L (in the lab frame) will be favored over the non-rotating state if the angular frequency of the trap exceeds a critical value given by

$$\Omega_c = \frac{E_L - E_0}{L_z}$$

The numerator is just the vortex excitation energy given by Eq. (12.1) under the Thoma-Fermi limit. Using (12.1) and (12.2) we can calculate the critical frequency as

$$\Omega_c = \frac{5}{2}\frac{\hbar}{mR^2}\ln\left(0.671\frac{R}{\xi}\right)$$

For faster and faster rotation, more and more vortices will be created. These vortices form a triangular Abrikosov lattice.

12.5 vortex lattice in fast rotating trap

Let us consider a 2D case. The condensate is confined in the xy-plane by a harmonic trap $V = m\omega_\perp^2\rho^2/2$, and rotates along the symmetry z-axis with angular momentum Ω. The energy functional E' in the rotating frame is related to that in the lab frame E by

$$E' = E - \langle \Omega L_z \rangle = \int d^2\rho \left[\psi^*(h_\perp - \Omega L_z)\psi + \frac{1}{2}Ng|\psi|^4\right]$$

where

$$h_\perp = -\frac{\mathbf{p}_\perp^2}{2m} + V = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\omega_\perp^2(x^2+y^2)$$

Since $\mathbf{L} = \mathbf{r}\times\mathbf{p}$, we have $L_z = xp_y - yp_x$, therefore

$$H_\perp = h_\perp - \Omega L_z = \frac{\mathbf{P}_\perp^2}{2m} + V_{\text{eff}}(\rho) = \frac{(\mathbf{p} - m\Omega\hat{z}\times\boldsymbol{\rho})^2}{2m} + \frac{1}{2}m(\omega_\perp^2 - \Omega^2)\rho^2 \tag{12.3}$$

Two observations. 1) The rotating frequency Ω cannot exceed the trapping frequency $\omega_\perp$. Otherwise, the trap cannot balance the centrifugal force. 2) If we rewrite $H_\perp$ as $H_\perp = h_\perp - \Omega L_z = H_L + (\omega_\perp - \Omega)L_z$ where

$$H_L = h_\perp - \omega_\perp L_z = \frac{(\mathbf{p}_\perp - m\omega_\perp\hat{z}\times\boldsymbol{\rho})^2}{2m}$$

Recall that the Hamiltonian describing an electron of charge e and mass m moving in the xy-plane under the influence of a magnetic field $\mathbf{B} = B\hat{z}$ with vector potential $\mathbf{A} = \mathbf{B}\times\boldsymbol{\rho}/2$ is given by

$$H_\text{e} = \frac{(\mathbf{p}_\perp - e\mathbf{A})^2}{2m}$$

Therefore if we make the identification

$$\omega_\perp = \frac{eB}{2m}$$

, then the two Hamiltonian are completely equivalent. The eigenstates and eigenvalues of H_e (hence H_L)are well-known. The eigenstates are called Landau levels with wave function

$$h_{n,m}(\boldsymbol{\rho}) = \frac{e^{|u|^2/(2a_\perp^2)}\partial_+^m\partial_-^n e^{-|u|^2/a_\perp^2}}{\sqrt{\pi a_\perp^2 n!m!}}$$

and the associated eigenenergy is

$$E_{n,m} = \hbar\omega_\perp(2n+1)$$

where

$$u = \frac{x+iy}{a_\perp}, \quad a_\perp = \sqrt{\frac{\hbar}{m\omega_\perp}}, \quad \partial_\pm = \frac{a_\perp}{2}(\partial_x \pm i\partial_y)$$

Since $h_{n,m}$ are also eigenstates for L_z with eigenenergy $\hbar(m-n)$, they are also eigenstates for $H_\perp$ with eigenfrequency

$$\omega_{n,m} = n(\omega_\perp + \Omega) + m(\omega_\perp - \Omega) + \omega_\perp$$

In the limit $\Omega \to \omega_\perp$, the states with same n but different m become degenerate. In particular, the lowest Landau level (LLL) with $n = 0$ should be dominantly occupied and we reach the 2D *quantum Hall* regime.

Chapter 13

Spinor BEC

13.1 Two-component BEC

Consider a two-component condensate with collision interactions between them. The energy functional of the system reads $E = E_1 + E_2 + E_{12}$ where

$$\begin{aligned} E_i &= N_i \int d^3r \left[\frac{\hbar^2}{2m_i} |\nabla \psi_i|^2 + V_i |\psi_i|^2 + \frac{N_i g_i}{2} |\psi_i|^4 \right] \\ E_{12} &= N_1 N_2 g_{12} \int d^3r \, |\psi_1|^2 \, |\psi_2|^2 \end{aligned}$$

where $g_i = 4\pi\hbar^2 a_i/m_i$ and $g_{12} = 2\pi\hbar^2 a_{12}/m_r$ with m_r being the reduced mass. Both N_1 and N_2 are conserved independently. And the chemical potentials are in general different for the two components.

13.1.1 miscible and immiscible states

Let us consider a homogeneous system with $g_i > 0$, trapped within volume V. One obvious choice for the ground state is that both components have uniform density distribution spread over the whole volume, the so-called *miscible state*. Hence we have $n_i = N_i/V$. The energy of the miscible state is

$$E_{\text{ho}} = \frac{N_1^2}{2V} g_1 + \frac{N_2^2}{2V} g_2 + \frac{N_1 N_2}{V} g_{12}$$

For sufficiently large and positive g_{12}, the two components want to stay away from each other (i.e., phase-separated). So they may occupy non-overlapping volumes V_1 and $V_2 = V - V_1$, respectively, in the so-called *immiscible state*. Thus we have $n_i = N_i/V_i$ and the energy of the system becomes (there is no inter-species interaction energy)

$$E_{\text{in}} = \frac{N_1^2}{2V_1} g_1 + \frac{N_2^2}{2V_2} g_2 = \frac{N_1^2}{2V_1} g_1 + \frac{N_2^2}{2(V - V_1)} g_2$$

which can be minimized with

$$V_1 = \frac{N_1\sqrt{g_1}}{N_1\sqrt{g_1} + N_2\sqrt{g_2}} V, \quad V_2 = \frac{N_2\sqrt{g_2}}{N_1\sqrt{g_1} + N_2\sqrt{g_2}} V$$

The minimized energy is given by

$$E_{\text{in}} = \frac{N_1^2}{2V} g_1 + \frac{N_2^2}{2V} g_2 + \frac{N_1 N_2}{V} \sqrt{g_1 g_2}$$

Compare $E_{\rm ho}$ and $E_{\rm in}$, we find that the phase-separated system has a lower energy (i.e., $E_{\rm in} < E_{\rm ho}$) when

$$g_{12} > \sqrt{g_1 g_2}$$

With the inclusion of trapping potentials, the above phase separation criterion still serves as a good estimate.

13.1.2 dynamical instability of the miscible state

When the condition $g_{12} > \sqrt{g_1 g_2}$ is satisfied, we know that the miscible state is *energetically unstable*, i.e., it is no longer the lowest energy state. We will now show that under the same condition, the miscible state is also *dynamically unstable*, i.e., it possesses excitation modes with complex excitation frequencies.

The two coupled GPEs are given by

$$\begin{aligned} i\hbar\dot{\psi}_1 &= -\frac{\hbar^2}{2m}\nabla^2\psi_1 + N_1 g_1|\psi_1|^2\psi_1 + N_2 g_{12}|\psi_2|^2\psi_1 && (13.1)\\ i\hbar\dot{\psi}_2 &= -\frac{\hbar^2}{2m}\nabla^2\psi_2 + N_2 g_2|\psi_2|^2\psi_2 + N_1 g_{12}|\psi_1|^2\psi_2 && (13.2)\end{aligned}$$

Decompose the wave functions as

$$\psi_i(\mathbf{r},t) = \left[\frac{1}{\sqrt{V}} + \delta_i(\mathbf{r},t)\right] e^{-i\mu_i t/\hbar}$$

with $\mu_1 = g_1 n_1 + g_{12} n_2$ and $\mu_1 = g_2 n_2 + g_{12} n_1$ being the two chemical potentials for the miscible state.

Putting this decomposition into the GPEs, keeping up to the linear fluctuation terms, we have

$$\begin{aligned} i\hbar\dot{\delta}_1 &= -\frac{\hbar^2}{2m}\nabla^2\delta_1 + g_1 n_1(\delta_1+\delta_1^*) + g_{12}n_2(\delta_2+\delta_2^*)\\ i\hbar\dot{\delta}_2 &= -\frac{\hbar^2}{2m}\nabla^2\delta_2 + g_2 n_2(\delta_2+\delta_2^*) + g_{12}n_1(\delta_1+\delta_1^*)\end{aligned}$$

Seeking solutions with the form

$$\delta_i(\mathbf{r},t) = u_i\, e^{i\mathbf{k}\cdot\mathbf{r}+i\omega t} + v_i^*\, e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t}$$

we have

$$\begin{aligned} -\hbar\omega u_1 &= \epsilon_k^0 u_1 + g_1 n_1(u_1+v_1) + g_{12}n_2(u_2+v_2)\\ \hbar\omega v_1 &= \epsilon_k^0 v_1 + g_1 n_1(u_1+v_1) + g_{12}n_2(u_2+v_2)\\ -\hbar\omega u_2 &= \epsilon_k^0 u_2 + g_2 n_2(u_2+v_2) + g_{12}n_1(u_1+v_1)\\ \hbar\omega v_2 &= \epsilon_k^0 v_2 + g_2 n_2(u_2+v_2) + g_{12}n_1(u_1+v_1)\end{aligned}$$

with $\epsilon_k^0 = \hbar^2k^2/(2m)$. Define the following quantities

$$f_\pm = u_1 \pm v_1, \quad h_\pm = u_2 \pm v_2$$

we have

$$\begin{aligned} -\hbar\omega f_- &= (\epsilon_k^0 + 2g_1 n_1)f_+ + 2g_{12}n_2 h_+\\ -\hbar\omega f_+ &= \epsilon_k^0 f_-\\ -\hbar\omega h_- &= (\epsilon_k^0 + 2g_2 n_2)h_+ + 2g_{12}n_1 f_+\\ -\hbar\omega h_+ &= \epsilon_k^0 h_-\end{aligned}$$

Eliminate f_- and h_-, we have

$$\begin{aligned}\hbar^2\omega^2 f_+ &= \epsilon_k^0(\epsilon_k^0+2g_1n_1)f_+ + 2g_{12}n_2\epsilon_k^0 h_+ \\ \hbar^2\omega^2 h_+ &= \epsilon_k^0(\epsilon_k^0+2g_2n_2)h_+ + 2g_{12}n_1\epsilon_k^0 f_+\end{aligned}$$

The condition for the above equations to have non-trivial solutions is

$$\begin{vmatrix} \hbar^2\omega^2-\epsilon_k^0(\epsilon_k^0+2g_1n_1) & -2g_{12}n_2\epsilon_k^0 \\ -2g_{12}n_1\epsilon_k^0 & \hbar^2\omega^2-\epsilon_k^0(\epsilon_k^0+2g_2n_2)\end{vmatrix} = 0$$

which can be solved as

$$\hbar^2\omega_\pm^2 = \epsilon_k^0(\epsilon_k^0+g_1n_1+g_2n_2) \pm \sqrt{\left(\epsilon_k^0\right)^2(\epsilon_k^0+g_1n_1+g_2n_2)^2 + 4g_{12}^2n_1n_2\left(\epsilon_k^0\right)^2 - \left(\epsilon_k^0\right)^2(\epsilon_k^0+2g_1n_1)(\epsilon_k^0+2g_2n_2)}$$

The argument of the square root is non-negative, hence ω_+^2 is always positive. However, when $g_{12}^2 > g_1g_2$, ω_-^2 becomes negative for long-wavelength excitations, i.e., the miscible state becomes dynamically unstable.

13.2 Spin-1 condensate

In magnetic traps usually only one internal state (weak-field seeking state) can be trapped, therefore the atomic spin degrees of freedom is not available. Such a condensate is called the *scalar condensate*. The JILA group first created a *spinor BEC* in a magnetic trap by trapping two states of ^{87}Rb of different hyperfine levels. The bare energy of these two states are separated by about 7 GHz, hence the two spin components are not free to convert into each other without external couplings (RF field).

Here we want to study a spinor condensate made possible by optical trapping. When a condensate is transferred to an optical dipole trap, all magnetic sublevels experience essentially the same trapping potential. Thus the spin degrees of freedom are fully released. Here we focus on a condensate with hyperfine angular quantum number $f = 1$. The three magnetic sublevels (spins) have spin projection quantum number $m_f = -1$, 0 and +1.

13.2.1 Hamiltonian

Let us first derive the second-quantized Hamiltonian of the system.

The two-body interaction potential is given by

$$U(\mathbf{r}_1,\mathbf{r}_2) = \delta(\mathbf{r}_1,\mathbf{r}_2)\sum_{F=0}^{2} g_F\mathcal{P}_F$$

Here F is the total spin of the two spin-1 particles, hence F can take values 0, 1 and 2.

$$\mathcal{P}_F = \sum_{m_F=-F}^{F} |F,m_F\rangle\langle F,m_F|$$

is the projection operator which projects the two spin-1 atoms into a state with total spin F. $g_F = 4\pi\hbar^2 a_F/m$ is the interaction strength in F-channel. For bosonic atoms, the total wave function has to be symmetrized. Due to the δ contact potential, the spatial wave function is symmetric. Therefore the spin wave function has to be symmetric too. This means only even-F channels contribute and we can thus neglect $F = 1$ spin channel. Hence we have

$$U(\mathbf{r}_1, \mathbf{r}_2) = \delta(\mathbf{r}_1, \mathbf{r}_2)(g_0\mathcal{P}_0 + g_2\mathcal{P}_2)$$

In quantum mechanics, the most usual way to describe the interaction between two spins $\mathbf{f}_1$ and $\mathbf{f}_2$ has a form $\mathbf{f}_1 \cdot \mathbf{f}_2$, which can be written in the form

$$\mathbf{f}_1 \cdot \mathbf{f}_2 = \sum_F \frac{1}{2}[F(F+1) - f_1(f_1+1) - f_2(f_2+1)]\,\mathcal{P}_F$$

Now using $F = 0$, 2 and $f_1 = f_2 = 1$, we have

$$\mathbf{f}_1 \cdot \mathbf{f}_2 = \mathcal{P}_2 - 2\mathcal{P}_0$$

Together with $\mathcal{P}_0 + \mathcal{P}_1 = 1$, we have finally

$$U(\mathbf{r}_1, \mathbf{r}_2) = \delta(\mathbf{r}_1, \mathbf{r}_2)\,(c_0 + c_2\,\mathbf{f}_1 \cdot \mathbf{f}_2)$$

with

$$c_0 = \frac{g_0 + 2g_2}{3}, \quad c_2 = \frac{g_2 - g_0}{3}$$

We can then write the total Hamiltonian as

$$\begin{aligned} H_{\rm sp} &= \int d\mathbf{r}\,\hat{\psi}^\dagger_\alpha(\mathbf{r})\left(-\frac{\hbar^2\nabla^2}{2m} + V\right)\hat{\psi}_\alpha(\mathbf{r}) + \frac{c_0}{2}\int d\mathbf{r}\,\hat{\psi}^\dagger_\alpha(\mathbf{r})\hat{\psi}^\dagger_\beta(\mathbf{r})\hat{\psi}_\alpha(\mathbf{r})\hat{\psi}_\beta(\mathbf{r}) \\ &+\frac{c_2}{2}\int d\mathbf{r}\,\hat{\psi}^\dagger_\alpha(\mathbf{r})\hat{\psi}^\dagger_{\alpha'}(\mathbf{r})\mathbf{f}_{\alpha\beta}\cdot\mathbf{f}_{\alpha'\beta'}\hat{\psi}_\beta(\mathbf{r})\hat{\psi}_{\beta'}(\mathbf{r}) \end{aligned} \tag{13.3}$$

where all the repeated indices are summed over, $\hat{\psi}_\alpha$ represents the field operator for magnetic sublevel $m_f = \alpha$, and $\mathbf{f}_{\alpha\beta}$ is the density matrix of angular momentum operator with $f = 1$. Explicitly, we have (in the basis of $m_f = 1, 0, -1$)

$$f^x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad f^y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad f^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

13.2.2 single mode approximation

For alkali atoms, the values of a_0 and a_2 are very close to each other and both are positive. Hence $|c_2| \ll c_0$. This suggests that in the mean-field treatment, the spatial wave function of the condensate is determined by the first and second term in (14.1). Since these two terms are spin-symmetric, we expect the spatial wave functions are the same for different m_f. So we can invoke the single mode approximaiton (SMA)

$$\hat{\psi}_\alpha(\mathbf{r}) = \phi(\mathbf{r})a_\alpha$$

where the wave function $\phi(\mathbf{r})$ satisfies

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V + c_0N|\phi|^2\right)\phi = \mu\phi$$

Under the SMA, we can write (14.1) as

$$H_{\rm sp} = \mu N - c_0' N(N-1) + c_2'\, a_\alpha^\dagger a_{\alpha'}^\dagger \mathbf{f}_{\alpha\beta}\cdot\mathbf{f}_{\alpha'\beta'} a_\beta a_{\beta'} \tag{13.4}$$

where $N = a_\alpha^\dagger a_\alpha$ and

$$c_F' = \frac{c_F}{2}\int d\mathbf{r}\,|\phi(\mathbf{r})|^4$$

Let us take a look at the last term in (13.4).

$$\begin{aligned} a_\alpha^\dagger a_{\alpha'}^\dagger \mathbf{f}_{\alpha\beta}\cdot\mathbf{f}_{\alpha'\beta'} a_\beta a_{\beta'} &= a_\alpha^\dagger \mathbf{f}_{\alpha\beta}\cdot a_{\alpha'}^\dagger a_\beta \mathbf{f}_{\alpha'\beta'} a_{\beta'} \\ &= a_\alpha^\dagger \mathbf{f}_{\alpha\beta}\cdot (a_\beta a_{\alpha'}^\dagger - \delta_{\alpha'\beta})\mathbf{f}_{\alpha'\beta'} a_{\beta'} \\ &= a_\alpha^\dagger \mathbf{f}_{\alpha\beta} a_\beta \cdot a_{\alpha'}^\dagger \mathbf{f}_{\alpha'\beta'} a_{\beta'} - a_\alpha^\dagger \mathbf{f}_{\alpha\beta}\cdot\mathbf{f}_{\beta\beta'} a_{\beta'} \\ &= \mathbf{L}^2 - 2N \end{aligned}$$

where

$$\mathbf{L} = a_\alpha^\dagger \mathbf{f}_{\alpha\beta} a_\beta$$

is the total many-body angular momentum operator of the system whose components are

$$L_z = a_1^\dagger a_1 - a_{-1}^\dagger a_{-1}, \quad L_- = L_x - iL_y = \sqrt{2}\,(a_0^\dagger a_1 + a_{-1}^\dagger a_0), \quad L_+ = L_x + iL_y = \sqrt{2}\,(a_1^\dagger a_0 + a_0^\dagger a_{-1})$$

which satisfy the commutation relations

$$[L_+, L_-] = 2L_z, \quad [L_z, L_\pm] = \pm L_\pm$$

The total Hamiltonian under the SMA is therefore:

$$H_{\rm sp} = \mu N - c_0' N(N-1) + c_2'(\mathbf{L}^2 - 2N)$$

13.2.3 ground state

In an isolated system, the total particle number operator N is a constant of motion. Hence we can neglect terms proportional to N in the Hamiltonian, since these terms only give the wave function a constant phase. Therefore the Hamiltonian has the following simple form:

$$H = c_2'\mathbf{L}^2$$

It is instructive to write down $\mathbf{L}^2$ in the form:

$$\mathbf{L}^2 = N + (N_1 - N_{-1})^2 + N_0 + 2N_0N_1 + 2N_0N_{-1} + 2a_0^\dagger a_0^\dagger a_1 a_{-1} + 2a_0 a_0 a_1^\dagger a_{-1}^\dagger$$

The first two terms at the r.h.s. are constants of motion, the last two terms represent the spin-exchange interactions, which are the source of all kinds of interesting behaviors (spin mixing, spin entanglement, etc.) of spinor BEC.

The eigenstates and eigenenergies of this Hamiltonian are

$$\mathbf{L}^2|l, m_l\rangle = l(l+1)|l, m_l\rangle, \quad L_z|l, m_l\rangle = m_l|l, m_l\rangle$$

The allowed values of l are $l = 0, 2, 4, ..., N$ if N is even and $l = 1, 3, 5, ..., N$ if N is odd; and the allowed values of m_l are $m_l = 0, \pm 1, \pm 2, ..., \pm l$.

The ground state $|G\rangle$ is completely determined by the sign of c_2' (assume N even):

$$|G\rangle = \begin{cases} |0,0\rangle, & \text{if } c_2' > 0 \\ |N, m_N\rangle, & \text{if } c_2' < 0 \end{cases}$$

The interaction is anti-ferromagnetic for $c_2' > 0$, and ferromagnetic for $c_2' < 0$.

In a classical picture, the ground state of a ferromagnetic spinor condensate is like a spin with maximum length, pointing to any arbitrary direction, which can be fixed by any magnetic field.

The ground state of an antiferromagnetic spinor condensate is a spin singlet state (assume even total number), which can be expanded onto the Fock state basis $|N_1, N_0, N_{-1}\rangle$ as

$$|0,0\rangle = \sum_k c_k \left| \frac{1}{2}(N-2k), 2k, \frac{1}{2}(N-2k) \right\rangle$$

where the coefficients are given by

$$c_k = (-1)^k \sqrt{\frac{(2k-1)!!N!!}{(2k)!!(N+1)!!}}$$

from which we can show that in this state, all three spin states are equally populated with $\langle N_1\rangle = \langle N_0\rangle = \langle N_{-1}\rangle = N/3$. It can also be shown that this state is a *fragmented* state. This is an extremely fragile state: a very week external field will destroy it. The spin Hamiltonian including the effect of a magnetic field along z-direction reads:

$$H = c_2'\mathbf{L}^2 - hL_z$$

with $h = \gamma B$ (γ is the gyromagnetic ratio). Without loss of generality, we take $h > 0$. For antiferromagnetic condensate ($c_2' > 0$), the ground state now becomes $|G\rangle = |\ell_0, \ell_0\rangle$ with $\ell_0 = [h/(2c_2') + 0.5]$.

Chapter 14

Atomic Diffraction

14.1 Elements of linear atom optics

Collimators, lens, mirrors... very simple

14.2 Atomic diffraction

Consider an atomic beam propagating along x-direction with velocity v_x, there is a standing wave laser light along z-direction. Assume that v_x is sufficiently large such that the atom-light interaction does not affect v_x, but changes the atomic velocity along z. So we only need to treat the problem as a 1D system. Further assume the atom is a two-level atom with ground state $|g\rangle$ and excited state $|e\rangle$. The light is detuned from the atomic transition by Δ. The Hamiltonian for the system in the interaction region (in the rotating frame) is

$$H = \frac{p_z^2}{2m} - \hbar\Delta|e\rangle\langle e| + \frac{\hbar\Omega}{2}\cos(kz)(|e\rangle\langle g| + |g\rangle\langle e|) \tag{14.1}$$

The problem can be divided into three regimes according to the relations among three length scales: the width of the atomic beam along z, w_z; the period of the standing laser light, λ; and the width of the interaction region, L.

14.2.1 Raman-Nath Regime

In the Raman-Nath regime, we have $w_z \gg \lambda$ (so the atom experiences the full periodic structure of the light potential) and L is sufficiently small such that during the interaction, the kinetic energy (along z) of the atom does not change very much. Hence we can simply neglected in the Hamiltonian. The Hamiltonian in the rotating frame becomes

$$H = -\hbar\Delta|e\rangle\langle e| + \hbar\Omega\cos(kz)(|e\rangle\langle g| + |g\rangle\langle e|)$$

Express the state vector of the atom in momentum space,

$$|\Psi(p,t)\rangle = \psi_e(p,t)|e\rangle + \psi_g(p,t)|g\rangle$$

Here is p is the momentum along z. We can then derive the equations of motion for the amplitudes ψ_e and ψ_g as

$$\begin{aligned} i\dot{\psi}_e(p,t) &= -\Delta\psi_e(p,t) + \frac{\Omega}{2}[\psi_g(p+\hbar k,t) + \psi_g(p-\hbar k,t)] \\ i\dot{\psi}_g(p,t) &= \frac{\Omega}{2}[\psi_e(p+\hbar k,t) + \psi_e(p-\hbar k,t)] \end{aligned} \tag{14.2}$$

Since the momentum state p is only coupled to states $p \pm \hbar k$, we can do the following expansion:

$$\psi_e(p,t) = \sum_n \psi_e^n(t)\,\delta(p - n\hbar k), \quad \psi_g(p,t) = \sum_n \psi_g^n(t)\,\delta(p - n\hbar k)$$

If initially the atom is in the ground state with momentum $p = 0$, then the initial condition is

$$\psi_e^n(0) = 0, \quad \psi_g^n(0) = \delta_{n0}$$

- *On-resonance case* From Eqs. (14.2), we have $(\Delta = 0)$

  $$i\dot{x}_n = \frac{\Omega}{2}(x_{n-1} + x_{n+1})$$

  where $x_n = \psi_e^n$ for odd n and $x_n = \psi_g^n$ for even n. The solution for the above equation is the nth-order Bessel functions of the the first kind:

  $$x_n = (-i)^n J_n(\alpha)$$

  with $\alpha(t) = \int_0^t dt'\Omega(t')$, and J_n being the Bessel function of the first kind.

- *Far-off-resonance case* In this case, we can adiabatically eliminate the excited state as $\psi_e(p,t) = (\Omega/2\Delta)[\psi_g(p+\hbar k,t) + \psi_g(p-\hbar k,t)]$, then the equation of motion for the ground state amplitude becomes

  $$i\dot{\psi}_g(p,t) = \frac{\Omega^2}{4\Delta}\,[\psi_g(p+2\hbar k,t) + 2\psi_g(p,t) + \psi_g(p-2\hbar k,t)]$$

  The ground state atom changes its momentum in units of $2\hbar k$. Let $\psi_g(p,t) = \sum_m \psi_g^m(t)\delta(p - 2m\hbar k)$ with initial condition $\psi_g^m(0) = \delta_{m0}$, then we have

  $$\psi_g^m(t) = (-1)^m\, e^{i(-\alpha + m\pi/2)}\, J_m(\alpha)$$

  with $\alpha(t) = \int_0^t dt'\Omega^2(t')/(2\Delta)$.

The treatment above neglects the photon recoil and the spontaneous emission, which tend to wash out the diffraction pattern.

14.2.2 Bragg Regime

In the Bragg Regime, we still have $w_z \gg \lambda$. But here L is sufficiently large that the interaction with laser light significantly changes the kinetic energy of the atom, so we can no longer neglect it in the Hamiltonian.

With the kinetic energy term included, the equations of motion becomes

$$\begin{aligned} i\dot{\psi}_e(p,t) &= \frac{p^2}{2m}\psi_e(p,t) + \frac{\Omega}{2}[\psi_g(p+\hbar k,t) + \psi_g(p-\hbar k,t)] - \Delta\psi_e(p,t) \\ i\dot{\psi}_g(p,t) &= \frac{p^2}{2m}\psi_g(p,t) + \frac{\Omega}{2}[\psi_e(p+\hbar k,t) + \psi_e(p-\hbar k,t)] \end{aligned} \tag{14.3}$$

For far-off resonance light, $\hbar\Delta \ll \hbar\Omega, p^2/(2m)$, we can adiabatically eliminate the excited state amplitude using the first of Eqs. (14.3),

$$\psi_e(p,t) = \frac{\Omega}{2\Delta}[\psi_g(p+\hbar k) + \psi_g(p-\hbar k)]$$

Putting this into the second equation, we have

$$i\dot{\psi}_g(p,t) = \left(\frac{p^2}{2m} + \frac{\Omega^2}{2\Delta}\right)\psi_g(p,t) + \frac{\Omega^2}{4\Delta}[\psi_g(p+2\hbar k,t) + \psi_g(p-2\hbar k,t)] \tag{14.4}$$

The above equation shows that momentum conservation requires that an atom with initial momentum p_i is connect to final momentum state $p_f = p_i + 2n\hbar k$ through a $2n$-photon process. The energy difference between these two states are

$$\Delta E = \frac{1}{2m}\left[(p_i + 2n\hbar k)^2 - p_i^2\right]$$

The only two states that satisfy both momentum and energy conservation (phase matching) are

$$p_i = -p_f = -n\hbar k$$

In this case, we can neglect all other off-resonant momenta states and keep only these two resonant states. The resulting coupled equation can be easily solved. Let $p_i = \hbar k$, denote $g_{\pm n}(t) = \psi_g(\pm n\hbar k, t)$, then

$$g_{-n}(t) = \exp[-i(n^2\omega_r t + 2\theta)]\,\cos(\theta), \quad g_{+n}(t) = i\exp[-i(n^2\omega_r t + 2\theta)]\,\sin(\theta)$$

with $\omega_r = \hbar k^2/(2m)$ and $\theta(t) = \int_0^t dt'\Omega^2(t')/(4\Delta)$. Hence the atom oscillates between $n\hbar k$ and $-n\hbar k$.

To resonantly connect an arbitrary p_i to $p_f = p_i + 2n\hbar k$, we have to apply for the energy mismatch ΔE. This can be done by detuning the frequency of the two laser beams that form the standing wave. Suppose the two beams are detuned by $\Delta\omega$. The $2n$-photon process involves absorbing n-photon from one beam and emitting n-photon to the other beam. Each absorption-emission cycle will add an extra energy $\hbar\Delta\omega$ to the atom. Therefore to make the state p_i and p_f resonance with the $2n$-photon process, we need to have

$$n\hbar\Delta\omega = \Delta E \tag{14.5}$$

We can also view this laser detuning from the following perspective: The two beams detuned from each other by Δ will form a *moving* standing wave which moves at the velocity $v = \Delta\omega/(2k)$. In this moving frame, the initial momentum of the atom is shifted to $p_i' = p_i - mv$. When the resonance condition (14.5) is satisfied, $p_i' = -n\hbar k$ which becomes resonant with the final state $p_f' = p_f - mv = n\hbar k$ through a $2n$-photon process.

Bragg diffraction can also be performed on a condensate [J. Stenger *et al.*, PRL **82**, 4569 (1999)]. A Bragg pulse is applied to create excitation with $k > c_s$, so the excitation is free-particle excitation with energy $\epsilon_k^0 + n_0 g$, the second term being the mean-field interaction energy. The signal is plotted as a function of laser detuning, by comparing it with the result of a non-interacting condensate (Bragg pulse is applied after the cloud is released from the trap and the interaction energy has converted to the kinetic energy), one can deduce the value of $n_0 g$. The width of the signal, which is determined by the momentum width of the sample) can also be used to detect the condensation phase transition. For a thermal cloud at temperature T, the momentum width is about $(\Delta p)_{\text{thermal}} \sim \sqrt{2mkT}$, whereas for a condensate, it is given by $(\Delta p)_{\text{BEC}} \sim \hbar/R$ with R being the size of the condensate. For non-interacting condensate confined in harmonic trap, R is about the harmonic oscillator length, hence $(\Delta p)_{\text{BEC}} \sim \sqrt{\hbar m\omega}$. The ratio of the thermal and condensate width is

$$\frac{(\Delta p)_{\text{BEC}}}{(\Delta p)_{\text{thermal}}} = \sqrt{\frac{\hbar\omega}{2kT}}$$

which is about 5% for $\omega = 2\pi \times 100\text{Hz}$ and $T = 1\mu\text{K}$ (typical critical temperature). For a repulsive condensate, the size is larger than the harmonic oscillator length, this ratio is smaller still. Experimentally, it was shown that the Bragg width is indeed inversely proportional to the size of the condensate. This is Heisenberg uncertainty principle at work at a macroscopic level! For this reason, a condensate is truly a macroscopic quantum mechanical object.

14.2.3 Stern-Gerlach Regime

In the Stern-Gerlach regime, $w_z \ll \lambda$, i.e., the atomic beam is localized in z-direction such that the atom sees a local potential rather than the full periodic potential.

Again, we assume the laser light is on-resonant with the atomic transition, i.e., $\Delta = 0$. The eigenstates of the interaction Hamiltonian is the dressed states

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|g\rangle \pm |e\rangle)$$

with associated energy

$$E_\pm = \pm\frac{\hbar\Omega}{2}\cos(kz)$$

If initially the atom is in its ground state $|\psi(0)\rangle = |g\rangle$, which in terms of the dressed states can be decomposed as $|\psi(0)\rangle = (|+\rangle + |-\rangle)/\sqrt{2}$, then the two components will experience opposite forces with equal magnitude: $F_\pm = -\nabla E_\pm = \mp(\hbar\Omega k/2)\sin(kz)$. Hence the atomic wavepacket splits into two spatial components, just as in the original Stern-Gerlach experiment atoms split into several spatial components in an inhomogeneous magnetic field due to different magnetic spin components.

Chapter 15

Four Wave Mixing in BEC

15.1 mixing of matter waves

The wave function of a scalar condensate satisfies the GPE

$$i\hbar\frac{\partial}{\partial t}\phi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r}) + Ng|\phi(\mathbf{r},t)|^2\right]\phi(\mathbf{r},t) \tag{15.1}$$

which has the same form as a Schrödinger equation with a cubic nonlinear term. The same type of nonlinearity appears in many other physical system. In particular, in nonlinear optics, where a light beam going through a Kerr nonlinear medium, the equation governing the propagation of the light has the same mathematical form.

It is well-known, in the context of nonlinear optics, that such nonlinear term gives rise to wave-mixing. Therefore it is rather intuitive to expect same phenomenon also occurs in condensate. In 1999, W. D. Phillips' group at NIST successfully demonstrated four-wave mixing in an atomic condensate [Nature **398**, 218 (1999)]. In that experiment, a condensate is first released from the trap, then optical pulses are applied to Bragg scatter part of the original condensate in momentum state $\mathbf{k}_1 = 0$ into finite momenta states $\mathbf{k}_2 = k(\hat{x}+\hat{y})$ and $\mathbf{k}_3 = 2k\hat{x}$. These three modes initially overlap with each other and interact nonlinearly to produce a fourth mode at momentum $\mathbf{k}_4 = \mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 = k(\hat{x}-\hat{y})$.

The time it takes to create states $\mathbf{k}_2$ and $\mathbf{k}_3$ using the Bragg pulses is very short, and it can thus be taken to be instantaneous. As a result, all different momentum modes have the same spatial distribution. We write the wave function for different momentum states as

$$\psi_i(\mathbf{r},t) = \varphi_i(\mathbf{r},t)\, e^{i(\mathbf{k}_i\cdot\mathbf{r}-\omega_i t)}$$

with $\omega_i = \hbar k_i^2/(2m)$. In the above expression, the envelope function $\varphi_i(\mathbf{r},t)$ is assumed to be slowly varying in space and time on the scales of $1/k_i$ and $1/\omega_i$, respectively, and are normalized as $\int d\mathbf{r}\, \sum_i |\varphi_i(\mathbf{r},t)|^2 = 1$. Different modes are approximately orthogonal to each other. Such *slowly varying envelope approximation* is necessary to restrict the momentum components only to those around the central momentum of each of the wave packets and allows efficient numerical simulations as it separates out explicitly the fast oscillating phase factors representing the central momentum. The total wave function is therefore

$$\phi(\mathbf{r},t) = \sum_{i=1}^{4} \varphi_i(\mathbf{r},t)\, e^{i(\mathbf{k}_i\cdot\mathbf{r}-\omega_i t)}$$

Put this into the GPE ($V = 0$), collecting terms with the same phase factors, eliminating rapidly varying terms and keeping only the phase-matched terms, we finally have

$$i\left(\frac{\partial}{\partial t} + \frac{\hbar\mathbf{k}_i}{m}\cdot\nabla - i\frac{\hbar}{2m}\nabla^2\right)\varphi_i(\mathbf{r},t) = \frac{Ng}{\hbar}\sum_{j,m,n}\delta_{\mathbf{k}_i+\mathbf{k}_j,\mathbf{k}_m+\mathbf{k}_n}\delta_{\omega_i+\omega_j,\omega_m+\omega_n}\varphi_j^*(\mathbf{r},t)\varphi_m(\mathbf{r},t)\varphi_n(\mathbf{r},t), \quad (15.2)$$

The indices take any value from 1 to 4. The two δ-functions ensure momentum and energy conservations, respectively. They are automatically satisfied if $i = j = m = n$, which gives rise to the so-called *self-phase modulation* terms; or if $i = m \neq j = n$ or $i = n \neq j = m$, which gives rise to the *cross-phase modulation* terms. These two types of terms do not generate new modes as they do not involve particle exchange between different modes. The term responsible for four-wave mixing must involve all four different modes. To gain more insight, let us write down the explicit form for $i = 4$, the mode which is created by the nonlinear interaction:

$$i\left(\frac{\partial}{\partial t} + \frac{\hbar\mathbf{k}_4}{m}\cdot\nabla - i\frac{\hbar}{2m}\nabla^2\right)\varphi_4(\mathbf{r},t) = \frac{Ng}{\hbar}\left(|\varphi_4|^2 + 2|\varphi_1|^2 + 2|\varphi_2|^2 + 2|\varphi_3|^2\right)\varphi_1 + 2\frac{Ng}{\hbar}\varphi_2^*\varphi_1\varphi_3$$

The last term at the r.h.s. is the wave-mixing term that generates this mode. In general, Eqs. (15.2) have to be solved numerically.

15.2 mixing between light and matter waves

Nonlinear wave mixing can also occur between light and matter waves. The first demonstration on this was reported by Ketterle's group [PRL **82**, 4569 (1999)]. A cigar-shaped condensate is illuminated by an off-resonant laser beam with wave number k_L propagating perpendicular to its long axis z. After absorbing the photon from the laser beam, the atom gets a recoil momentum along y, the laser propagation direction. Subsequent spontaneous emission gives the atom another momentum kick. Normally the spontaneous emission is isotropic. However it can shown that for a cigar-shape atomic ensemble, spontaneous emission occurs preferentially along the z-axis, the so-called *end-fire* modes. After one such absorption-emission cycle, the atom is now in momentum state $\mathbf{k} = k_L(\hat{y} \pm \hat{z})$. Now we have two light waves (the laser and the spontaneously emitted light) and two matter waves (the original zero-momentum condensate and the recoiled atoms). The two lights waves interfere with each other and form a grating which scatters condensate atoms into the recoil mode; while the two matters waves also form a grating which scatters the light waves. The two gratings thus strengthen each other until the condensate gets sufficiently depleted. Successive atomic momentum side modes are being built up by this process.

Chapter 16

Solitons

16.1 Discovery of the solitary wave and the soliton

The first documented observation of a solitary wave wave was made by a Scottish engineer, John Scott Russel, in 1834, when he saw a rounded smooth heap of water detach itself from a boat and propagate without change of shape or speed for over two miles along the canal (he chased the wave on horseback). After that, he went back and performed some wave-tank experiments. In 1895, Korteweg and de Vries derived a model equation which describes the unidirectional propagation of long waves in shallow water. This equation has become much celebrated and is now known as the KdV equation, and can be written as

$$\frac{\partial h}{\partial t} + h\frac{\partial h}{\partial z} + \frac{\partial^3 h}{\partial z^3} = 0$$

The second and third term describe nonlinearity and dispersion, respectively. KdV found both a periodic and a localized solution to the equation.

In the 1960's, inspired by the Fermi-Pasta-Ulam recursion problem, Zabusky and Kruskal reinvestigated the KdV equation numerically, and found that robust pulse-like waves can propagate in a system modelled by such an equation. These solitary waves, which can pass through each other and preserve their shapes and speed after the collision, are called **solitons**. The soliton solution of the KdV equation is given by

$$h(t,z) = 3v\,\mathrm{sech}^2\frac{\sqrt{v}}{2}(z - vt)$$

16.2 The soliton concept in physics

A **solitary wave**, as discovered by Russel, is a localized wave that propagates along one space direction with undeformed shape.

A **soliton**, as discovered numerically by Zabusky and Kruskal, is a large-amplitude coherent pulse or very stable solitary wave, the exact solution of a wave equation, whose shape and speed are not altered by a collision with other solitary waves.

Thus, to a mathematician the word soliton has a quite specific and ideal connotation in the context of systems with exact analytical solutions (such systems are called *integrable systems*). There are roughly about 100 different types of partial differential equations that support soliton solutions. Physicists, on the other hand, normally use the word soliton in a much loose sense. In the dictionary of a physicist, soliton and solitary wave are usually inter-changeable.

Qualitatively, the solitary wave or soliton can be understood as representing a balance between the effect of dispersion and that of nonlinearity.

16.3 Bright soliton for an attractive condensate

Consider an attractive condensate in a uniform 1D geometry. After rescaling, the GPE reads

$$i\frac{\partial \psi}{\partial t} + \frac{1}{2}\frac{\partial^2 \psi}{\partial z^2} + |\psi|^2\psi = 0 \tag{16.1}$$

16.3.1 modulational instability of a plane wave

The above equation has a solution with constant density:

$$\psi(z,t) = u_0\, e^{iu_0^2 t}$$

where u_0 is a constant. Let's check if this state is stable. To this end we add small perturbation to both amplitude and phase:

$$\psi(z,t) = [u_0 + a(z,t)]e^{iu_0^2 t + i\phi(z,t)}$$

Put this back into the equation and linearized with respect to small variables $a(z,t)$ and $\phi(z,t)$, to obtain the linearized equations as

$$\dot{\phi} - 2u_0 a - \frac{1}{2u_0}a'' = 0, \quad \dot{a} + \frac{1}{2}u_0\phi'' = 0$$

It has the solution with form

$$a(z,t) = a_0 e^{i(kz-\omega t)}, \quad \phi(z,t) = \phi_0 e^{i(kz-\omega t)}$$

Putting this into the equations for a and ϕ, we have

$$\begin{aligned} \left(\frac{k^2}{2u_0} - 2u_0\right)a_0 - i\omega\phi_0 &= 0 \\ i\omega a_0 + \frac{k^2}{2}u_0\phi_0 &= 0 \end{aligned}$$

Nontrivial solutions exist only when

$$\begin{vmatrix} \frac{k^2}{2u_0} - 2u_0 & -i\omega \\ i\omega & \frac{k^2}{2} \end{vmatrix} = 0$$

or

$$\omega^2 = \frac{k^2}{2}\left(\frac{k^2}{2} - 2u_0^2\right)$$

Hence the long wavelength excitations with $k < 2u_0$ possess complex frequencies, and are therefore dynamically unstable. Such instability is called *modulational instability.* Note that the above dispersion relation is nothing but the excitation frequency of a uniform condensate.

16.3.2 localized soliton solution

We want to find the localized stationary solution of the GPE with the form

$$\psi(z,t) = \sqrt{\rho(z)}e^{-i\mu t}$$

Put this into the GPE, we have

$$-\frac{1}{8}\frac{1}{\rho^2}\left(\rho'\right)^2 + \frac{1}{4\rho}\rho'' + \rho + \mu = \frac{1}{8}\frac{d}{d\rho}\left[4\rho^2 + \frac{1}{\rho}\left(\rho'\right)^2\right] + \mu = 0$$

where $\rho' = d\rho/dz$. Integrate over ρ, we have $\left(\rho'\right)^2 = -4\rho^3 - 8\mu\rho^2 + c\rho$, where c is an integral constant.

The condition of localization means that when $z \to \infty$, ρ and its derivatives should all vanish. Take derivative w.r.t. z for the above equation, we have $2\rho'\rho'' = -12\rho^2\rho' - 16\mu\rho\rho' + c\rho'$ or

$$2\rho'' = -12\rho^2 - 16\mu\rho + c$$

The boundary condition at ∞ requires that $c = 0$. Hence we have $\left(\rho'\right)^2 = -4\rho^3 - 8\mu\rho^2$ or

$$\rho' = 2\rho\sqrt{\rho_0 - \rho}$$

with $\rho_0 = -2\mu$, which gives

$$\rho(z) = \rho_0 \operatorname{sech}^2(\sqrt{\rho_0}z)$$

In general, the equation also supports solutions stationary in a moving frame:

$$\psi(z,t) = \eta \operatorname{sech}\left[\eta(z - vt - \theta_0)\right] \exp\left[ivz + \frac{i}{2}(\eta^2 - v^2)t - i\sigma_0\right]$$

The parameter η represents the amplitude and width of the solitary wave, v represents its speed, and θ_0 and σ_0 are two phase constants. It can be shown that these localized solutions are dynamically stable.

16.3.3 discussion

The existence of stable soliton solutions suggests the fate of the uniform system under molulational instability. For an initially uniform system, any localized disturbance will seed the unstable modes. The most unstable one (the one with largest $\mathrm{Im}(\omega)$) occurs at $k_0 = \sqrt{2}u_0$. In real condensate parameters, this is $k_0 = \sqrt{8\pi n_0|a|}$. Thus, one may expect that in vicinity of the disturbance arises the region of oscillations with a wavelength on the order of $\lambda_0 = 2\pi/k_0$ (For a scattering length of -1.4nm, $n_0 = 10^{14}/\mathrm{cm}^3$, the most unstable wavelength is about 3.3μm). Formation of this oscillation region will saturate the instability and a condensate with length L will eventually break into a train of solitons with the number of solitons $\sim L/\lambda_0$.

Indeed, such experiments have been carried out: K. E. Strecker *et al.*, Nature (London) **417**, 150 (2002); L. Khaykovich *et al.*, Science **296**, 1290 (2002). In both experiments, a condensate of ^{7}Li is created with the help of Feshbach resonance such that the scattering length of the condensate is tuned to be positive in the beginning. Then the scattering length is changed to be negative, and out come solitons. The former shows a soliton train, while the latter creates a single soliton.

16.4 Dark soliton for a repulsive condensate

Consider a repulsive condensate in a uniform 1D geometry. After rescaling, the GPE reads

$$i\frac{\partial\psi}{\partial t} + \frac{1}{2}\frac{\partial^2\psi}{\partial z^2} - |\psi|^2\psi = 0 \tag{16.2}$$

We look for a solution such that the density approaches a constant value but its derivatives tend to zero for $|z| \to \infty$.

16.4.1 general solution

The general non-normalized solutions are

$$\psi(z,t) = \left\{ iv - \sqrt{1-v^2}\tanh\left[\sqrt{1-v^2}(z-vt)\right]\right\} e^{-it}$$

where the real parameter v is the velocity of the dark soliton and takes values from 0 to 1. v also determines both the width ($= 1/\sqrt{1-v^2}$) and the "darkness" of the soliton since the minimum density at the center of soliton (occurs at $z = vt$) is v^2. The density approaches the constant 1 far away from the minimum.

- $v = 0$, this is a stationary dark soliton, and the wave function is simplified as $\psi(z,t) = \tanh(z)e^{-it}$. The width of the dark soliton is the healing length (in our units, =1).
- $0 < v < 1$, this is also called the *grey soliton*.
- $v = 1$, in this case, $\psi(z,t) = ie^{-it}$, hence the density is uniform and this is actually the homogeneous ground state of the system. Note that in our units, the Bogoliubov sound velocity is given by $c_s = 1$. So c_s is the maximum speed of the dark soliton.
- The function $\tanh(x)$ changes signs across $x = 0$, hence the phase of the wave function changes across the density minimum. This phase slip is $2\tan^{-1}(\sqrt{1-v^2}/v)$ which is π for $v = 0$. This phase change is continuous for finite v, discontinuous for $v = 0$.

16.4.2 energy of a dark soliton

In our units, the chemical potential is fixed to $\mu = 1$. We need to calculated the free energy $K = E - \mu\int dz\,|\psi|^2 = (1/2)\int dz\,[|\psi'|^2 + |\psi|^4 - 2|\psi|^2]$ which can be found to be

$$K = K_0 + \frac{4}{3}(1-v^2)^{3/2}$$

where $K_0 = -(1/2)\int dz$ is the free energy of the ground state with wave function $\psi = ie^{-it}$.

- The free energy of a dark soliton with $0 \le v < 1$ is higher than that of the ground state, as expected.
- The free energy of a dark soliton decreases as its velocity increases. In this sense, one may say that *dark solitons have negative kinetic energy*!

- The above property suggests the fate of a dark soliton in realistic experiment. The inelastic collisions between the dark soliton and background atoms accelerates the former towards the sound velocity and the dark soliton continuously transforms itself into the ground-state condensate. So dark solitons decay via acceleration. But at sufficiently low temperature, the lifetime of a dark soliton should be quite long such that it can be observed experimentally.

- Experimental observation of dark soliton was report by Burger *et al.* in PRL **83**, 5198 (1999). The dark soliton was created using the phase imprinting method: a far-off-resonant laser light is applied over half of the condensate, which imprints a phase difference $\sim \pi$ between the two halves.