# Homework of Lectures on Cold Atom Physics

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#### 1 Atomic Structure

Exercise 1 Consider 87Rb and 6Li atom in magnetic field B2. The Hamiltonian can be written as

$$\hat{H} = B(\mu_B J_z + \mu_N I_z) + \alpha \mathbf{J} \cdot \mathbf{I}$$

- (1) Solve the full energy spectrum *E* as a function of *B*.
- (2) Analyze how E depends on B for small B and find out linear and quadratic Zeeman shift. For linear Zeeman field, one can also use Wigner-Eckart theorem to determine the coefficient  $g_F$ .
- (3) Analyze the spin structure at large *B*.

This exercise is very important for magnetic trapping[2] and later discussion of spinor condensate.

#### Solution:

<sup>87</sup>Rb and <sup>6</sup>Li are all alkali atoms. Thus they have spin S=1/2 and orbital angular momentum L=0. Thus J=1/2.  $^1$ 

**General discussion.** The limit behaviours when  $B/\alpha \to 0$  or  $\infty$  are easily to guess. We expect that when B is very small, the energy spectrum is determined mainly by the *spin nuclear-spin coupling* term. Choosen the total spin representation, where the Hamiltonian would be almost diagonalized, we see directly that energy levels could be roughly labeled by the total spin quantum number F. To see this,

$$\mathbf{J} \cdot \mathbf{I} = \frac{1}{2} (\mathbf{F}^2 - \mathbf{I}^2 - \mathbf{J}^2)$$

While at the other limit that magnetic field B is quite large compared with coupling term, the first term, named *Zeeman energy*, would dominate.  $I_z$ ,  $J_z$  representations are good for estimate. The total energy is determined mainly by  $B(\mu_B J_z + \mu_N I_z)$  while  $\alpha \mathbf{J} \cdot \mathbf{I}$  could be treat as small perturbation. Energy levels could be approximately labeled by  $m_I$  and  $m_I$  quantum number.

We see this clearly from 1Fig. 1 (a) and 1Fig. 1 (b).

### For <sup>87</sup>Rb, nuclear spin is I = 3/2.

The direct-product space for total spin is thus 8 dimensions. To see this,

$$F = I + I, ..., |I - I| = 2, 1$$

$$\dim F = \dim F_2 \oplus F_1 = 5 + 3 = 8$$

or

$$\dim I_{3/2} \otimes J_{1/2} = (2 \times 3/2 + 1) \times (2 \times 1/2 + 1) = 4 \times 2 = 8$$

Since there are no simultaneous eigenstates for Zeeman-term and spin nuclear-spin coupling term for different magnitude of *B*, we solve the energy spectrum no matter in which representation. An

<sup>&</sup>lt;sup>1</sup>We solve this problem for consider the Hamiltonian as a perturbation to Coulomb potential. It is meaningful only to the ground state (or only some particular energy level) of atom. Thus L = 0 is the only case we consider here. And J = 1/2.

easy way is to choose  $J_z$ ,  $I_z$  representation, where the coupling term could be written as

$$\mathbf{I} \cdot \mathbf{J} = I_z J_z + \frac{1}{2} (I_+ J_- + I_- J_+)$$

with

$$I_{\pm} = I_x \pm iI_y$$
$$I_{+} = I_x \pm iI_y$$

Angular momentum theory shows that [7]

$$J_{\pm}|j,m\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}|j,m\pm 1\rangle$$

which enabled us to write  $I_{\pm}$  and  $J_{\pm}$  in  $I_z$ ,  $J_z$  representation <sup>2 3</sup> , like

$$J_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad J_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$I_{+} = egin{pmatrix} 0 & \sqrt{3} & 0 & 0 \ 0 & 0 & 2 & 0 \ 0 & 0 & 0 & \sqrt{3} \ 0 & 0 & 0 & 0 \end{pmatrix} \qquad I_{-} = egin{pmatrix} 0 & 0 & 0 & 0 \ \sqrt{3} & 0 & 0 & 0 \ 0 & 2 & 0 & 0 \ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$

Total Hamiltonian in the direct product space of  $I_z$  and  $J_z$  thus writes

$$\hat{H} = B(\mu_B J_z + \mu_N I_z) + \alpha \mathbf{J} \cdot \mathbf{I}$$
  
=  $B(\mu_B J_z + \mu_N I_z) + \alpha I_z J_z + \frac{\alpha}{2} (I_+ J_- + I_- J_+)$ 

(take direct product of evolved matrices)

where  $\bar{B} = \frac{\mu_B B}{\alpha \hbar^2}$  is the dimensionless magnitude of magnetic field, and  $\bar{\mu} = \mu_N/\mu_B \sim 10^{-3}$ . And hereinafter, we use hyperfine energy scale  $\epsilon_0 = \alpha \hbar^2$  as unit.

Diagonalize this Hamiltonian matrix gives directly the full energy spectrum. See Fig. 1 (a) .

<sup>&</sup>lt;sup>2</sup>Hereinafter, we take the convention to arrange basekets in terms of  $m_j$ , from large to small. For examply, when I = 3/2, we arrange basekets in this order,  $|3/2\rangle$ ,  $|1/2\rangle$ ,  $|-1/2\rangle$ ,  $|-3/2\rangle$ , to write down our matrix of operators.

<sup>&</sup>lt;sup>3</sup>And we set some constants, like  $\hbar$ , to be 1, whenever conveniently.

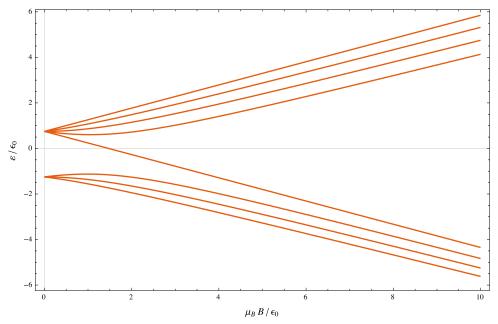


Fig. 1 (a) Full energy spectrum of  ${}^{87}Rb$  in a Zeeman field with different magnetic field. We take  $\epsilon_0 = \alpha \hbar^2$  as unit, which is actually the energy scale of spin nuclear-spin coupling. Two starting point correspond to F = 2 and F = 1, respectively.

### For $^6$ Li, nuclear spin is I = 1.

The direct-product space for total spin is thus 6 dimensions. To see this,

$$F = I + I, ..., |I - I| = 3/2, 1/2$$

$$\dim F = \dim F_{3/2} \oplus F_{1/2} = 4 + 2 = 6$$

or

dim 
$$I_1 \otimes J_{1/2} = (2 \times 1 + 1) \times (2 \times 1/2 + 1) = 3 \times 2 = 6$$

Similarly we solve it in "direct-product" representation. Different is, I=1 and space spanned by nuclear freedom is of dimension 3. Easily to calculate that

$$I_{+} = egin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \qquad I_{-} = egin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

and Hamiltonian matrix turns out to be

Diagonalize this Hamiltonian matrix gives directly the full energy spectrum of <sup>6</sup>Li. See Fig. 1 (b) .

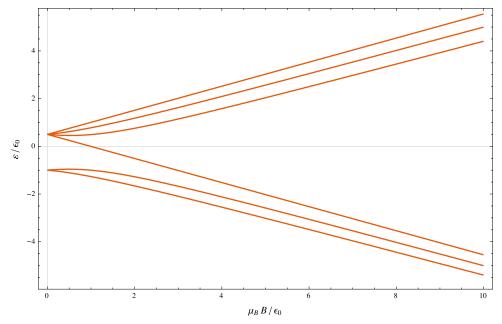


Fig. 1 (b) Full energy spectrum of  $^6Li$  in a Zeeman field with different magnetic field. Two starting point correspond to F = 3/2 and F = 1/2, respectively.

**Physics at small** B. Without loss of generality, we choose  ${}^{87}Rb$  to discuss here. When B is small compared with spin nuclear-spin hyperfine energy, a proper way for analysis is to consider it in *total angular momentum representation* ( $F = I \oplus J$ ). As we can see from Hamiltonian matrix above, (we could always write down a matrix in whatever representation, especially for calculation), the exists of nonzero off-diagonal elements mixes different direct-product state and gives energy shifts. Within each  $m_F$  space, one- or two-dimensional matrix could be diagonalized easily.

 $F=\pm 2$ :  $|3/2,1/2\rangle$  and  $|-3/2,-1/2\rangle$  spaces are both one-dimensional. These two states do not mix with any others. And they are the only two gives *linear Zeeman shift*:

$$E(3/2,1/2) = \frac{3}{4} + (\frac{1}{2} + \frac{3}{2}\bar{\mu})\bar{B}$$
$$E(-3/2,-1/2) = \frac{3}{4} - (\frac{1}{2} + \frac{3}{2}\bar{\mu})\bar{B}$$

These two states correspond to (1,1) and (8,8) element in matrix, and the  $1^{st}$  and  $5^{th}$  energy level (from the topmost) in Fig. 1 (a), respectively.

All other states exhibit *quadratic Zeeman shift* as could be seen from following:  $m_F = 1$ :  $|3/2, -1/2\rangle$  and  $|1/2, 1/2\rangle$ . Hamiltonian in  $m_F = 1$  subspace is

$$\left( \begin{array}{ccc} \bar{B}(-\frac{1}{2}+\frac{3}{2}\bar{\mu})-\frac{3}{4} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \bar{B}(\frac{1}{2}+\frac{1}{2}\bar{\mu})+\frac{1}{4} \end{array} \right) \Longrightarrow E = -\frac{1}{4}+\bar{\mu}\bar{B}\pm\sqrt{\frac{3}{4}+\frac{1}{4}\Big[1+(1+\bar{\mu})\bar{B}\Big]^2}$$

 $m_F = 0$ :  $|-1/2,1/2\rangle$  and  $|1/2,-1/2\rangle$ . Hamiltonian in F = 0 subspace is

$$\left( \begin{array}{cc} \bar{B}(-\frac{1}{2} + \frac{1}{2}\bar{\mu}) - \frac{1}{4} & 1 \\ 1 & \bar{B}(\frac{1}{2} - \frac{1}{2}\bar{\mu}) - \frac{1}{4} \end{array} \right) \Longrightarrow E = -\frac{1}{4} \pm \sqrt{\frac{3}{4} + \frac{1}{4} \left[ (1 - \bar{\mu})\bar{B} \right]^2}$$

 $m_F=-1$  is similar as  $m_F=1$ . Just take  $\bar{B} \to -\bar{B}$  .

When  $\bar{B}$  is sufficiently small,  $\bar{B} \ll 1$ ,  $\sqrt{1 + (\dots \bar{B})^2}$  could be expanded as  $1 + (1/2)(\dots \bar{B})^2$ , quadratic as seen.

We see that to first order in magnetic field, the energy may be written as

$$E(F, m_F) = E(F) + m_F g_F \mu_B B$$

To get  $g_F$ , we make use of the Wigner-Eckart theorem such that

$$\langle F, F_z'|J_z|F, F_z\rangle = \frac{\langle F, F_z'|(\mathbf{J} \cdot \mathbf{F})F_z|F, F_z\rangle}{F(F+1)}$$

$$= \frac{\langle F, F_z'|\frac{1}{2}(\mathbf{F}^2 + \mathbf{J}^2 - \mathbf{I}^2)F_z|F, F_z\rangle}{F(F+1)}$$

$$= \frac{F(F+1) + J(J+1) - I(I+1)}{2F(F+1)} m_F \delta_{m_F', m_F}$$

While

$$g_F = \frac{m_J + \bar{\mu} m_I}{m_F} = \frac{(1 - \bar{\mu}) m_J + \bar{\mu} (m_J + m_I)}{m_F}$$
$$= (1 - \bar{\mu}) \frac{m_J}{m_F} + \bar{\mu}$$

Thus we obatin

$$g_F = (1 - \bar{\mu}) \frac{F(F+1) + J(J+1) - I(I+1)}{2F(F+1)} + \bar{\mu}$$

**Physics at large** B. At large B, atoms polarized, splitting into two major beams with their electronic spin parallel or anti-parallel to Zeeman field. The reason is  $\mu_N \ll \mu_B$ , which is a direct result of  $m_p \gg m_e$ . Thus, mainly the electronic magnetic momentum dominates. Witnin each beams, there would be further splitting, corresponding to different hyperfine energy levels. As we said before, in this strong-field limit, *direct-product representation* ( $I_z \otimes I_z$ ) would be appropriate for discussion.

This exercise refers to [1, 2, 7].

*Exercise* 2 Recently a new atomic species Ho has been cooled by laser cooling. In the future it can be made to quantum degenerate by further evaporative cooling. Please analyze the electronic structure of Ho and find out the total electronic spin (S + L) of ground state of Ho.

#### Solution:

Holmium is the number 67 element in Periodic Table[3, 4]. Its electronic configuration is

$$(1s^22s^22p^63s^23p^63d^{10}4s^24p^64d^{10}5s^25p^6)4f^{11}6s^2$$

Hund's rule states that (i) the lowest energy atomic state is the one that maximizes the sum of the S values for all of the electrons in the open subshell; (ii) as for orbital angular momentum, ground state is the one that maximizes *L* for the case that number of electrons in the valance shell exceeds

half filling.

The 6s shell gives total spin S = 0 and total angular momentum L = 0.

The 4f shell gives total spin S=3/2 while total angular momentum L=6. To see this, I sketch here

Thus the total electronic spin J = S + L of ground state of Ho is

$$^{4}I_{15/2}$$

Here we use the popular atomic label  ${}^{2S+1}L_I$  to denote it.

More words about this. From the sketch above we see clearly the value of  $\hat{S}_z$  and  $\hat{L}_z$ , i.e. quantum number  $m_z$  and  $m_l$ , a rough way of applyiny Hund's rule to decide the ground state of total electronic angular momentum. But how about S and L? When we write  ${}^4I_{15/2}$ , we definitely mean 2S+1=4 and J=15/2, where S and J are quantum numbers for  $S^2$  and  $J^2$ , respectively. But how do we conclude this, just from a roughly sketch about actually the magnetic quantum number?

This is what have ever confused me for a long time during my first study Atomic Physics while not so understanding about Quantum Mechanics. It seems like we just do simply algebraic addition and subtraction: we add the total  $m_z$  to get the S, and add all of the  $m_l$  then obtain the L (=6).

Actaully, the argument above is right not for coincidence. In principle, it could be derived from the most rigorous calculation of angular momentum combination[5], which equals to working out all the CG coefficients. This could be done via one-by-one addition of all the valence electron angular momentum (all the Ls and all the Ss). However, there exists a easier way to see this.

Hund's rule says that, for exceeding half filling cases, lowest energy state tends to maximize angular momentum. From my sketch above we see that, what I draw here is the very configuration that a state get the largest z-component of angular momentum. Could not be larger. But from the theory of angular momentum we know that  $m_J$  can equals only to -J, -J + 1, ..., J - 1, J. Thus J could not exceed the largest value of  $m_J$ . Meanwhile J could not be less than a possible value of  $m_J$ . Thus, for this case, J equals this largest  $m_J$ , and itself arrive at a maximized value. And our primary-school-level algebraic addition works.

By the way, the logic above is L-S coupling. In fact, for atom of large atomic number, we do not know the way of coupling. However, the argument works no matter this.

This exercise refers to [3, 4, 5].

### 2 Atom-Light Interaction

*Exercise* Consider two counter propagating Raman beams. One is along  $\hat{x}$  direction with frequency  $\omega$  and polarization along  $\hat{y}$ , i.e.  $E = E_0 \cos(k_0 x - \omega t) \mathbf{e}_y$ , the other is along  $-\hat{x}$  with frequency

 $\omega + \delta \omega$  and polarization along  $\hat{z}$ , i.e.  $\mathbf{E} = E_0 \cos(-k_0 x - (\omega + \delta \omega)t)\mathbf{e}_z$ . An alkali atom is illuminated in these two lights, and the vector coupling can be written in the form as  $\mathbf{B}_{\text{eff}} \cdot \mathbf{S}$ , where

$$B_{\text{eff}} = B_{\text{eff.0}} + B_{\text{eff.+}} e^{i\delta\omega t} + B_{\text{eff.-}} e^{-i\delta\omega t}$$

Please give the explicit form of  $B_{\text{eff}}$ .

#### Solution:

To make use of the conclusion we obtained in class, I rewrite the electronic vector **E** in complex form.

$$\mathbf{E}_r = E_0 e^{\mathrm{i}(k_0 x - \omega t)} \hat{\mathbf{e}}_y$$

$$\mathbf{E}_l = E_0 e^{\mathrm{i}(-k_0 x - (\omega + \delta \omega)t)} \hat{\mathbf{e}}_y$$

We have already derived the form of the effective Hamiltonian for dipole interaction between electromagnetic field and atom. That is[1]

$$H_{\rm eff} = u_s |\mathbf{E}|^2 + \mathrm{i} u_v (\mathbf{E}^* \times \mathbf{E}) \cdot \mathbf{S}$$

where  $u_s = -(1/12\Delta_e)|\langle l=0|\mathbf{d}|l=1\rangle|^2$  is the scalar polarizability and  $u_v = \alpha\hbar u_s$  is the vector polarizability of an atom. **S** is the atom's spin.

Thus the vector coupling could be written as

$$\mathcal{H}_{\text{eff}} = iu_v(\mathbf{E}^* \times \mathbf{E}) \cdot \mathbf{S}$$

It turns out that

$$\mathbf{E}^* \times \mathbf{E} = E_0^2 (e^{-(\mathrm{i}2k_0x + \delta\omega t)} - e^{(\mathrm{i}2k_0x + \delta\omega t)}) \hat{\mathbf{e}}_x$$

If we write the effective Hamiltonian as

$$\mathcal{H}_{\text{eff}} = \mathbf{B}_{\text{eff}} \cdot \mathbf{S}$$

with

$$B_{\text{eff}} = B_{\text{eff,0}} + B_{\text{eff,+}} e^{i\delta\omega t} + B_{\text{eff,-}} e^{-i\delta\omega t}$$

We see clearly here that

$$B_{\rm eff,0} = 0$$
 ,  $B_{\rm eff,\pm} = \mp i u_v E_0^2 e^{\pm i k_0 x}$ 

Actually we could take the dipole approximation (which is our starting point of this section) to omit the  $k_0x$ .

Physically,  $B_{\text{eff,0}} = 0$  is a direct result of the linear polarization of th propogating light beams (along  $\mathbf{e}_{v}$  and  $\mathbf{e}_{z}$ , see the context of this exercise). We already learned in class that if it is circular

polarized then

$$\mathbf{E}^* \times \mathbf{E} == 2\mathrm{i} E_0^2 \mathbf{e}_z$$

which gives rise to a light-induced Zeeman energy proportional to  $u_s E_0^2 S_z$  [1]. Generally[6],

$$\mathcal{B}_{\text{eff}} = \frac{\mathrm{i} u_v(\tilde{\mathbf{E}}^* \times \tilde{\mathbf{E}})}{\mu_B g_J}$$

and

$$\mathcal{B}_{\text{eff,0}} = \frac{\mathrm{i}u_v}{\mu_B g_J} \Big( \mathbf{E}_{\omega,-}^* \times \mathbf{E}_{\omega,-} + \mathbf{E}_{\omega,+}^* \times \mathbf{E}_{\omega,+} \Big)$$
$$\mathcal{B}_{\text{eff,\pm}} = \frac{\mathrm{i}u_v}{\mu_B g_J} \mathbf{E}_{\omega,\pm}^* \times \mathbf{E}_{\omega,\mp}$$

where  $\omega$ , + and  $\omega$ , - correspond to the  $\omega$  and  $\omega + \delta \omega$  propagating light.

This section refers to [1, 6].

### 3 Interaction between Two Atoms

*Exercise* University of two-body bound states.

Consider two interaction potentials:

- (I) a square well  $V(r) = -U_0$  for  $r < r_0$  and V(r) = 0 for  $r > r_0$ .  $U_0 > 0$ ; and
- (II) a well plus a barrier  $V(r) = -W_0$  for  $r < r_1$ ,  $V(r) = W_1$  for  $r_1 < r < r_2$  and V(r) = 0 for  $r > r_2$ .  $W_0 > 0$ ,  $W_1 > 0$ .

Show the condition when model (I) and model (II) give the same s-wave scattering length  $a_s$ . Further compare the shallow bound state energy of these two models when both of them give same  $a_s \gg r_0, r_1, r_2$ .

#### Solution:

For potential with rotation symmetry, the wave function could be partial-waves expanded as

$$\Psi(\mathbf{r}) = \sum_{l=0}^{+\infty} \frac{\chi_{kl}(r)}{kr} P_l(\cos(\theta))$$

Substituting it into<sup>4</sup>

$$\left[ -\frac{\hbar^2 \nabla^2}{2\bar{m}} + V(\mathbf{r}) - E \right] \Psi(\mathbf{r}) = 0$$

<sup>&</sup>lt;sup>4</sup>written in relative coordinate here

leaves a separated radial equation that

$$\frac{d^2}{dr^2}\chi_{kl} - \frac{l(l+1)}{r^2}\chi_{kl} + \frac{2\bar{m}(E - V(r))}{\hbar^2}\chi_{kl} = 0$$

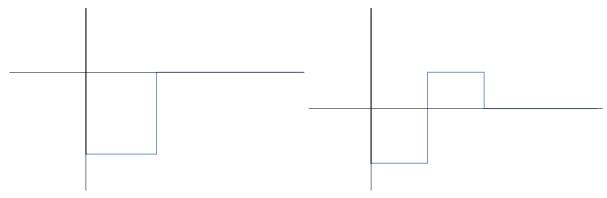


Fig. 2 (a) (I). V(r)

Fig. 2 (b) (II). V(r)

**Consider scattering states first.** For s-wave, l = 0, it becomes

$$\frac{d^2}{dr^2}\chi_{kl} + \frac{2\bar{m}(E - V(r))}{\hbar^2}\chi_{k0} = 0$$

(I) For

$$V(r) = \begin{cases} -U_0, & r < r_0 \\ 0, & r > r_0 \end{cases}$$

We have

$$\frac{d^2}{dr^2} \chi_k + \frac{2\bar{m}(E + U_0)}{\hbar^2} \chi_k = 0 \quad \text{for} \quad r < r_0$$
 (1a)

$$\frac{d^{2}}{dr^{2}}\chi_{k} + \frac{2\bar{m}(E + U_{0})}{\hbar^{2}}\chi_{k} = 0 \quad \text{for} \quad r < r_{0}$$

$$\frac{d^{2}}{dr^{2}}\chi_{k} + \frac{2\bar{m}E}{\hbar^{2}}\chi_{k} = 0 \quad \text{for} \quad r > r_{0}$$
(1a)

Introducing

$$k^2 = \frac{2\bar{m}E}{\hbar^2}$$
 and  $\kappa^2 = \frac{2\bar{m}(E + U_0)}{\hbar^2}$ 

Eq.(1) could be rewritten as

$$\frac{d^2}{dr^2}\chi_k + \kappa^2 \chi_k = 0 \qquad \text{for} \quad r < r_0$$
 (2a)

$$\frac{d^2}{dr^2}\chi_k + \kappa^2\chi_k = 0 \qquad \text{for} \quad r < r_0$$

$$\frac{d^2}{dr^2}\chi_k + k^2\chi_k = 0 \qquad \text{for} \quad r > r_0$$
(2a)

Easily to show that

$$\chi_k(r) \sim \begin{cases} \sin(\kappa r), & r < r_0 \\ A\sin(kr + \delta_k), & r > r_0 \end{cases}$$
(3)

Boundary condition at  $r = r_0$  should be matched approaching either from left and right, which gives

$$\left. \frac{\chi_k'(r)}{\chi_k(r)} \right|_{r=r_0^-} = \frac{\chi_k'(r)}{\chi_k(r)} \right|_{r=r_0^+}$$

Thus

$$\frac{\kappa \cos(\kappa r)}{\sin(\kappa r)} = \frac{k \cos(kr + \delta_k)}{\sin(kr + \delta_k)}$$

or

$$\kappa \cot(\kappa r) = k \cot(kr + \delta_k)$$

This determines the *phase shift*  $\delta_k$  given certain incident energy.

Take low energy limit gives s-wave scattering length  $a_s$  that

$$-\frac{1}{a_s} = \lim_{k \to 0} \frac{k}{\tan \delta_k} \tag{4}$$

Calculation shows

$$a_s = -r_0 \left( \frac{\tan(k_0 r_0)}{k_0 r_0} - 1 \right) = r_0 \left( 1 - \frac{\tan(\kappa r_0)}{\kappa r_0} \right)$$
 (5)

where we define  $k_0^2 = 2\bar{m}U_0/\hbar^2$ . Note that in the zero-energy limie,  $\kappa \to k_0$ , thus we have Eq.(5) above.

(II) For

$$V(r) = egin{cases} -W_0, & r < r_1 \ W_1, & r_1 < r < r_2 \ 0, & r > r_2 \end{cases}$$

we solve for zero-energy state to get the  $a_s$ .

$$\chi_0(r) \sim egin{cases} \sin(kr)\,, & r < r_1 \ e^{\kappa r} + B e^{-\kappa r}\,, & r_1 < r < r_2 \ A(1 - r/a_s)\,, & r > r_2 \end{cases}$$

where<sup>5</sup>

$$\frac{\hbar^2 k^2}{2\bar{m}} = W_0 \quad \text{and} \quad \frac{\hbar^2 \kappa^2}{2\bar{m}} = W_1$$

Boundary conditions:

$$\frac{k}{\tan(kr_1)} = \kappa \cdot \frac{e^{\kappa r_1} - Be^{-\kappa r_1}}{e^{\kappa r_1} + Be^{-\kappa r_1}} \quad \text{and} \quad \kappa \cdot \frac{e^{\kappa r_2} - Be^{-\kappa r_2}}{e^{\kappa r_2} + Be^{-\kappa r_2}} = \frac{1}{r - a_s}$$
 (6)

<sup>&</sup>lt;sup>5</sup>Notice the zero-energy condition here

Two equations with two variables (B and  $a_s$ ). From Eq.(6) we directly solved

$$a_{s} = r_{2} \left[ 1 - \frac{1}{\kappa r_{2}} \left( 1 - \frac{2}{1 - \frac{e^{2\kappa(r_{2} - r_{1})}(\kappa + k\cot(kr_{1}))}{\kappa - k\cot(kr_{1})}} \right) \right]$$
 (7)

The condition for same scattering length  $a_s$  in two potentials is determined by

$$r_0 \left( 1 - \frac{\tan(\sqrt{U_0}r_0)}{\sqrt{U_0}r_0} \right) = r_2 \left[ 1 - \frac{1}{\sqrt{W_1}r_2} \left( 1 - \frac{2}{1 - \frac{e^{2\sqrt{W_1}(r_2 - r_1)}(\sqrt{W_1} + \sqrt{W_1}\cot(\sqrt{W_0}r_1))}{\sqrt{W_1} - \sqrt{W_0}\cot(\sqrt{W_0}r_1)}} \right) \right]$$
(8)

where we have set  $\hbar = 1$ ,  $2\bar{m} = 1$ .

**Shallow bound states** For both two cases, same  $a_s(\gg r_0, r_1, r_2)$  gives same shallow bound state energy  $-\hbar^2/ma_s^2$ .

#### 4 Bose-Einstein Condensate

*Exercise* Discuss the Bose-Einstein condensation temperature for free bosons at one- and two-dimension.

### Solution:

There is no Bose-Einstein Condensation in one- or two-dimensions (or low dimensions) for free particles. This is determined by the behavior of *Density of States* (DOS) in different dimensions. To see this, we suppose there are some critical tempraturs for BEC. Then we would have an integral as follow

$$n = \int \frac{\mathcal{D}(\varepsilon)d\varepsilon}{e^{\varepsilon/kT_c} - 1}$$

This integral must be integrable for a  $T_c$  to exist.

The Density of States of one-, two- and tree-dimensions are

$$\mathcal{D}_1(\varepsilon) = \frac{1}{2\pi\hbar} (2m)^{1/2} \varepsilon^{-1/2} \propto \varepsilon^{-1/2}$$

$$\mathcal{D}_2(\varepsilon) = \frac{1}{2\pi\hbar^2} m \, d\varepsilon = \text{some constant}$$

$$\mathcal{D}_3(\varepsilon) = \frac{1}{4\pi^2\hbar^3} (2m)^{3/2} \varepsilon^{1/2} \propto \varepsilon^{1/2}$$

It turns out to be integrals like

$$\int \frac{x^{1/2}}{e^x - 1} dx$$
,  $\int \frac{1}{e^x - 1} dx$ ,  $\int \frac{1}{x^{1/2}(e^x - 1)} dx$ ,

for tree-, two-, and one-dimensions, respectively. We see clearly from Figure 3 that for one- or two-dimensions the integral is divergent.

Integrate 
$$[\mathbf{x}^{\wedge}(1/2)/(\mathbf{e}^{\wedge}\mathbf{x}-1), \{\mathbf{x}, 0, \infty\}]$$
Integrate  $[\mathbf{x}^{\wedge}(0)/(\mathbf{e}^{\wedge}\mathbf{x}-1), \{\mathbf{x}, 0, \infty\}]$ 
Integrate  $[\mathbf{x}^{\wedge}(-1/2)/(\mathbf{e}^{\wedge}\mathbf{x}-1), \{\mathbf{x}, 0, \infty\}]$ 

Out[1]=  $\frac{1}{2}\sqrt{\pi}$  Zeta  $\left[\frac{3}{2}\right]$ 
Integrate::idiv: Integral of  $\frac{1}{-1+e^{\chi}}$  does not converge on  $\{0, \infty\}$ .  $\gg$ 

Out[2]=  $\int_0^{\infty} \frac{1}{-1+e^{\chi}} d\mathbf{x}$ 
Integrate::idiv: Integral of  $\frac{1}{(-1+e^{\chi})\sqrt{\chi}}$  does not converge on  $\{0, \infty\}$ .  $\gg$ 

Out[3]=  $\int_0^{\infty} \frac{1}{(-1+e^{\chi})\sqrt{\chi}} d\mathbf{x}$ 

Fig. 3: Do integrals using Mathematica

No BEC in 1d and 2d (free bosons).

### 5 Bogoliubov Theory

*Exercise* Write down the explicit form of ground state wave function of the Bogoliubov Hamiltonian in term of boson operators  $\hat{a}_{\mathbf{k}}$ , which should satisfy  $\langle \hat{a}_{\mathbf{k}} \rangle = \sqrt{N_0}$  and  $\hat{a}_{\mathbf{k}} | \Phi \rangle = 0$ .

### Solution:

The ground state should be coherent state of ak = 0:

$$|g\rangle = \frac{1}{\exp N_0} \exp\left(\sqrt{N_0} a_0^{\dagger}\right) |0\rangle$$

from which we see clearly that

$$a_0|g\rangle = \sqrt{N_0}|g\rangle$$
  $a_{k\neq 0}|g\rangle = 0$  (for  $a_k$  commutes with  $a_0$  here)

Thus  $\langle \hat{a}_{\mathbf{k}} \rangle = \sqrt{N_0}$  and  $\hat{a}_{\mathbf{k}} | \Phi \rangle = 0$  satisfied.

### 6 BEC in a Harmonic Trap

*Exercise* Determine Bose condensation temperature of free bosons in a general trap  $V(\mathbf{r}) = \hbar \omega (r/a)^n$ , where  $\hbar \omega$  and a are characteristic energy and length scales, respectively.

#### Solution:

Actually, the critical temperature  $T_c$  for Bose-Einstein condensation is determined by the integral

gives *n* (or N). To condensate, it needs to evaluate <sup>6</sup>

$$n = \int \frac{\mathcal{D}(\epsilon)d\epsilon}{e^{\epsilon/k_BT} - 1}$$

and exhibit a  $n_0$  comparable to total n.

$$N = \frac{1}{(2\pi)^3} \int d^3 \mathbf{r} d^3 k \frac{1}{e^{(\hbar^2 k^2 / 2m + \hbar\omega(r/a)^n)/k_B T_c} - 1}$$

By introducing dimensionless variables

$$\bar{r} = \left(\frac{\hbar\omega}{a^n k_B T_c}\right)^{1/n} r \qquad \bar{k} = \left(\frac{\hbar^2}{2m k_B T_c}\right)^{1/2} k$$

We reduce the integral to

$$N = \frac{1}{(2\pi)^3} \left(\frac{a^n k_B T_c}{\hbar \omega}\right)^{3/n} \left(\frac{2m k_B T_c}{\hbar^2}\right)^{3/2} \int d^3 \mathbf{r} d^3 \bar{k} \frac{1}{e^{\bar{k}^2 + \bar{r}^2} - 1} \sim T_c^{3n + 6/2n}$$

The integral is a constant. Or other except  $T_c$  is constant. Thus  $T_c = N^{\frac{2n}{3n+6}} \times$  some constant.

### 7 Topological Excitations

*Exercise* Solve single-particle Hamiltonian<sup>7</sup>

$$\hat{H}_0 = \frac{\hbar^2 k^2}{2m} + \frac{1}{2}m\omega^2 r^2 - \Omega \hat{L}_z$$

by introducing

$$\hat{a}_x = \frac{1}{\sqrt{2}} \left( \frac{x}{a} + ik_x a \right) \qquad \hat{a}_x^{\dagger} = \frac{1}{\sqrt{2}} \left( \frac{x}{a} - ik_x a \right)$$

$$\hat{a}_y = \frac{1}{\sqrt{2}} \left( \frac{y}{a} + ik_y a \right) \qquad \hat{a}_y^{\dagger} = \frac{1}{\sqrt{2}} \left( \frac{y}{a} - ik_y a \right)$$

and

$$\hat{a}_{\pm}=rac{\hat{a}_x\mp\hat{a}_y}{\sqrt{2}} \qquad \qquad \hat{a}_{\pm}^{\dagger}=rac{\hat{a}_x^{\dagger}\mp\hat{a}_y^{\dagger}}{\sqrt{2}}$$

with harmonic length  $a=\sqrt{\hbar/(m\omega)}$ . Find out all energy spectrum and the wave function<sup>8</sup>

$$\psi_m \propto r^m e^{\mathrm{i}m\theta} e^{-r^2/(2a^2)} = z^m e^{-|z|^2/(2a^2)}$$

<sup>&</sup>lt;sup>6</sup>In fact, for bosons in isotropic trap, the critical temprature is determined by  $\mu = V(r = 0) = 0$ 

<sup>&</sup>lt;sup>7</sup>See Eq. (19) on [1], Page 77.

<sup>&</sup>lt;sup>8</sup>See Eq. (20) on [1], Page 77.

### Solution:

PS: I do not use the  $\hat{a}_{\pm}$  and  $\hat{a}_{\pm}^{\dagger}$  given above. I will define new ones later.

**Energy levels** To solve this rotational invariant 2D harmonic oscillator plus rotation Hamiltonian, introducing creation and annhiliation operators like  $\hat{a}_x$ ,  $\hat{a}_y$ , and  $\hat{a}_x^{\dagger}$ ,  $\hat{a}_y^{\dagger}$  would be much helpful. There physical meaning could be seen as lowering (raising) the state one energy level, with energy decreasing (increasing)  $\hbar\omega$ , along  $\hat{x}$  or  $\hat{y}$  direction. Easily seeing that

$$H_0 = (a_x^{\dagger} a_x + a_y^{\dagger} a_y + 1)\hbar\omega - \mathrm{i}(a_x^{\dagger} a_y - a_y^{\dagger} a_x)\hbar\Omega$$

Obviously it is not diagonalized in  $\hat{a}_x$ ,  $\hat{a}_y$ ,  $\hat{a}_x^{\dagger}$ ,  $\hat{a}_y^{\dagger}$  representations. This is clear because the total Hamiltonian is rotational invariant while creating (destroying) an energy quanta along some particular axis would certainly break this symmetry.

To solve it, one way is to directly diagonalize the Hamiltonian matrix, which is not smart, and violate the goodness of this problem. So I better choose another way, to look into the diagonalized representation where energy levels would be easily find.

Now I define new operators using these xy-operators.

$$\hat{a}_{\pm}=rac{1}{\sqrt{2}}ig(\hat{a}_{x}\pm\mathrm{i}\hat{a}_{y}ig)$$

$$\hat{a}_{\pm}^{\dagger}=rac{1}{\sqrt{2}}ig(\hat{a}_{x}^{\dagger}\mp\mathrm{i}\hat{a}_{y}^{\dagger}ig)$$

I define them because I expect the Hamiltonian would be diagonalized in this representation. I expect this because the original Hamiltonian is obviously something products  $\sigma_y$ . Actually, these two could be compared to *left(right) circularly polarized light*. See Sakurai [8]. No focus on which one is left and which is right, because I don't remember either.

Easily to show that

$$H_0 = (a_+^{\dagger} a_+ + a_-^{\dagger} a_- + 1)\hbar\omega + (a_+^{\dagger} a_+ - a_-^{\dagger} a_-)\hbar\Omega$$

Clearly

$$E = n_{+}\hbar(\omega + \Omega) + n_{-}\hbar(\omega - \Omega) + \hbar\omega$$

where  $n_+$  is the number of  $a_+^{\dagger}$ -like circular polarized energy quanta while  $n_-$  is the number of  $a_-^{\dagger}$ -like circular polarized energy quanta.

A traditional way works out

$$E = (n+1)\hbar\omega - m\hbar\Omega$$

where n is the principle quantum number, equal to total number of energy quanta along  $\hat{x}$  and  $\hat{y}$ , and m labels z-component angular momentum. Comparing these two expression we got

$$n_{+} + n_{-} = n$$

$$n_+ - n_- = -m$$

**Wave function** To get the wave function we introduce complex variables, i.e.

$$z = x + iy$$
,  $\partial_z = \partial_x - i\partial_y$   
 $\bar{z} = x - iy$ ,  $\partial_{\bar{z}} = \partial_x + i\partial_y$ 

such that

$$a_{+} = \frac{1}{2}(\frac{z}{a} + ia\partial_{\bar{z}})$$
  $a_{-} = \frac{1}{2}(\frac{\bar{z}}{a} + ia\partial_{z})$ 

Ground state wave function satisfied

$$a_-f_0(z,\bar{z}) = 0$$
  
$$a_+f_0(z,\bar{z}) = 0$$

which gives  $f_0(z,\bar{z}) \propto \exp(-|z|^2/2a^2)$ . Wave function of excited states could be created by  $a_-^{\dagger} f_n$  and  $a_+^{\dagger} f_n$ . Calculation shows

$$\psi_m \propto r^m e^{\mathrm{i}m\theta} e^{-r^2/(2a^2)} = z^m e^{-|z|^2/(2a^2)}$$

More words on this. Hamiltonian like this is of great interests, or at least needs to be worked out in details, for some reason. One might be that it is related to gauge transformation in some way. Actually, when  $\Omega = \omega = \omega_0/2$ , it realises

$$H_0 = H\left(\frac{\omega_0}{2}, m\right) - \frac{\omega_0}{2} L_z$$

which recovers landau levels. It is equivalent to adding a homogeneous magnetic field  $\mathbf{B} = B\hat{z}$  to a free particle.

For details, see Shankar, Principle of Quantum Mechanics 2nd ed.[7], Page 317-318, Exercise 12.3.8.

This section refers to [7, 8].

### 8 Phase Coherence and Fragmentation

*Exercise* Numerically solve the Hamiltonian<sup>9</sup>

$$\hat{H} = -t(\hat{a}_1^{\dagger} \hat{a}_2 + \hat{a}_2^{\dagger} \hat{a}_1) + \frac{U}{2}(\hat{n}_1(\hat{n}_1 - 1) + \hat{n}_2(\hat{n}_2 - 1))$$

for finite number of particles, and discuss the wave function, density matrix, relative particle fluctuations in three regimes

- (i) U > 0 and  $U \lesssim t$ ;
- (ii) U > 0 and  $U \gg t$ ;
- (iii) U < 0 and  $|U| \gg t$ .

<sup>&</sup>lt;sup>9</sup>See Eq. (1) on Page 115 of [1]

In regime (iii), please also discuss the excitation gap between the first excited state and the ground state as a function of total particle number *N*.

#### Solution:

According to the lectures given in class[1], if we solve it in Fock space, we obtain the following Shrödinger equations

$$E\Psi_l = -t_{l+1}\Psi_{l+1} - t_l\Psi_l + Ul^2\Psi_l$$

where

$$t_l = t\sqrt{(\frac{N}{2} + l)(\frac{N}{2} - l + 1)}$$

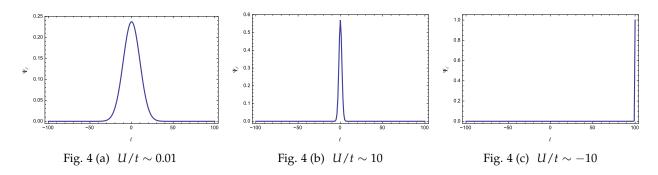
Note that here we have chosen  $|N/2 + l, N/2 - l\rangle$  as our bases. Wave function could be written as

$$\psi = \sum_{l} \Psi_{l} \left| \frac{N}{2} + l, \frac{N}{2} - l \right>$$

This could be written down as a matrix and we simply diagonalize it under three different assumptions. We expect, and result also shows that

- (i) U > 0 and  $U \lesssim t$ . Interaction within a well is less important than the hopping term between two wells. System would favor coherent states. Gaussian distribution would be most likely to occur if we look at  $\Psi_l l$ . Fig. 4 (a)
- (ii) U > 0 and  $U \gg t$ . With very large repulsive interaction, system favor a fifty-fifty staying. Fig. 4 (b)
- (iii) U < 0 and  $|U| \gg t$ . The interaction is attractive and more important than the hopping term. Particles would be mostly possible staying in either one well. Fig. 4 (c)

Here plot some cases. Given different U/t, density matrices appears different, showing fragmenta-



tion macroscopic occupying. Here are some certain cases.

$$\hat{\rho} = \begin{pmatrix} 99.99 & 0.10 \\ 0.10 & 0.10 \end{pmatrix} \begin{pmatrix} 99.98 & 1.01 \\ 1.01 & 1.01 \end{pmatrix} \begin{pmatrix} 1.03 & 10.10 \\ 10.10 & 10.10 \end{pmatrix} \begin{pmatrix} 50. & 49.99 \\ 49.99 & 49.99 \end{pmatrix} \begin{pmatrix} 50. & 49.78 \\ 49.78 & 49.78 \end{pmatrix} \begin{pmatrix} 50. & 48.67 \\ 48.67 & 48.67 \end{pmatrix} \begin{pmatrix} 50. & 44.86 \\ 44.86 & 44.86 \end{pmatrix}$$

for U/t = -10, -1, -0.1, 0.001, 0.1, 1, 10, respectively. (the results are unnormalised with 100, which is our total number.) We see clearly that the results of numerical simulation agree highly with our expectation. Relative particle fluctuation is very small in case (ii) and (iii), while large in case (i).

For details, see Mueller [9].

### 9 Two-Fluid Hydrodynamics

*Exercise* Show  $c_2^2 = c_1^2/3$  from Equation<sup>10</sup> (30)

$$c_1^2 = \frac{\partial P}{\partial \rho}$$
  $c_2^2 = \frac{\rho_s T \tilde{s}^2}{\rho_n \tilde{c}}$ 

assuming a linear dispersion for low-energy phonon dispersion.

### Solution:

For interacting Bose gas, the ground state energy in the low-temperature limit  $T \to 0$  is given by  $E_0 = \frac{N^2 U_0}{2V}$ . The pressure is then

$$P = -\frac{\partial E_0}{\partial V} = \frac{1}{2}U_0n^2 = \frac{U_0\rho^2}{2m^2}$$

Thus we obtain the first sound velocity to be

$$c_1^2 = \frac{\partial P}{\partial \rho} = \frac{nU_0}{m}$$

As for  $c_2$ , the entropy and specific heat for phonons are related by  $\tilde{s} = \tilde{c}/3$  and  $\tilde{c} = 3\rho_n s^2/T\rho$ . Thus we obtain

$$c_2^2 = \frac{s^2}{3} = \frac{nU_0}{3m} = \frac{1}{3}c_1^2$$

### 10 Feshbach Resonance

No Exercises

### 11 Fermi Liquid

No Exercises

### 12 BEC-BSC Crossover

**Exercise** Discuss the self-consistent solution of BEC problem

$$H_{\rm BCS} = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \mu_{\sigma}) c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k}} \Delta c_{\mathbf{k},\uparrow}^{\dagger} c_{-\mathbf{k},\downarrow}^{\dagger} + \sum_{\mathbf{k}} \Delta^{*} c_{\mathbf{k},\uparrow} c_{-\mathbf{k},\downarrow}$$

<sup>&</sup>lt;sup>10</sup>See [1], page 140.

when  $\mu_{\uparrow} \neq \mu_{\downarrow}$ , and compare the energy of BCS state with free Fermi gas for different  $h = \mu_{\uparrow} - \mu_{\downarrow}$ .

#### Solution:

The Hamiltonian could be written as

$$H_{BCS}(\mathbf{k}) = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \mu_{\sigma}) c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k}} \Delta c_{\mathbf{k},\uparrow}^{\dagger} c_{-\mathbf{k},\downarrow}^{\dagger} + \sum_{\mathbf{k}} \Delta^{*} c_{\mathbf{k},\uparrow} c_{-\mathbf{k},\downarrow}$$

$$= (c_{\mathbf{k},\uparrow}^{\dagger}, c_{-\mathbf{k},\downarrow}) \begin{pmatrix} \epsilon_{\mathbf{k}} - \mu_{\uparrow} & \Delta \\ \Delta & -\epsilon_{\mathbf{k}} + \mu_{\downarrow} \end{pmatrix} \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c_{-\mathbf{k},\downarrow}^{\dagger} \end{pmatrix}$$

$$= \phi(\mathbf{k})^{\dagger} \left[ (\epsilon_{\mathbf{k}} - \frac{\mu_{\uparrow} + \mu_{\downarrow}}{2}) \sigma_{z} + \Delta \sigma_{x} - \frac{\mu_{\uparrow} - \mu_{\downarrow}}{2} \right] \phi(\mathbf{k})$$

using *Nambu representation*. Here we set  $\Delta$  to be real, with *Nambu basis*  $\phi(\mathbf{k})^{\dagger} = (c_{\mathbf{k},\uparrow}^{\dagger}, c_{-\mathbf{k},\downarrow})$ . Fermionic system could be directly diagonalized to obtain

$$E(\mathbf{k}) = \pm \sqrt{(\epsilon_{\mathbf{k}} - \frac{\mu_{\uparrow} + \mu_{\downarrow}}{2})^2 + \Delta^2} - h$$

Comparing this with free fermion case, we see that, the energy gain is positive if  $|h| < 2\Delta$ . Otherwise the pairing instability at zero momentum is prohibited. The different chemical potential of two spin species can be resulted from an effective magnetic field B. If B is too large, the zero-momentum pairing is not favored. We need a finite momentum pairing to connect two seperate fermi sheets.

### 13 BEC-BCS Crossover at Finite Temperature

No Exercises

### 14 Time-Dependent Ginzburg-Landau Theory of BEC-BCS Crossover

No Exercises

#### 15 Bose-Hubbard Model

Exercise Consider a relativistic nonlinear equation

$$\frac{\hbar^2 \partial^2 \varphi}{\partial t^2} = -\frac{\hbar^2 \nabla^2}{2m} \varphi + g|\varphi|^2 \varphi$$

Study small amplitude oscillation of phase and amplitude of wave function  $\varphi$ , and obtain a gapless Goldstone mode and a gapped Higgs mode from the real and imaginary parts of this equation.

### Solution:

Assume  $\varphi = \rho e^{i\phi}$ . Given some small oscillation of amplitude  $\rho$  and phase  $\phi$ , we have

$$\rho = \rho_0 + \delta \rho$$
$$\phi = \phi_0 + \delta \phi$$

Substituting it into  $\frac{\hbar^2 \partial^2 \varphi}{\partial t^2} = -\frac{\hbar^2 \nabla^2}{2m} \varphi + g |\varphi|^2 \varphi$  gives

$$\begin{split} \frac{\partial^2}{\partial t^2} \varphi &= e^{\mathrm{i}\phi_0} \left( \frac{\partial^2}{\partial t^2} \delta \rho + \mathrm{i}\rho_0 \frac{\partial^2}{\partial t^2} \delta \phi - \rho (\partial_t \delta \phi)^2 \right) \\ &= -\frac{1}{2m} \left( e^{\mathrm{i}\phi_0} \nabla^2 \delta \rho + \mathrm{i}\rho_0 \nabla^2 \delta \phi - \rho (\nabla \delta \phi)^2 \right) + \rho_0^3 e^{\mathrm{i}\phi_0} \end{split}$$

Equating the real and imaginary parts separatedly, we immediately read out the gapless Goldstone mode with dispersion  $\omega^2 = k^2/2m$  which corresponds to the phase fluctuations and a gapped Higgs mode corresponds to the amplitude fluctuation.

#### 16 Fermion Hubbard Model

*Exercise* 1 Consider a two-dimensional Fermion Hubbard model without interactions (U = 0), and for a nonmagnetic state ( $n_{\uparrow} = n_{\downarrow}$ ), discuss how the Fermi surface evolves when filling number n increases from zero to two.

#### Solution:

With U = 0, we have a reduced Fermion Hubbard model to be

$$H = -t \sum_{\mathbf{n.n.},\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} \tag{9}$$

Note two things.

- 1. We consider only the nearest neighbouring hopping, with an universal hopping amplitude.
- 2. There are no polarizing in spin, which is to say that it is diagonalized in spin space. Direct-producting the spin space with coordinate space to get the whole Hilbert space, we could actually trace out the spin degree of freedom (for they are seperable). Thus in the following I'll omit the  $\sigma$  index. In fact, stated in the context given above,  $n_{\uparrow}=n_{\downarrow}$  is what we would expect, which is a physical result of  $\mu_{\uparrow}=\mu_{\downarrow}$ .

General physics Actually, this is the simplest model in *Solid State Physics*, one of our college course of undergraduate level, named *Tight-binding model* to solve a crystall's energy spectrum, which gives rise to the general *band structure* explaning most kinds of *band metal*, *band insulator*, and predicting *band semi-insulator*—the foundation of Computor Science and one of the greatest achievements in 20th century.

Just a simple model. (yet universal, elegant, and relevant to applications)

So you see, through this general discussion, we have already got what we expect to get. Following is merely formalise it. (this is where math do jobs)

**Solving tight-binding model** To get the dispersion relationship, we do Fourier transformation.

$$c_{\mathbf{k}} = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{a}} c_{\mathbf{k}}$$
$$c_{\mathbf{k}}^{\dagger} = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{a}} c_{\mathbf{k}}^{\dagger}$$

where  $k \in FBZ$ . Substituating it into Eq.(9), we obtain

$$\mathcal{H}(\mathbf{k}) = -t \sum_{\mathbf{n}.\mathbf{n}.\mathbf{n},\sigma} c_{i\sigma}^{\dagger} c_{j\sigma}$$
$$= -t \sum_{\mathbf{k} \in \text{fbz}} 2\cos(\mathbf{k} \cdot \mathbf{a}) c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}}$$

For two-dimensional case,

$$\mathcal{H}(\mathbf{k}) = -2t \sum_{\mathbf{k} \in \text{fbz}} \left[ \cos(\mathbf{k} \cdot \mathbf{a_i}) + \cos(\mathbf{k} \cdot \mathbf{a_j}) \right] c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}}$$

where  $\mathbf{a}_i(\mathbf{a}_i)$  denotes lattice vectors along  $\hat{x}(\hat{y})$  direction.

Clearly, the dispersion is no more *quadratic* as free fermion case, but becomes cos form within a band (and open gap between bands). This also change the effective mass. See Ashcroft [10].

When filling number n increases from zero to two, the Fermi surface raising correspondingly, the corresponding material changes from insulator to metal then to insulator again. n=1 corresponds to half-filling, with the greatest ability of conductance. And the Fermi surface is within the band. While n=2, this is the case of full-filling. Fermi surface jumps to lie in gap (between bands). Excitation energy is finite. Thus insulator. This is the most difference with free fermi gases, where the Fermi surface continuously raising, and excitation energy is always infinitesimal. Sketch of Fermi surface see Fig. 4

*Exercise* 2 Discuss the Hanbury-Brown-Twiss effect for noninteractiong fermions and compare its difference with bosons.

### Solution:

The density operator is defined as <sup>11</sup>

$$\rho(\mathbf{r}) = \langle \psi^{\dagger}(\mathbf{r})\psi(\mathbf{r}) \rangle$$

If we expand the field operator as

$$\hat{\psi}(r) = \hat{a}_1 \phi_1(r) + \hat{a}_2 \phi_2(r)$$

we have

$$\rho(\mathbf{r}) = \langle \psi^{\dagger}(\mathbf{r})\psi(\mathbf{r})\rangle = n_1|\phi(\mathbf{r})|^2 + n_2|\phi(\mathbf{r})|^2$$

<sup>&</sup>lt;sup>11</sup>Here we write field operator as  $\psi$  while not  $\Psi$  for it looks more beautiful in the font I choose for this context.

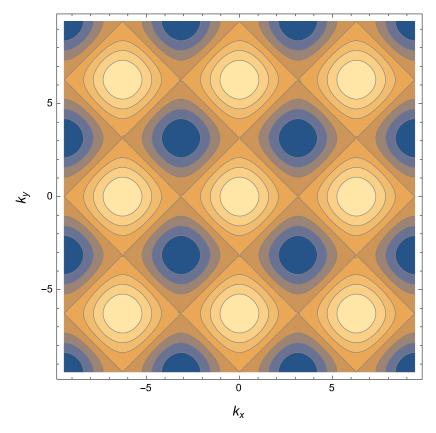


Fig. 4: Fermi surface for 2D tight-binding model

with  $n_1 = \langle a_1^{\dagger} a_1 \rangle$  and  $n_2 = \langle a_2^{\dagger} a_2 \rangle$ .

If we go on considering second-order density correlation, which is actually the essential of *Hanbury-Brown-Twiss Effect* [11],

$$\langle \psi^{\dagger}(r)\psi(r)\psi^{\dagger}(r')\psi(r')\rangle = \rho(r)\rho(r') + \langle a_{2}^{\dagger}a_{1}a_{1}^{\dagger}a_{2}\rangle(\phi_{1}^{*}(r')\phi_{1}^{*}(r)\phi_{2}(r)\phi_{1}(r) + h.c.)$$

$$= \rho(r)\rho(r') - n_{1}n_{2}(\phi_{1}^{*}(r')\phi_{1}^{*}(r)\phi_{2}(r)\phi_{1}(r) + h.c.)$$

Note the minus sign in front of the second term. This is the difference contrast with bosons.

This section refers to [1, 11].

## 17 Topological States in Optical Lattice

No Exercises

### Acknowledgement

I would like to thank Ruihua Fan for helpful discussion.

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