Les Houches Lecture Notes

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These are my lecture notes for the 2015 Les Houches Summer school which took place at the Centre de Physique des Houches in the French alps. They contain lectures by

- Jook Walraven

- Phillipe Verkerk

- Dmitry Petrov

- Helene Perrin

- Leticia Tarruell

- Thierry Lahaye

- Bruno Laburthe-Tolra

- Trey Porto

Many of the lectures included slides of experiments and other results and often these are not contained in these notes. There may be typos in these notes and they are by no means complete accounts of any of these subjects.

Contents

1 Elastic interactions (Jook Walraven)

1.1 Lecture 1

We know that the potentials of atoms usually looks something like the Morse potential which is strongly repulsive for short range and then attractive, going to zero at large r, where r is the internuclear separation. For many potentials (although not all, even important ones), we can define a typical distance r_0 and for $r > r_0$, we can ignore the potential to an extremely good approximation.

If we consider the Thermal de Broglie wavelength

$$\lambda_{dB} = \sqrt{\frac{2\pi\hbar^2}{mk_BT}}, \tag{1.1}$$

then we will need to use quantum mechanics when $\lambda_{dB} \gg r_0$. This means we do not need quantum degeneracy to have quantum effects. Now if we define

$$k = \frac{2\pi}{\lambda_{dB}}, \tag{1.2}$$

a wavevector, then we have the condition $kr_0 \ll 1$ for the regime in which we say we have ultracold collisions.

Now we can change our coordinates to center of mass and relative coordinates which will simplify the mathematics considerably. Consider two binary particles with position $\vec{r}_1, \vec{r}_2$ and velocities $\vec{v}_1, \vec{v}_2$. Then we can define

$$\vec{r} = \vec{r}_1 - \vec{r}_2 \,;\; \vec{v} = \vec{v}_1 - \vec{v}_2, \tag{1.3}$$

and in analogy to classical mechanics in a closed system, E and P are conserved, where

$$P = \vec{P}_1 + \vec{P}_1 \, E = \frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2}. \tag{1.4}$$

Note if we define $p = \mu\vec{v}$, where μ is the reduced mass, then we can also write

$$E = \frac{P^2}{2M} + \frac{p^2}{2\mu}, \tag{1.5}$$

where $M = m_1 + m_2$. [1]

1.1.1 Binary Collision Equation

We can define the general Hamiltonian of the relative motion of the atoms (we don't really care about center of mass motion as this will just be normal plane waves) as

$$H = \frac{p^2}{2\mu} + V(\vec{r}) = -\frac{\hbar^2}{2\mu}\nabla^2 + V(\vec{r}). \tag{1.6}$$

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[1]This only strictly works if p is the canonical momentum, which means that electromagnetic fields will slightly alter this approximation. However, it will still be quite good.

Confining ourselves to the case of a central potential (spherically symmetric around $r = 0$), we can write $V(\vec{r}) = V(|\vec{r}|) = V(r)$. Transforming to separated spherical coordinates, we can write the Hamiltonian as

$$H = \frac{1}{2\mu} \left(p_r^2 + \frac{L^2}{r^2} \right) + V(r). \tag{1.7}$$

We need to be careful about the case $r = 0$ as in general the solutions to this separated equation will not be solutions to the original Hamiltonian at this point. [2]

Now we can solve the Shrodinger equation $H\psi = E\psi$

$$\left[\frac{1}{2\mu} \left(p_r^2 + \frac{L^2}{r^2} \right) + V(r) \right] \psi = E\psi, \tag{1.8}$$

and since L^2 commutes with the Hamiltonian, we can separate variables and write our solution as

$$\psi_{lm}(r) = R_l(r)Y_l^m(\theta, \phi). \tag{1.9}$$

where Y_l^m are the spherical Harmonics which we know solve the angular part of a centrally symmetric potential.

Now we use the eigenvalue of the L^2 operator ($L^2 Y_l^m = \hbar^2 l(l+1)$), to write

$$\left[\frac{1}{2\mu} \left(p_r^2 + \frac{\hbar^2 l(l+1)}{r^2} \right) + V(r) \right] R_l(r) = E R_l(r), \tag{1.10}$$

where we have divided the spherical Harmonics out of the problem. This is known as the radial equation and is the primary object we will be dealing with since the angular part is already known. Plugging in our definition of p_r in radial coordinates, we get

$$\left[-\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} \right) + \frac{l(l+1)\hbar^2}{2\mu r^2} + V(r) \right] R_l(r) = E R_l(r). \tag{1.11}$$

Now we switch to wavenumber notation where we define $\hbar^2 \epsilon = 2\mu E$ and $\hbar^2 U(r) = 2\mu V(r)$, which reduces our equation to

$$R_l'' + \frac{2}{r}R_l' + \left[\epsilon - U(r) - \frac{l(l+1)}{r^2} \right] R_l = 0. \tag{1.12}$$

1.1.2   S-Wave Regime

First we define an effective potential

$$U_{eff} = U(r) + \underbrace{\frac{l(l+1)}{r^2}}_{\text{centrifugal barrier}}, \tag{1.13}$$

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[2]This is due to the $1/r^2$ term in the angular momentum part which is undefined at zero.

which we can see reduces to $U(r)$ in the case of $l = 0$. For $l > 0$, we have a classical turning point defined as

$$k^2 = \frac{l(l+1)}{r^2} \implies kr_0 = \sqrt{l(l+1)}\frac{r_0}{r_{cl}}, \tag{1.14}$$

where r_{cl} is the classical turning point. Now since we are operating under the assumption that $kr_0 \ll 1$, we know this will be a small number. This implies that

$$r_{cl} \gg r_0, \tag{1.15}$$

and thus for $l > 0$ we can essentially ignore the potential as the particle will never be in a regime where it will matter. We only care about $l = 0$ scattering which is also known as s-wave scattering.

1.1.3   Solutions of Scattering Equation

If we consider the solutions for $U(r) = 0$, we have the spherical Bessel equation whose solutions are given as

$$R_l = \alpha_l j_l(kr) + \beta_l n_l(kr), \tag{1.16}$$

where j_l and n_l are the spherical Bessel and spherical Neumann functions of order l. We can use these as a basis to write different functions, for example a palne wave can be written as

$$e^{ikz} = \sum_{l=0}^{\infty}(2l+1)i^l j_l(kr)Y_l^0(\theta, \phi), \tag{1.17}$$

and we can also substitute $Y_l^0(\theta, \phi) = P_l(\cos\theta)$, where P_l are the Legendre polynomials.

We can rewrite the radial equation into a one dimensional equation by writing $u_l(r) = rR_l(r)$, which gives us that

$$u_l'' + \left[\epsilon - U(r) - \frac{l(l+1)}{r^2}\right]u_l = 0, \tag{1.18}$$

and for $l = 0$ and $\epsilon > 0$, we can write this as

$$u_0'' + [k^2 - U(r)]u_0 = 0, \tag{1.19}$$

where $k^2 = \epsilon$.

For a free particle $U(r) = 0$, the solutions are simple, and given as

$$u_0 = \alpha\sin(kr) + \beta\cos(kr). \tag{1.20}$$

If we make the substitutions $\alpha \to A\cos\eta_0$ and $\beta \to A\sin\eta_0$, then

$$u_0 = A\cos\eta_0\sin(kr) + A\sin\eta_0\cos(kr) = A\sin(kr + \eta_0), \tag{1.21}$$

and η_0 is the phase shift. For free particles $\eta_0 = 0$ since the solution must be regular at the origin.[3]

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[3] $R = u_0/R$ and so as $k \to 0$, $R \to A\sin(\eta_0)/r$, thus $\sin(\eta_0) = 0 \implies \eta_0 = 0$ for regularity at the origin.
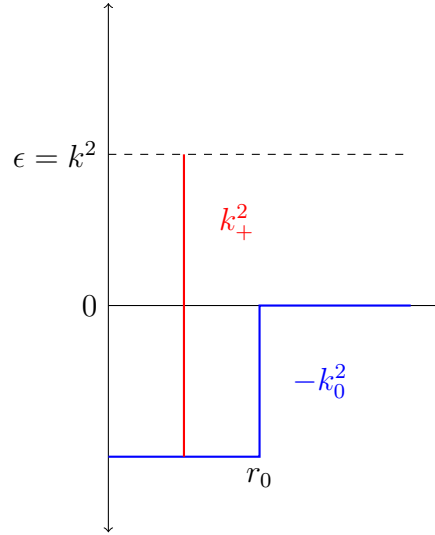
Figure 1: Square well potential well.

1.1.4   Hard Wall Potential

If we consider a potential which is infinite at some point a, then we consider the wavefunction for $r > a$. The solution is that of a free particle, however, we no longer require the solution be regular at the origin, and require that $u_0(a) = 0$. This means that

$$\sin(ka + \eta_0) = 0, \tag{1.22}$$

which implies that $\eta_0 = -ka + n\pi$. Restricting to the case that $n = 0$, we have that

$$R_0(r) = \frac{A}{kr}\sin(k(r - a)), \tag{1.23}$$

and in the limit that $k \to 0$, we have that

$$R_0 = r\left(1 - \frac{a}{r}\right). \tag{1.24}$$

1.1.5   Spherical Square Well

Here we consider a spherical well with $\epsilon > 0$ (continuum states). This is shown in Figure 1. The well depth is $-k_0^2$ and we define $k_+^2 = k^2 + k_0^2$. Restricting to $l = 0$, we can write the potential as

$$U(r) = \begin{cases} 0 & r > r_0 \\ k_0^2 & r < r_0 \end{cases} \tag{1.25}$$

We can solve both inside and outside the well. First outside the well, we can use the solution we found before, namely

$$u_0(r)^{r>r_0} = A\sin(kr + \eta_0), \tag{1.26}$$

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and inside the well, we can note that the equation we seek to solve is

$$u_0'' + k_+^2 u = 0, \tag{1.27}$$

and since this must be regular at the origin, we have

$$u_0^{r < r_0} = B \sin(k_+ r). \tag{1.28}$$

With our two solutions, we now impose the boundary conditions that the wavefunction and its derivative must be continuous at r_0. Since we are after the phase, we can simply match the logarithmic derivatives of the wavefunctions at r_0, which gives

$$k \cot(k r_0 + \eta_0) = k_+ \cot(k_+ r_0), \tag{1.29}$$

which we can rearrange to solve for η_0 as

$$\eta_0 = \arctan\left(\frac{k}{k_+} \tan(k_+ r_0)\right) - k r_0, \tag{1.30}$$

a function of k, r_0 and the well depth. Now we can write $\eta_0(k) = -k a(k)$ and thus

$$a(k) = r_0 - \frac{1}{k} \arctan\left[\frac{k}{k_+ \cot(k_+ r_0)}\right], \tag{1.31}$$

and in the limit $k \to 0$, we have that $k_+ \to k_0$ nd thus

$$a(k) = r_0 - \frac{1}{k_+ \cot(k_+ r_0)}, \tag{1.32}$$

and thus

$$k_+ \cot(k_+ r_0) = \frac{1}{r - a}, \tag{1.33}$$

which allows us to define the scattering length a as

$$a = \lim_{k \to 0} a(k) = -\lim_{k \to 0} \frac{\eta_0(k)}{k}. \tag{1.34}$$

In terms of the well parameter $\gamma = k_0 r_0$, we can write

$$a = r_0\left(1 - \frac{\tan \gamma}{\gamma}\right). \tag{1.35}$$

This result is plotted in Figure 2.

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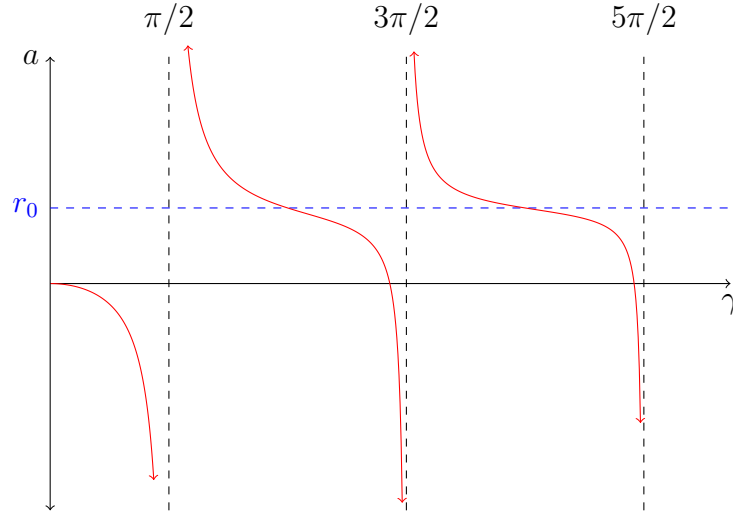
Figure 2: Plot of $a = r_0 \left(1 - \frac{\tan \gamma}{\gamma}\right)$, the scattering length in a spherical square well potential.

1.2 Lecture 2

1.2.1 Previous Summary

We first summarize results from the previous lecture

1. $kr_0 \ll 1$ implies ultracold regime.

2. Solved radial wave equation for $l = 0$ and $u(r) = 0$ to get that

$$R_0(r) = \frac{A}{kr} \sin(kr + \eta_0). \tag{1.36}$$

3. For the spherical well

$$\eta_0 = -kr_0 + \tan^{-1}\left[\frac{k}{k_+ \cot(k_+ r_0)}\right]. \tag{1.37}$$

4. In limit $k \to 0$, $k_+ \to k_0$ and thus

$$\eta_0 = -ka(k), \tag{1.38}$$

where a is a function of k given as

$$a(k) = r_0 - \frac{1}{k} \tan^{-1}\left[\frac{k}{k_+ \cot(k_+ r_0)}\right] \tag{1.39}$$

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5. The scattering length is given as

$$a = \lim_{k \to 0} a(k). \tag{1.40}$$

And so if we define $\gamma = k_0 r_0$, then

$$a = r_0 \left(1 - \frac{\tan \gamma}{\gamma} \right). \tag{1.41}$$

1.2.2　Bound States

We now want to answer the questions, what happens when $\gamma = \pi/2 + n\pi$. We can understand this by examining bound states, We now let a bound state have energy $\epsilon = -\kappa^2$, $(\kappa > 0)$ and define k_-^2, where

$$k_-^2 = k_0^2 - \kappa^2, \tag{1.42}$$

We can now solve this problem in a similar way to the unbound state. For the case $r < r_0$, $U = -k_0^2$, which implies that our radial equation is

$$u_0'' + k_-^2 u_0 = 0, \tag{1.43}$$

which can be solved as

$$u_0^{r<r_0} = A \sin(k_- r), \tag{1.44}$$

as there can be no phase shift to ensure regularity at the origin.

Now for $r > r_0$, we have $U(r) = 0$ and thus our equation is

$$u_0'' - \kappa^2 u_0 = 0, \tag{1.45}$$

which gives that

$$u_0^{r>r_0} = B e^{-\kappa r}, \tag{1.46}$$

where we must discard the other solution for normalization.

We can use the boundary conditions to match logarithmic derivatives as

$$k_- \cot(k_- r_0) = -\kappa. \tag{1.47}$$

In the lower binding limit $\kappa \to 0$, $k_- \to k_0$, we get that

$$k_0 \cot(k_0 r_0) = -\kappa \implies \gamma \cot \gamma = -\kappa r_0, \tag{1.48}$$

and so $\gamma = \pi/2 + n\pi$, which implies that the divergence corresponds to the formation of a bound state.

In this case, a large positive scattering length supports a bound state, but a negative scattering length does not.

We now consider the *halo state*, which is a very weakly bound state. At this point, the tail of the exponential decay extends much further than the size of the
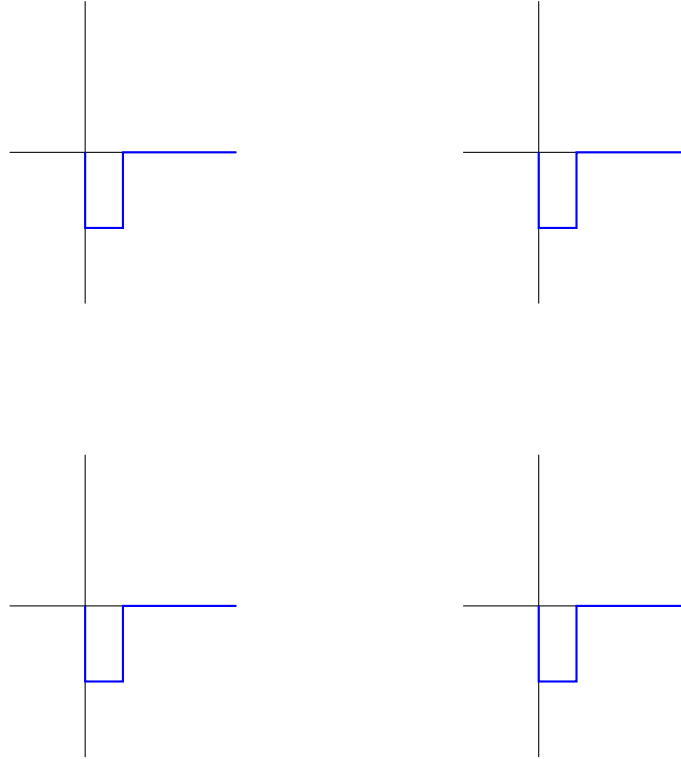
Figure 3: Caption

well. In this case, we can ignore the well part and extend the exponential through the well. This is universal in the sense that it does not care about the details of the well. This is the case when $k_0 r_0 \approx \pi/2$.

We can conserve the ratio of $k_0 r_0$ and take the limit as $r_0 \to 0$. Although we lose information about all other bound states, we retain the binding energy of the last state. It can be used to investigate problems where we do not know the potential.

In this case, $\kappa = 1/a$ and $\epsilon \sim -1/a^2$. So in the weakly bound state, the binding energy is independent of the sign of a.

This potential is important because except in pathological cases, it describes most of the physical properties of realistic potentials.

To interpret the scattering length, we can first look at the case for $a > 0$. Then in the low energy limit, the wavefunction has a node at $r = a$. If we let $a \to \infty$ and go through a resonance, $a \to -\infty$, and continuing on, we have a node at negative distance $(a < 0)$. This is called a virtual node, and supports an almost bound state called a virtual bound state. **finish PLOTS**

1.2.3   Effective Range

We have already found that

$$\eta_0(k) = \underbrace{-kr_0}_{\text{regular}} + \underbrace{\tan^{-1}\left[\frac{k}{k_+\cot(k_+r_0)}\right]}_{\text{resonant}}, \tag{1.49}$$

which we have divided into two sections. We ask for the leading k dependence of this expression. To manipulate this, we will use the fact that

$$\tan(a+b) = \frac{\tan a + \tan b}{1 - \tan a \tan b}, \tag{1.50}$$

and also that

$$\tan x = x + \frac{1}{3}x^3 + \cdots = x\left(1 + \frac{1}{3}x^2\right), \tag{1.51}$$

the usual Taylor expansion of x. This will give

$$k\cot\eta_0 = \frac{k_+\cot(k_+r_0) + k^2 r_0^2}{1 - r_0\left(1 + \frac{1}{3}k^2 r_0 + \dots\right)k_+\cot(k_+r_0)} \tag{1.52}$$

and note that

$$k_+ r_0 = r_0\sqrt{k^2 + k_0^2} = k_0 r_0\left(1 + \frac{1}{2}\frac{k^2}{k_0^2} + \dots\right) = \gamma + \frac{1}{2}\frac{k^2 r_0^2}{\gamma}, \tag{1.53}$$

which allows us to write for $a \neq 0$

$$k\cot\eta_0 = -\frac{1}{a} + \frac{1}{2}k^2 \underbrace{r_0\left(1 - \frac{3ar_0 + \gamma^2 r_0^2}{3\gamma^2 a^2}\right)}_{r_e}, \tag{1.54}$$

where r_e is the effective range.

In the limit that $a = 0$, we can expand for $a \ll r_0$, in this case

$$\frac{1}{a\cot\eta_0} = -a + \frac{1}{6}k^2 r_0^3\left[1 - 3\left(\frac{a}{r_0}\right)^2 + \frac{3}{\gamma^2}\left(\frac{a}{r_0}\right)\right] + \dots \tag{1.55}$$

Now we will analyze some specific situations. If $a = |r_0|$, then

$$k\cot\eta_0 = -\frac{1}{a} + \frac{1}{3}k^2 r_0 + \dots \tag{1.56}$$

This is usually referred to as a "regular" scattering length where the order of the range and the order of the scattering and the range are the same. We can see that the second term is small in the ultracold regime and thus the scattering length is a

constant independent of energy. This is the typical case in cold atom experiments. In this case $r_e \approx 2r_0/3$.

Now we consider the case that $|a| \to \infty$, which yields

$$k \cot \eta_0 = -\frac{1}{a} + \frac{1}{2}k^2 r_0, \tag{1.57}$$

and $r_e = r_0$.

If $a \to 0$, then

$$r_e = -\frac{1}{3}r_0 \left(\frac{r_0}{a}\right)^2, \tag{1.58}$$

and

$$k \cot \eta_0 = \frac{6}{k^2 r_0^3} + \ldots \tag{1.59}$$

and so there is a very strong k dependence of the scattering length.

We now turn to the meaning of the effective range which is a quantity which describes the k dependence of the interaction. It is named as a distance because it was originally used to calculate the size of the nucleus in many atoms. This value can become negative in more complicated models.

1.3   Lecture 3

We are going to start with the effective range and talk about different types of important resonances.

1.3.1   S-wave Resonance

We start by looking at the resonance contribution to the phase shift

$$\tan \eta_{res}(a) = \frac{k}{k_+ \cot(k_+ r_0)}, \tag{1.60}$$

where $k_+ r_0 = (m + 1/2)\pi$. We will now look at the continuum for the square well and note that the "least bound" state (highest energy) contains information about the continuum. we can write

$$k_+ = \sqrt{k_0^2 + k^2} = \sqrt{k_0^2 + (k_{res} + \delta k)^2} = \sqrt{K_{res}^2 + 2k_{res}\delta k + \delta k^2} \tag{1.61}$$

where $K_{res} = k_0^2 + k_{res}^2$. We can look near the resonance and find that

$$k_+ = K_{res} + \delta k \frac{k_{res}}{K_{res}}, \tag{1.62}$$

We can see that in this approximation

$$k_+ \cot k r_0 \approx K_{res} \cot k_+ r_0. \tag{1.63}$$

We can write

$$\frac{k}{k_+ \cot(k_+ r_0)} \approx -\frac{1}{\delta k r_0} = -\frac{k + k_{res}}{(k^2 - k_{res}^2) r_0} \approx -\frac{2 k_r es}{(\epsilon - \epsilon_{res}) r_0} = -\frac{\Gamma/2}{E - E_{res}}, \quad (1.64)$$

where $\Gamma/2 = k_{res} \hbar^2/\mu r_0$. In the case where $\Gamma/2 \ll (E - E_{res})$. This gives rise to the following equation

$$\sin^2 \eta_{res} = \frac{(\Gamma/2)^2}{(E - E_{res})^2 + (\Gamma/2)^2}, \quad (1.65)$$

which is the Breit-Wigner lineshape.[4]

These resonances are generally at high energies and do not need to be worried about except when the first resonance is very close to the zero. The problem is that the lineshape is only well developed far from the origin and it is quite complicated and asymmetric near the origin.

We can think of the resonance enhancement of a near the threshold. We can write

$$a(k) = -\frac{\eta(k)}{k} = r_0 - \frac{1}{r} \arctan \left[\frac{k}{k_+ \cot(k_+ r_0)} \right], \quad (1.66)$$

and for a weakly bound state $k_+ \to k_0$ and thus $k_0 \cot(k_0 r_0) \to -\kappa$. Thus we can write

$$a(k) = r_0 + \frac{1}{k} \arctan \left[\frac{k}{\kappa + \frac{1}{2}\kappa^2 r_0} \right] \quad (1.67)$$

and we can rewrite this using the resonant scattering length as

$$a(k) = r_0 + \frac{1}{k} \arctan \left[\frac{k a_{res}}{1 + \frac{1}{2}k r_0^2 a_{res}} \right]. \quad (1.68)$$

One might ask how the resonance could be made more narrow even though are linked to the size of the well. One way to do it is to add a delta function potential at the edge of the well. This allows the wavefunction to build up in the well and you can get arbitrary phase shift.

1.3.2   General Short-Range Potentials

We have discussed the spherical square well, but it can be generalized to arbitrary short-range potential. We assume nothing about the shape beyond the fact that there is some range r_0. Thus, the radial equation can be written as

$$R_l'' + \frac{2}{r}R' + \left[k^2 - U(r) - \frac{l(l+1)}{r^2} \right] R_l = 0, \quad (1.69)$$

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[4]This is the same as the Lorentzian distribution for non-relativistic particles, which we are certainly dealing with in ultra-cold physics.

and first we look at $r \gg r_0$ in which case $U(r) = 0$ and we can write the radial wave equation as

$$R_l'' + \frac{2}{r}R' + \left[k^2 - \frac{l(l+1)}{r^2}\right]R_l = 0, \tag{1.70}$$

If we look at conditions where $kr \ll 1$. In this case, we can ignore the k dependence of the wavefunction and the potential as

$$R_l'' + \frac{2}{r}R' + \left[-\frac{l(l+1)}{r^2}\right]R_l = 0. \tag{1.71}$$

and so if $kr_0 \ll kr \ll 1$, which is equivalent to the condition

$$r_0 \ll r \ll \frac{1}{k}, \tag{1.72}$$

and in this region, Eq. (1.70) and Eq. (1.71) must coincide. We can solve Eq. (1.70) as

$$R_l(r) = \alpha_l j_l(kr) + \beta_l n_l(kr) = \alpha_l \frac{(kr)^l}{(2l+1)!!} + \beta_l \frac{(2l+1)!!}{2l+1}\left(\frac{1}{kr}\right)^{l+1}, \tag{1.73}$$

where we have used asymptotic forms and we can solve Eq. (1.71) as

$$R_l(r) = c_{1l}r^l + c_{2l}\left(\frac{1}{r}\right)^{l+1}, \tag{1.74}$$

and changing variables to $\alpha_l = A_l \cos \eta_l, \beta_l = A_l \sin \eta_l$, and equating equations, we get that

$$A_l \cos \eta_l = c_{1l}(2l+1)!!k^{-l} \tag{1.75}$$

$$A_l \sin \eta_l = c_{2l}\frac{(2l+1)}{(2l+1)!!}k^{l+1}, \tag{1.76}$$

and by taing the ratio of these terms and taking $kr \to 0$, we get that

$$\tan \eta_l = -\frac{2l+1}{[(2l+1)!!]^2}(ka_l)^{2l+1}, \tag{1.77}$$

where $a_l^{2l+1} = -a_{2l}/a_{1l}$. So for $l = 0$, we have for $kr \to 0$

$$\tan \eta_0 = -ka_0. \tag{1.78}$$

This approximation breaks down for $l > 1$, in other words, there is no phase shift independent of the potential for higher partial waves. For something like the Van der Waals potential, it is only valid for $l = 0, 1$.

If we write a potential as

$$U(r) = \frac{c_s}{r^s}, \tag{1.79}$$

the finite range is valid for $l < \frac{1}{2}(s-3)$. It can be shown that these high partial waves generally scale as

$$\sin \eta_l \sim (kr_c)^{s-2}(\kappa_c, r_c) 3\pi \frac{(2l+3-s)!!}{(2l+5)!!}, \tag{1.80}$$

where everything with subscript c is a constant.

This makes it very clear that dipole-dipole interactions are not short range.

1.3.3   Elastic Scattering of Unlike Atoms

We have two particles which are not identical and we want to examine the scattering. We know we can write the wavefunction for the relative motion of two particles at large r after scattering as a plane wave and an outgoing spherical wave

$$\psi(\vec{r}) \sim \underbrace{e^{ikz}}_{\psi_{in}} + \underbrace{f(\theta)\frac{e^{ikr}}{r}}_{\psi_{sc}}, \tag{1.81}$$

and we have already solved the relevant stationary wave equations, we can write the general solution

$$\psi(r,\theta) = \sum_{l=0}^{\infty} c_l (2l+1) i^l R_l(k,r) P_l(\cos\theta), \tag{1.82}$$

and we can compare this with the plane wave,

$$\psi_{in} = e^{ikz} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta), \tag{1.83}$$

which allows us to write

$$\psi_{sc} = \psi - \psi_{in} = \sum_{l=0}^{\infty} (2l+1) i^l Q_l(k,r) P_l(\cos\theta), \tag{1.84}$$

where

$$Q_l(k,r) = c_l R_l(k,r) - j_l(kr). \tag{1.85}$$

Far from the scattering center, we can use asymptotic forms, so

$$\lim_{r \to \infty} Q_l(kr) = \frac{1}{kr} \left[c_l \sin(kr + \eta_l(k) - l\pi/2) - \sin(kr - l\pi/2) \right], \tag{1.86}$$

and we must choose c_l to only get outgoing spherical waves as incoming spherical waves are not physics. We can use the complex forms of the sin function [5] to get that

$$\lim_{r \to \infty} Q_l(kr) = \frac{1}{2ikr} \left[c_l i^{-l} e^{ikr} e^{i\eta_l} - i^l e^{-ikr} e^{-i\eta_l} c_l - i^{-l} e^{ikr} + i^l e^{-ikr} \right], \tag{1.87}$$

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[5]$\sin x = \frac{1}{2i}(e^{ix} - e^{-ix})$; $e^{i\pi/2} = i$

and thus we must set

$$c_l = i^{i\eta_l}, \tag{1.88}$$

which produces only outgoing spherical waves. We get that

$$\lim_{r\to\infty} \psi_{sc} = \frac{e^{ikr}}{r} \underbrace{\frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)(e^{2i\eta_l} - 1)P_l(\cos\theta)}_{f(\theta)}, \tag{1.89}$$

which means that we can write

$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) f_l P_l(\cos\theta), \tag{1.90}$$

where we can write f_l in four different ways

$$\begin{aligned} f_l &= \frac{1}{2ik}(e^{2i\eta_l} - 1) \\ &= \frac{1}{k} e^{i\eta_l} \sin\eta_l \\ &= \frac{1}{k\cot\eta_l - ik} \\ &= \frac{1}{k}\left(\sin\eta_l \cos\eta_l + i\sin^2\eta_l\right). \end{aligned} \tag{1.91}$$

We can write the s-wave scattering as

$$\eta_0 = -ka \implies f_0 = -\frac{1}{k}e^{-ika}\sin(ka), \tag{1.92}$$

which in the limit of $k \to 0$ is just $f_0 = -a$.

1.4 Lecture 4

From last lecture, we have four different forms of the scattering amplitude. Now we calculate the imaginary part of the forward scattering amplitude

$$Im[f(0)] = \frac{1}{k} \sum_{l=0}^{\infty} (2l+1)\sin^2\eta_l. \tag{1.93}$$

Now we consider p wave scattering. We start with the expression for $l = 1$ phase shift

$$\eta_1 = -\frac{1}{3}(ka_1)^3, \tag{1.94}$$

If we substitute this into the equation for f_1 and then take the limit as $k \to 0$, we get

$$f_1 = -\frac{1}{3}k^2 a_1^3. \tag{1.95}$$

This means that the p-wave scattering scales as k^2, thus at low energy, there is no p-wave scattering.

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1.4.1   Cross Sections

Consider the situation where there are plane waves going towards the scattering potential and scattered into spherical ways. We consider a differential surface $dS = r^2 d\Omega$ as some angle θ, where Ω is the solid angle, thus $d\Omega = \sin\theta\, d\theta d\phi$. We look at the probability curent, which is given as

$$\vec{j} = \frac{i\hbar}{2\mu}(\psi\nabla\psi^* - \psi^*\nabla\psi), \tag{1.96}$$

and We can compute j_{in} and j_{sc}, which are vectors in the z direction. We can easily compute

$$j_{in} = \hat{z}\frac{\hbar k}{\mu} = v_z, \tag{1.97}$$

and similarly we can compute the scattered current [6]

$$j_{sc} = \frac{v_r}{r^2}|f(\theta)|^2 \tag{1.98}$$

We can look at the current scattered through surface dS which is given by

$$dI = j_r(r)dS = \frac{v_r}{r^2}|f(\theta)|^2 r^2 d\Omega = v|f(\theta)|^2 d\Omega. \tag{1.99}$$

Now we define $d\sigma$ as

$$d\sigma = \frac{dI}{j_i n} = |f(\theta)|^2 d\Omega \implies \frac{d\sigma}{d\Omega} = |f(\theta)|^2, \tag{1.100}$$

where the last term is the differential cross section. Since our potential is spherically symmetric, we can write the partial cross section as

$$d\sigma = 2\pi|f(\theta)|^2 \sin\theta\, d\theta, \tag{1.101}$$

and if we substitute in the expression for the scattering amplitude, we are left with

$$d\sigma = 2\pi\sin\theta\sum_{l=0}^{\infty}\sum_{l'}^{\infty}(2l+1)(2l'+1)f_l f_{l'}^* P_l(\cos\theta)P_{l'}(\cos\theta)\, d\theta, \tag{1.102}$$

and if we are interested only in the total cross section, the situation simplifies, since if we integrate both sides, we have

$$\sigma = 2\pi\sum_{l=0}^{\infty}(2l+1)^2|f_l|^2\int_0^{\pi}[P_l(\cos\theta)^2\sin\theta\, d\theta = 4\pi\sum_{l=0}^{\infty}(2l+1)|f_l|^2 = \sum_{l=0}^{\infty}\sigma_l \tag{1.103}$$

where the off diagonal terms are zero in the integral due to the orthogonality of the Legendre polynomials. If we are interested in the angular dependence, there is no

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[6]The θ dependence of the scattering amplitude is real and thus does not contribute to the current.

integration and the cross terms still exist. A very nice expression for the total cross section is

$$\sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \eta_l. \tag{1.104}$$

Now referring back to eq. (1.93), we can see that

$$\sigma = \frac{4\pi}{k} Im[f(0)], \tag{1.105}$$

which is know as the *Optical Theorem*.

Now we look at the s-wave cross section, which is given as

$$\sigma_0 = \frac{4\pi}{k^2} \sin^2 \eta_0, \tag{1.106}$$

since we found in the limiting case that $\eta_0 = -ka$, then we get that

$$\lim_{k \to 0} \sigma_0 = 4\pi a^2. \tag{1.107}$$

There is an issue that this seems to allow infinite cross section, however looking back before the approximation, we see that $\sigma_{max} = 4\pi/k^2$ which is known as the unitary limit. This cross section will be zero at about $kr_0 \approx 1$, also called a *Ramsauer-Townsend minimum*.

IF $a \neq 0$, we can write

$$k \cot \eta_0 = -\frac{1}{a} + \frac{1}{2} r_l k^2 + \dots \tag{1.108}$$

and we can write

$$\sigma_0 = 4\pi \left| \frac{1}{k \cot \eta_0 - ik} \right|^2 = \frac{4\pi}{k^2 \cot^2 \eta_0 + k^2}, \tag{1.109}$$

and we can look at several cases:

- For $a = 0$, we can write $\sigma_0 = \frac{1}{2} \pi r_0^2 (kr_0)^4$, but since $kr_0 \ll 1$, this will be negligible.

- If we look at $a = r_0$, then we have that $r_l = 2r_0/3$ which means that

$$\sigma_0 = \frac{4\pi a^2}{1 + (ka)^2/3}. \tag{1.110}$$

- For the case that $|a| \gg r_0$, then $r_l = r_0$ and

$$\sigma_0 = \frac{4\pi a^2}{1 + (ka)^2 (1 - r_0/a)} \approx \frac{4\pi}{k^2} \tag{1.111}$$

1.4.2   Identical Particle Scattering

For identical bosons (fermions), we must symmetrize (anti-symmetrize) the wave-function and consider incoming waves in two directions. We cannot distinguish scattering from θ and $\pi - \theta$. thus, we have for bosons

$$d\sigma(\theta) = 2\pi \sin\theta |f(\theta) + f(\pi - \theta)|^2, \tag{1.112}$$

where

$$f(\theta + f(\pi - \theta) = \sum_{l=0}^{\infty}(2l+1)f_l\left[P_l(\cos\theta) + P_l(-\cos\theta)\right] = 2\sum_{l=0 \text{ (even)}}^{\infty}(2l+1)f_lP_l(\cos\theta). \tag{1.113}$$

In the case of fermions, we have

$$d\sigma(\theta) = 2\pi \sin\theta |f(\theta) - f(\pi - \theta)|^2, \tag{1.114}$$

where

$$f(\theta - f(\pi - \theta) = \sum_{l=0}^{\infty}(2l+1)f_l\left[P_l(\cos\theta) - P_l(-\cos\theta)\right] = 2\sum_{l=1 \text{ (odd)}}^{\infty}(2l+1)f_lP_l(\cos\theta). \tag{1.115}$$

It is sort of odd to talk about identical fermions because we can't really have two particles in the same spin state that would be considered identical, but the scattering math still works out.

For fermions, s-wave scattering is not allowed among identical particles. For identical bosons, we can integrate and find

$$\sigma_0 = 8\pi a^2. \tag{1.116}$$

1.4.3   Two Potentials

The Feshbach Resonance comes out of the desire to vary the scattering length. If there is a single species in a single internal state, then the potential is given and there isn't anyway to tune the scattering length. If there is more than one species, or more than one internal state, it is possible to be tuned.

Thus, one needs two potential to tune the scattering length. Here we will develop a method to reduce two potentials into a single potential so that we can apply the tools of scattering which we have developed.

WE start with the Hamiltonian as before and note that two atoms can bind in an $^1\Sigma_g^+$ state or a $^3\Sigma_u^+$ state. The triplet state is non-binding, but does have the attractive tail of the Van der Walls interaction and the singlet state is quite tightly bound. These potential depend on the electronic spin state (symmetric is triplet, anti-symmetric is singlet), we can write a potential

$$V_s(r) = \begin{cases} V_1 & S = 1 \text{ (triplet)} \\ V_0 & S = 1 \text{ (singlet)} \end{cases} \tag{1.117}$$

and We must extend our Hilbert space $|\psi_{lm}\rangle = |R_l\rangle \otimes |lm\rangle \otimes |S, m_s\rangle$. We can write an effective spin Hamiltonian as

$$V(r) = V_D(r) + J(r)\vec{S}_1 \cdot \vec{S}_2, \tag{1.118}$$

and if we define $V_D(r) = \frac{1}{4}[V_0 + 3V_1]$ and we define $J = V_1 - V_0$, then this Hamiltonian has

$$V(r)|0,0\rangle = V_0(r)|0,0\rangle \tag{1.119}$$
$$V(r)|1, m_s\rangle = V_1(r)|1, m_s\rangle, \tag{1.120}$$

and we can use all the machinery we have developed.

1.5   Lecture 5

1.5.1   Feshbach Resonance Hamiltonian

For interactions between alkali atoms, we have two electrons and thus can have $S = 1, 0$. So this means that we have two potentials, either a singlet V_0 potential, or an $S = 1$ V_1 triplet potential. So the exchange determines interatomic interaction. Thus we can construct the spin Hamiltonian from the previous lecture.

Now we add in a magnetic field, which adds a Zeeman Hamiltonian

$$H_z = \gamma_e \vec{S}_1 \cdot \vec{B} + \gamma_e \vec{S}_2 \cdot \vec{B} = \gamma_e \vec{S} \cdot \vec{B} = \gamma_e B S_z, \tag{1.121}$$

where we have chosen the z axis as our magnetization axis and also can write $\gamma_e = g_s \mu_B / \hbar$. This gives rise to an energy difference $\Delta E_z = g_s \mu_B B M_S$, where $M_s = m_{s_1} + m_{s_2}$ is a good quantum number. So the Hamiltonian

$$H \frac{1}{2\mu}\left(p_r^2 + \frac{L^2}{r^2}\right) + V_S(r) + \gamma_e B S_z, \tag{1.122}$$

with good basis states $|\psi\rangle = |R_l\rangle|lm_l; \psi_e\rangle|S, M_s\rangle$. We solve the radial equation for given l, S, M_s, where the radial equation is given as

$$R_{S,l}, M_s'' + \frac{2}{r}R_{S,l,M_s}' + [\epsilon - U_{S,l,M_s}(r)]R_{S,l,M_s} = 0, \tag{1.123}$$

where

$$U_{S,l,M_s}(r) = U_S(r) + \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2}\gamma_e B M_s, \tag{1.124}$$

and therefore the magnetic field lifts the degeneracy of the triplet potential which allows us to shift it with respect to the singlet potential.

There is a least bound state in both the triplet and singlet potential. Weak singlet-triplet coupling induces resonance, this is referred to as *Feshbach resonance.* However, the Hamiltonian we have currently been studying does not couple the potentials as it is diagonal in the $|S, M_s\rangle$ basis. We need to add in another term.

In the simplest case, we have a two channel model where one state is in the continuum relative to the other potential. Actual calculations are difficult, however, asymptotic solutions can be mapped to models which give the same phase shifts. We can solve our Hamiltonian for continuum states $\epsilon > 0$ as

$$\epsilon_k = k^2 + \frac{2\mu}{\hbar^2}\gamma_e BM_s, \tag{1.125}$$

and if there are bound states $\epsilon < 0$ and

$$\epsilon_{v,l}^S = -\kappa_{v,S}^2 + l(l+1)\mathbf{R}_{v,l}^S + \frac{2\mu}{\hbar^2}\gamma_e BM_s, \tag{1.126}$$

where $\mathbf{R}_{v,l}^S = \langle R_{v,l}^S|r^{-2}|R_{v,l}^S\rangle$. Now we can add nuclear Zeeman terms (first for unlike atoms), with Hamiltonian

$$H_z = -\gamma_1 \vec{I}_1 \cdot \vec{B} - \gamma_2 \vec{I}_2 \cdot \vec{B}, \tag{1.127}$$

and then we must extend our basis to describe the nuclear spin. Now the potential shift includes the nuclear component. For identical atoms, $\vec{I} = \vec{I}_1 + \vec{I}_2$ nd $M_I = m_1 + m_2$ and thus

$$H_z = -\gamma_n \vec{I} \cdot \vec{B}, \tag{1.128}$$

induces a potential shift of

$$U_{S,l,M_s}(r) = U_S(r) + \frac{l(l+1)}{r^2} + \frac{2\mu}{\hbar^2}[\gamma_e BM_s - \gamma_n BM_i], \tag{1.129}$$

and we can extend the basis sates by $|I, M_I\rangle$. Now we need to include the hyperfine interactions.

We can write the hyperfine interactions for unlike atoms

$$H_{hf} = \frac{a_1}{\hbar^2}\vec{I}_1 \cdot \vec{S}_1 + \frac{a_2}{\hbar^2}\vec{I}_2 \cdot \vec{S}_2. \tag{1.130}$$

Note that $M_F = M_S + M_I$ is a good quantum number, but S is not a good quantum number, we have a term which couples the singlet and triplet interactions!

To analyze the interaction we can write

$$H_{hf} = H_{hf}^+ + H_{hf}^-, \tag{1.131}$$

where

$$H_{hf}^{\pm} = \frac{a_1}{2\hbar^2}\vec{I}_1(\vec{S}_1 \pm \vec{S}_2) \pm \frac{a_2}{2\hbar^2}\vec{I}_2(\vec{S}_1 \pm \vec{S}_2). \tag{1.132}$$

For identical atoms

$$H_{hf}^+ = \frac{a_1}{2\hbar^2}\vec{I} \cdot \vec{S}, \tag{1.133}$$

since $a_1 = a_2$. Thus H_{hf} can change M_s but not S. However, H_{hf}^- converts singlet to triplet and triplet to singlet. We can write our total Hamiltonian as

$$H\frac{1}{2\mu}\left(p_r^2 + \frac{L^2}{r^2}\right) + V_S(r) + H_z + H_{hf}^+ + H_{hf}^- \tag{1.134}$$

1.5.2   Feshbach Resonances

So consider the triply degenerate triplet potential [7]. Consider $\epsilon^{1,0}_{v=-1} = \epsilon^1$,[8] where $S = 1, l = 0$ (s wave), the east bound state. Now consider the singlet $S = 0, l = 0$ state and its least bound state $\epsilon^{0,0}_{v=-1} = \epsilon^0$. It is hard to calculate these numbers, but we can measure them.

Now we need to calculate the hyperfine states of an atom. We will work with ^{6}Li. Consider a pair of atoms, one with $|F = 1/2, m_f = -1/2\rangle$, the other with $|F = 1/2, m_f = 1/2\rangle$. These are both Fermions, but not identical, so there can be collisions in the s-wave. This pair has $m_F = 0$, we can have $S = 0$, an anti-symmetric state, $X^1\Sigma_g^+$. For $S = 1$, we have the symmetric state $a^3\Sigma_u^+$. Note that our total I and l quantum numbers must retain the symmetry of the state. Thus for $S = 0, I = 0$, we can only have $l = 0, 2, 4, \ldots$.

Since we are in the s-wave regime, we must conserve $l = 0$, we only need to consider states $S = 0, I = 0, 2$ or $S = 1, I = 1$ by symmetry requirements. When we consider ϵ^1, ϵ^0 and consider the free atoms, we can simply average the magnetic field dependence of the two atoms we are considering (note not identical particles, so no need to symmetrize). If we add the contribution of the Zeeman terms, the $S = 1$ develops triplet structure, and the $S = 0$ has no effect. The triplet state is further split by the hyperfine interaction.

Most of the physics is simple spin physics, however, in a narrow range of fields where $S = 1, S = 0$ have noticeable coupling. There is a Feshbach resonance whenever the free atom energies are the same as one of the bound states, However, not all of the positions have anything to do with the hyperfine interaction.

Writing the Hamiltonian

$$H = \frac{1}{2\mu}\left(p_r^2 + \frac{\vec{L}^2}{r^2}\right) + V_S(r) + \gamma_e B S_z - (\gamma_1 I_{z_1} + \gamma_2 I_{z_2})B + H_{hf}^+ + H_{hf}^-, \quad (1.135)$$

and we need to solve

$$det|\langle\beta|H|\alpha\rangle - IE| = 0, \quad (1.136)$$

and if we assume the energy is found from solving the radial wave equation and given as $\epsilon_v^{S,l}$, we have for $l = 0$,

$$\langle\beta|H|\alpha\rangle = [\epsilon_v^{S,l} + (\gamma_e M_s - \gamma_1 m_1 + \gamma_2 m_2)B]\langle\beta|\alpha\rangle + \langle\beta|H_{hf}^+ + H_{hf}^-|\alpha\rangle$$

$$= \epsilon_v^{S,l}(B)\delta_{v,v'}\delta_{\sigma,\sigma'} + \underbrace{\langle\sigma|H_{hf}^+|\sigma\rangle}_{-0 \text{ for } S\neq S'}\delta_{v,v'} + \underbrace{\langle\sigma'|H_{hf}^-|\sigma\rangle}_{=0 \text{ for } S=S'}\underbrace{\langle R_{v'}^{S',l}|R_v^{S,l}\rangle}_{\text{Franck-Condon}}, \quad (1.137)$$

it is important to consider this last term because it could be a Halo state, which is universal and thus the Franck-Condon factor is large. For other states, we can calculate numerically.

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[7]Thats why its called triplet!

[8]$v = -1$ corresponds to the highest vibrational level

The relation to the scattering length is affected by the coupling to the closed channel. This means that a magnetic field allows us to change the scattering length since we can the binding energies with a magnetic field. This gives

$$a(B) = a \left(1 - \frac{\Delta}{B - B_0} \right),$$
(1.138)

where $\Delta = \gamma / u_{eff} a$, where a is the background scattering length (normal scattering length).
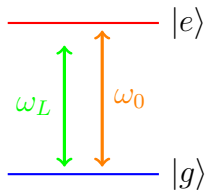
Figure 4: Two level atom

2 Laser Cooling and Trapping (Philippe Verkerk)

2.1 Lecture 1

The purpose of this lecture will be to explain when and why you can write the equation

$$\vec{F} - \alpha \vec{v}, \tag{2.1}$$

where $\vec{F}$ is some sort of friction force.

Laser cooling was developed in the 1980's and still widely used today. The first Magneto-Optical Trap (MOT) was realized in 1987. Some great lecture notes on this subject can be found by Helene Perrin. Also the 1990 Les Houches Lecture have some great work. The main difference is that here we will use Δ for detuning and they usually use δ.

Usually, we will picture the two level atom as in Figure 4. An atom is never actually a two level system, but we can treat it in such a way in certain approximations. Here we will consider one atom interacting with a light field characterized by a single frequency ω_L and it is an intense field (many photons) and we will be able to treat it classically. We will write it in the complex notation as

$$\vec{E}_L(t) = \frac{1}{2} \left(\vec{E}(\vec{r}) e^{-i\omega_L t} + \vec{E}^*(\vec{r}) e^{i\omega_L t} \right), \tag{2.2}$$

where $\vec{E}$ can depend on position. We can write it in a more useful form as

$$\vec{E}(\vec{r}) = \vec{\mathcal{E}} \underbrace{E(\vec{r}) e^{-i\phi(\vec{r})}}_{\text{real}}. \tag{2.3}$$

In the limit that the difference in frequencies of the levels ω_0 is close to ω_L and far from any other levels. So if define $\Delta = \omega_l - \omega_0$ and $|\Delta| \ll |\omega_L - \omega_j|$ where $|j\rangle$ is some other state.

An example atom is Cs which has a mass of 2.2×10^{-25}kg and a D_2 line of wavelength $\lambda_0 = 852$nm, corresponding to $\Gamma = 2\pi \times 5.22$MHz, which corresponds to a life time of 30ns. The mean velocity

$$\mu = \sqrt{\frac{k_B T}{M}} = 140 \text{ m/s}, \tag{2.4}$$

which can be compared to 300 m/s for Na. The recoil velocity is given as

$$v = \hbar k = 3.5 \text{ mm/s} , \tag{2.5}$$

and for Na, it is 30 mm/s. The comparison between these two velocities tells you how many photons you need to compensate for the velocity by exchanging photons. In particular for Cs, 10000 photons are required and it will take 3 ms to stop an atom at the maximal rate ($\Gamma/2$). However, to be exact, we would also need to include the Doppler broadening on the order of 10^9 rad/s which is much larger than Γ, which means that we need to play tricks in order to stay on resonance.

2.1.1   Hamiltonian

We can write the Hamiltonian for the atoms as

$$H_A = \hbar\omega_0 \,|e\rangle\langle e| + \frac{P^2}{2M} \tag{2.6}$$

and if we add the laser field, we introduce the dipolar effective interaction as

$$V_{AL} = -\vec{D} \cdot \vec{E}, \tag{2.7}$$

and also the vacuum field interaction as V_{AV}, and the vacuum field Hamiltonian as H_V. So the total Hamiltonian is

$$H = H_A + V_{AL} + H_V + V_{AV}, \tag{2.8}$$

and we will consider the momentum operator only when we need it.

Now introducing the reduced dipole elements

$$\vec{D} = \vec{d}\,|e\rangle\langle g| + \vec{d}^*\,|g\rangle\langle e| , \tag{2.9}$$

we write

$$\vec{d} = \left\langle e|\vec{D}|g\right\rangle . \tag{2.10}$$

We write

$$V_{AL} = -\vec{D} \cdot \vec{E}(\hat{R}, t) = V_{al}^{res} + V_{AL}^{non-res}, \tag{2.11}$$

where

$$V_{al}^{res} = -\frac{1}{2}(\vec{d} \cdot \vec{\mathcal{E}}(\vec{R}))E)L(\vec{R}\,) \,|e\rangle\langle g| \, e^{-i(\omega_L t + \phi(\vec{R}))} + h.c. \tag{2.12}$$

$$V_{al}^{non-res} = -\frac{1}{2}(\vec{d} \cdot \vec{\mathcal{E}}^*(\vec{R}))E_L(\vec{R}\,) \,|e\rangle\langle g| \, e^{i(\omega_L t + \phi(\vec{R}))} + h.c, \tag{2.13}$$

where $h.c$ stands for hermitian conjugate. Now we define the Rabi frequency Ω_1 as

$$\hbar\Omega_1 = -(\vec{d} \cdot \vec{\mathcal{E}}(\vec{r}))E_L(\vec{r}\,). \tag{2.14}$$

We can always make the Rabi frequency real and we will assume it is real for the rest of these notes.

We can now make the Rotating Wave Approximation (RWA). Introduce an operator $\Phi^+ = |e\rangle \langle g|$ and substitute this into the Heisenberg picture, so

$$\frac{d\Phi^+}{dt} = \frac{-i}{\hbar}[\Phi^+, H_A] = i\omega_0\Phi^+, \tag{2.15}$$

which means that the time propagator is $U = e^{i\omega_0 t}$. Now we note the time dependence of V_{AL}^{res} goes as $\Omega_1 e^{-i(\Delta t + \phi)}$ and the time dependence of $V_{AL}^{non-res}$ goes as $\Omega_1 e^{i((\omega_0+\omega_L)t+\phi)}$, and so if

$$|\Delta|, \Omega_1 \ll \omega_0, \omega_L, \tag{2.16}$$

[9] then $V_{AL} \approx V_{AL}^{res}$.

We can treat the vacuum H_v as

$$H_V = \sum_m \hbar\omega_m a_m^\dagger a_m, \tag{2.17}$$

and we can introduce $E_v = \sum_m (a_m^\dagger + a_m)$, and the vacuum atom interaction (keeping only the resonant part[10]) as

$$V_{AV} = V_{AV}^{res} \propto \sum_m \left[|g\rangle \langle e| a_m^\dagger + |e\rangle \langle g| a_m \right]. \tag{2.18}$$

2.1.2 Light Forces

In the semi-classical approximation, we consider the reduced wavelength

$$\lambda_r = \frac{\lambda}{2\pi} = k^{-1}, \tag{2.19}$$

which means that if $\Delta R \ll \lambda_r$, where R is the position operator, and $\Delta P \ll$ characteristic momentum , where P is the momentum operator, then we can use classical physics. In our case, we can write momentum condition as

$$k\frac{\Delta P}{M} \ll \Gamma, \tag{2.20}$$

which when combined with the Heisenberg equation gives

$$\hbar < \Delta R \Delta P \ll \frac{M\Gamma}{k^2}, \tag{2.21}$$

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[9]The magnitude of Δ is always satisfied by the conditions for a two level system. The size of the Rabi frequency will always be satisfied for optical radiation, but may not be for microwave radiation.

[10]Non-resonant terms can be disregarded as they do not conserve energy

and so the overall condition is that

$$\frac{\hbar^2 k^2}{M} \ll \hbar\Gamma, \tag{2.22}$$

which is known as the Broadband condition. For Cs, we can use the semi-classical picture. We can now switch to $\vec{r} = \langle R \rangle$ and $\vec{p} = \langle P \rangle$, the mean values of the operators.

The time-scales of this system can be broken into two times T_{int} and T_{ext}. For T_{int}, the relaxation time is Γ and so $T_{int} = \Gamma^{-1}$. For T_{ext}, we consider the exchange of photons, which gives a kick of momentum $\hbar k$ which a typical rate Γ[11], and a given as

$$a \sim \frac{\hbar k \Gamma}{M} = v_{recoil}\Gamma, \tag{2.23}$$

which leads to the conclusion that

$$ka T_{ex} \sim \Gamma, \tag{2.24}$$

and if we take our broadband condition from before, we can deduce that

$$T_{int} \ll T_{ext}. \tag{2.25}$$

Now we consider the force operator, which is given as

$$\vec{F} = \frac{d\vec{P}}{dt}, \tag{2.26}$$

and in the Heisenberg picture, we can write

$$\frac{d\vec{R}}{dt} = -\frac{i}{\hbar}[\vec{R}, H] = -\frac{i}{\hbar}\left[\vec{R}, \frac{P^2}{2M}\right] = \vec{v} \tag{2.27}$$

where we have noted that V_{AL}, H_V, V_{AV} do not depend on $\vec{P}$ and so will commute with R, and also that

$$\frac{d\vec{P}}{dt} = -\frac{i}{\hbar}[\vec{P}, H] = -\frac{i}{\hbar}[\vec{P}, V_{AL} + V_{AV}] = -\nabla V_{AL} - \nabla V_{AV}. \tag{2.28}$$

Now we will calculate the mean force for an atom at rest. We can write the mean force as

$$\vec{F}_{mean} = \left\langle \vec{F} \right\rangle = -\langle \nabla V_{AL} \rangle - \langle \nabla V_{AV} \rangle \tag{2.29}$$

where what is an operator and what is a vector is clear by context. We can say that $\langle \nabla V_{AV} \rangle$ since there is no preferential direction for emmitance of atom. Even if it is perturbed by a cavity, this will still hold, since there will always be paired emmiters. So

$$\vec{F} = -\langle \nabla V_{AL} \rangle. \tag{2.30}$$

---

[11]really $\Gamma/2$, but it doesn't matter here

2.2   Lecture 2

Now that we have calculated the force operator and taking the proper classical and semi-classical limits, we can now note that the internal degrees of freedom are the only dependence of the gradient operator acting on V_{AL}, thus

$$\nabla V_{AL} = \frac{\nabla \Omega_1(\vec{r})}{\omega_1(\vec{r})} V_{AL} - i\nabla \phi \frac{\hbar}{i} \Omega_1(\vec{r}) \left[|e\rangle \langle g| e^{-i(\omega_L t + \phi)} - h.c\right]. \tag{2.31}$$

Now we note that the mean value of an operator is given as

$$\left\langle \hat{A} \right\rangle = Tr[\hat{\sigma}\hat{A}], \tag{2.32}$$

where $\hat{\sigma}$ is the atomic density operator. We can rewrite the force as

$$F = -\langle \nabla V_{AL}^{res}\rangle = -\hbar \left[\nabla \Omega_1 \frac{\sigma_{ge} e^{-i(\omega_L t + \phi)} + c.c}{2} + \omega_1 \nabla \phi \frac{\sigma_{ge} e^{-i(\omega_L t + \phi)} - c.c}{2}\right], \tag{2.33}$$

and we can simply these by defining

$$u(t) = Re\left[\sigma_{ge} e^{-i(\omega_L t + \phi)}\right] \tag{2.34}$$

$$v(t) = Im\left[\sigma_{ge} e^{-i(\omega_L t + \phi)}\right] \tag{2.35}$$

$$w(t) = \frac{1}{2}(\sigma_{ee}(t) - \sigma_{gg}(t)) \tag{2.36}$$

Now we need to solve the Optical Bloch equations, however since $T_{int} \ll T_{ext}$ we are mainly interested in the stationary solution.

2.2.1   Optical Bloch Equations

The Optical Bloch equations can be written by considering

$$\sigma = \begin{pmatrix} \sigma_{ee} & \sigma_{ge} \\ \sigma_{eg} & \sigma_{gg} \end{pmatrix}, \tag{2.37}$$

with the restrictions $\sigma_{ee} + \sigma_{gg} = 1$ and $\sigma_{eg} = \sigma_{ge}^*$.[12] We can write down the master equation

$$\frac{d\sigma}{dt} = -\frac{i}{\hbar}[H_A + V_{AL}, \sigma] + \frac{d\sigma}{dt}, \tag{2.38}$$

and we will assume that

$$\frac{d\sigma}{dt} = -\Gamma \begin{pmatrix} \sigma_{ee} & \sigma_{ge}/2 \\ \sigma_{eg}/2 & -\sigma_{gg} \end{pmatrix} \tag{2.39}$$

---

[12]Note this is not the usual ordering, but we will remain consistent and the final answers will be the same.

and thus we can write

$$\dot{\sigma}_{ee} = -\Gamma \sigma_{ee} - i\frac{\Omega_1}{2}(\vec{r})\left(\sigma_{ge}e^{-i(\omega_L t + \phi)} - c.c\right)$$

$$\dot{\sigma}_{ge} = -\frac{\Gamma}{2}\sigma_{ge} + i\omega_0\sigma_{ge} + \frac{\Omega_1(\vec{r})}{2}(\sigma_{gg} - \sigma_{ee})e^{i(\omega_L t + \phi)}, \tag{2.40}$$

which are coupled equations with forcing terms. We are not interested in the general solution, but only in the stationary ones. [13] This gives

$$\sigma_{ee}^{stationary} = w + \frac{1}{2} \tag{2.41}$$

$$\sigma_{ge}^{stationary} = (u + iv)e^{i(\omega_L t = \phi)}, \tag{2.42}$$

and thus we can write down three new equations

$$0 = -\Gamma\left(w + \frac{1}{2}\right) + \Omega_1 v \tag{2.43}$$

$$0 = -\frac{\Gamma}{2} + \Delta v \tag{2.44}$$

$$0 = -\frac{\Gamma}{2} - \Delta u - \Omega_1 w, \tag{2.45}$$

which can be rearranged to solve for w, u, v as

$$w = \frac{\Omega_1}{\Gamma}v - \frac{1}{2} \tag{2.46}$$

$$u = \frac{2\Delta}{\Gamma}v \tag{2.47}$$

$$v = \frac{\Omega_1\Gamma}{4\Delta^2 + 2\Omega_1^2 + \Gamma^2} \tag{2.48}$$

$$\sigma_{ee} = \frac{\Omega_1^2}{4\Delta^2 + 2\Omega_1^2 + \Gamma^2}, \tag{2.49}$$

and We can now write the force by introducing the saturation parameter

$$s(\vec{r}) = \frac{\Omega_1^2/2}{\Delta^2 + \Gamma^2/4}, \tag{2.50}$$

and thus

$$\vec{F} = -\frac{s(\vec{r})}{1 + s(\vec{r})}\left[\hbar\Delta\frac{\nabla\Omega_1}{\Omega_1} + \frac{\hbar\Gamma}{2}\nabla\phi\right]. \tag{2.51}$$

Here the first term is related to the real part of the index of refraction in a quantum optics analogy and the second is related to absorption.

---

[13]We can also see why the non-resonant terms can be dropped by considering these terms in the perturbative limit where $\Omega_1 \ll \Gamma$.

2.2.2 Interpretation of Mean Force

We start by considering the radiation pressure which is related to the absorption and is a dissipative force we denote as F_{dis}. This is

$$\vec{F}_{dis} = -\frac{\hbar\Gamma}{2}\frac{s(\vec{(r)})}{1 + s(\vec{r})}\nabla\phi, \tag{2.52}$$

and so for an example, we will consider the plane wave. Here there is no positional dependence on the Rabi frequency ($\Omega_1(\vec{r}) = \Omega_1$ and $\phi = -\vec{k}\vec{r}$ which implies that $\nabla\phi = -\vec{k}$. Thus,

$$\vec{F}_{dis} = \hbar k \sigma_{ee}\Gamma, \tag{2.53}$$

which is the momentum change due to the dissipation of the photons. On resonance $\Delta = 0$ and thus $s = I/I_{sat}$, so

$$|\vec{F}_{dis}^{max}| = \frac{\hbar k\Gamma}{2}. \tag{2.54}$$

This will result in a Lorenztian distribution with a HWHM of $\sqrt{\Omega_1^2/2 + \Gamma^2/4}$. Again, this is much less than the Doppler width. We can compensate for this changing velocity to slow atoms using a Zeeman slower with a compensatory magnetic field.

The dipole force $\vec{F}_{dip}$ is given as

$$\vec{F}_{dip} = -\frac{s(\vec{r})}{1 + s(\vec{r})}\hbar\Delta\frac{\nabla\Omega_1}{\Omega_1}. \tag{2.55}$$

This force is conservative[14] and We know that $\Delta = 0 \implies \vec{F}_{dip} = 0$ and so the shape of the dispersion goes as $\Delta(4\Delta^2 + 2\Omega_1^2 + \Gamma^2)^{-1}$ and so the dipole force goes to zero slower than the dissipative force since it limits to $1/\Delta$ instead of $1/\Delta^2$. If the detuning is blue, the force is repulsive (atoms move away from light), if the detuning is red, the force is attractive.

2.2.3 Dressed Atom Picture

We can think of the laser as a quantum field, and so

$$H_L = \left(a_L^\dagger a_L + \frac{1}{2}\right)\hbar\omega_L, \tag{2.57}$$

and here

$$H = H_A + H_L + V_{AL}, \tag{2.58}$$

---

[14]To prove this note that $s \propto \Omega_1^2$ which means that $\nabla s/s = 2\nabla\Omega_1/\Omega_1$. Then noting that $\vec{F}_{dip} = -\nabla U(\vec{r})$, we can write down

$$\vec{F}_{dip} = -\hbar\Delta\nabla\ln(1 + s(\vec{r})). \tag{2.56}$$

and We can note that this splits into doublets of $|e, n\rangle$, $|g, n+1\rangle$ whose energy difference is just Δ. And so

$$E_{g,n} = n\hbar\omega_L + \frac{\hbar}{2}(\omega_L - \omega_) + \frac{1}{2}\hbar\omega_0, \tag{2.59}$$

and

$$E_{e,n-1} = n\hbar\omega_L - \frac{\hbar}{2}(\omega_L - \omega_) + \frac{1}{2}\hbar\omega_0 + n\hbar\omega_l + \frac{1}{2}\hbar\omega_0, \tag{2.60}$$

thus we can write

$$V_{AL}^{res} \frac{\hbar\Omega_0}{2}(a_l |e\rangle \langle g| + a_L^+ |g\rangle \langle e|), \tag{2.61}$$

which couples only levels in the same doublet. We can calculate

$$\langle g, n|V_{al}|e, n-1\rangle = \frac{\hbar\Omega_0}{2}\sqrt{n}, \tag{2.62}$$

and since we have an intense laser field, the mean number of photons $\bar{N} \gg 1$ and since we also have coherent fields, $\Delta^2 N = \bar{N}$, which allows us to replace $n \to \bar{N}$, as the maximum error scales as $\Delta N/N \ll 1$. The Hamiltonian can now be written in a very simple way,

$$H_n = \frac{\hbar}{2}\begin{pmatrix} -\Delta & \Omega_1 \\ \Omega_1 & \Delta \end{pmatrix} \tag{2.63}$$

where $\Omega_1 = \sqrt{\bar{N}}\Omega_0$. We can easily diagonalize this to find that

$$E_{n,\pm} = n\hbar\omega_L + \frac{1}{2}\hbar\omega_0 \pm \frac{\hbar}{2}\sqrt{\Delta^2 + \Omega_1^2}, \tag{2.64}$$

where the square root is sometimes referred to as the generalized Rabi frequency. This looks like a hyperbola and the separation at zero resonance is given as Ω_1.[15]

We can also write

$$|+, n\rangle = \sin\theta |g, n\rangle + \cos\theta |e, n-1\rangle \tag{2.65}$$

$$|-, n\rangle = -\cos\theta |g, n\rangle + \sin\theta |e, n-1\rangle, \tag{2.66}$$

where

$$\cos 2\theta = -\frac{\Delta}{\sqrt{\Delta^2 + \Omega_1^2}}. \tag{2.67}$$

---

[15]This can explain the restriction that $\Omega_1 \ll \omega_L$ for the rotating wave approximation to hold. This is so that the doublets when split by the Rabi frequency do not cross. This will never occur in the optical domain. In the microwave regime, this could occur.

2.2.4   Spontaneous Emission

The levels $|\pm, n\rangle$ are always mixtures of the ground and excited states. We will work in the secular limit which means that $\sqrt{\Delta^2 + \Sigma_1^2} \ll \Gamma$ and so the structure is not significantly changed by the emission. In this limit, the coupling between populations and coherence cancels. So the rate equations only depend on the populations in the levels. So if we define $\pi_\pm$ as the population in the $\pm$ state, we can write

$$\frac{d\pi_\pm}{dt} = -\Gamma_{\mp\pm}\pi_\pm + \Gamma_{\pm\mp}\pi_\mp, \tag{2.68}$$

and one can find that

$$\pi_+ - \pi_- = \frac{\Delta\Omega_1}{\Delta^2 + \Omega_1^2/2} \tag{2.69}$$

We can recalculate the diple force for an atom undergoes spontaneous emission by considering a general force

$$F = \pi_+ F_+ + \pi_- F_-, \tag{2.70}$$

to calculate the dipole force as

$$F_{dip} = -\frac{\hbar}{4}\left[\frac{\Delta}{\Delta^2 + \Omega_1^2/2}\right]\nabla\Omega_1^2. \tag{2.71}$$

2.3   Lecture 3

First we went over two questions from yesterday. There is first the dissipative force which arises from absorbing a photon in a single direction and emitting in a random direction, which gives gives rise to a momentum change of

$$\vec{q} = \vec{k}_L - \vec{k}_{sp}, \tag{2.72}$$

and in average only the $\vec{k}_L$ survives. This gives rise to the dissipative force. There is also stimulated emission, however, there is no momentum change for a single photon. For multiple photons, this is not true (this is why we need six MOT beams).[16]

The other point regarded the dressed atom where we introduce $\Gamma_{\pm\mp}$. If we wanted to calculate these quantities, we could note that we can change bases from $e, g, n \rightarrow +, -$ and write in a new form by introducing

$$\rho^+ = |e\rangle\langle g| \;;\; \rho^- = |g\rangle\langle e|, \tag{2.73}$$

which lets us write

$$\frac{d\sigma}{dt}\Big|_{\text{relax}} = -\frac{\Gamma}{2}(\rho^+\rho^-\sigma + \sigma\rho^+\rho^- - 2\rho^-\sigma\rho^+). \tag{2.74}$$
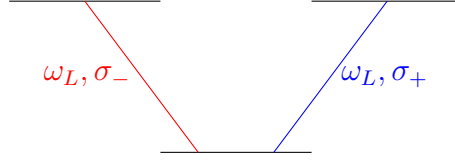
Figure 5: Three Level Atom
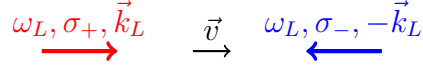
Figure 6: 1D mot illustration

2.3.1   Three Level Atom

We now consider the three level atom as shown in Figure 5, where we have two excited states with the same energy. If we are in a one dimensional magneto-optical trap, then two lasers with the same frequency will be detuned by the Doppler shift. So our two levels will be separated by $2\vec{k} \cdot \vec{v}$. We can consider the detuning

$$\Delta_\pm = \omega_L - \omega_0 \mp kv, \tag{2.75}$$

and if we add a magnetic field $\vec{B}$ across the system, we introduce another shift, which means the detuning is now give as

$$\Delta_\pm = \omega_L - \omega_0 \mp kv \mp \frac{g\mu_B B}{\hbar} = \Delta_\pm \delta, \tag{2.76}$$

and this picture is illustrated in Figure 6 We can write the forces for a single beam as

$$F_{dis} = \pm \frac{\Gamma}{2} \hbar \vec{k}_L \frac{s_\pm}{1 + s_\pm}, \tag{2.77}$$

and $F_{dip} = 0$, where

$$s_\pm = \frac{\Omega_\pm^2/2}{\Delta_\pm^2 + \Gamma^2/4}. \tag{2.78}$$

For two beams, we cannot just add up the forces from the $+$ and $-$.

We will work in the low saturation limit $s_\pm \ll 1$, which gives

$$F_{pm} = \pm \frac{\Gamma}{2} s_\pm \hbar \vec{k}_L, \tag{2.79}$$

and by assuming $\omega_+ = \Omega_- = \Omega_1$ and $|\delta| \ll |\Delta|, \Gamma$,

$$\vec{F} = \vec{F}_+ + \vec{F}_- = \frac{\Gamma}{2} \hbar \vec{k}_L \frac{\Omega_1^2}{2} \left(\frac{1}{(\Delta - \delta)^2 + \Gamma^2/4} - \frac{1}{(\Delta + \delta)^2 + \Gamma^2/4} \right), \tag{2.80}$$

---

[16]If the phases of the light are the same, then the force is zero.

again, this is only true in the this limit! We can expand these denominators to get a final expression for total force as

$$F = \frac{\Gamma\Omega_1^2\Delta\delta}{(\Delta^2 + \Gamma^2/4)^2}\hbar k_L,$$

(2.81)

where we have dropped the vectors with the understanding that in one dimension this is along the z axis. Note that the magnetic field is not uniform, rather $\delta = k_L v + g\mu bz/\hbar$, where $bz = B$ and thus we can write the force as

$$F = -\alpha v - \kappa z,$$

(2.82)

which is a friction force and a spring part. The coefficient α is given as

$$\alpha = \frac{-\Delta\Gamma\Omega_1\hbar k_L^2}{(\Delta^2 + \Gamma^2/4)^2}.$$

(2.83)

We can see that α increases with the intensity and is only positive if the detuning is negative. But, this expression is valid only until low saturation, so there is an upper limit on the size of α. Additionally, $\alpha = 0$ at resonance. Lastly, the wings of the distribution go as Δ^{-3} for constant laser detuning.

Now we will give a brief overview of the high intensity case. Writing the Hamiltonian as

$$H = \hbar \begin{pmatrix} 0 & \Omega_+ & \Omega_- \\ \Omega_-^* & \Delta_+ & 0 \\ \Omega_-^* & 0 & \Delta_- \end{pmatrix},$$

(2.84)

and we are using complex numbers for Ω, which means they are not really a frequency. We can solve the eigenvalue equation, but to get some idea of whats going on, we take $\delta = 0$, and our Hamiltonian becomes

$$H = \hbar \begin{pmatrix} 0 & \Omega_+ & \Omega_- \\ \Omega_-^* & \Delta & 0 \\ \Omega_-^* & 0 & \Delta \end{pmatrix},$$

(2.85)

which we can change to a couple level and an uncoupled level and write it as

$$H = \hbar \begin{pmatrix} 0 & \Omega & 0 \\ \Omega & \Delta & 0 \\ 0 & 0 & \Delta \end{pmatrix},$$

(2.86)

which is a two level system and can be solved easily. Going to nonzero δ, we can use first order perturbation theory to include its effects with a perturbation of

$$V = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & -\delta \end{pmatrix},$$

(2.87)

in the natural basis. We now calculate the atomic density matrix and then find the force as

$$F = \hbar k_L \Gamma (\sigma_{++} - \sigma_{--}), \tag{2.88}$$

and calculate first order corrections. The result is given (after a lengthy calculation)

$$F = -\alpha \vec{v}, \tag{2.89}$$

where

$$\alpha = 8\pi k_L^2 \frac{-\Delta\Gamma}{(4\Delta^2 + 2\Omega^2 + \Gamma^2)^2} \left[\Omega^2 + \frac{16|\Omega_+|^2|\Omega_-|^2\Gamma^2}{16\Gamma^2\Delta^2 + (2\Gamma^2 + \Omega^2)^2}\left(1 - \frac{\Omega^2}{4\Gamma^2}\right)\right], \tag{2.90}$$

which comes from the two states sharing a ground state and so the saturation conditions are coupled.

2.3.2　Limit Temperature

For now we just consider the classical friction force

$$F = -\alpha v, \tag{2.91}$$

which will bring the atom to rest classically. However, quantum mechanics does not allow this, we must have ignored something which is necessary quantum mechanically. This is due to the fact that F as considered here is the mean force. If we consider again the force operator, Eq. (2.28), thus we need to consider fluctuation part of the force to understand limits on temperature

$$\delta F = \delta F_l + \delta F_v. \tag{2.92}$$

To continue, we will make an analogy with Brownian motion and use somewhat loose argument to calculate the limit temperature. The Brownian motion considers the equation

$$\frac{dp}{dt} = -\gamma p + f(t), \tag{2.93}$$

where $f(t)$ is a fluctuating random force which has an average value of zero. To make an analogy with the case we are studying $\gamma = \alpha/M$.

We want to calculate the correlation function

$$C(t, t') = \overline{f(t)f(t')} \neq 0. \tag{2.94}$$

We can also write this as

$$C(\tau) = \overline{f(t)f(t+\tau)}. \tag{2.95}$$

The vacuum correlation time is quite small compared to the internal time and therefore the external time. After several cycles of absorption and spontaneous emission, the correlation will be lost, we can say that for $T_{int} \ll \tau \ll T_{ext}$,

$$C(\tau) = 2D\delta(\tau), \tag{2.96}$$

where $2D = \int d\tau \, \overline{f(t)f(t-\tau)}$. This allows us to write

$$p(t) = \underbrace{p_0 e^{-\gamma t}}_{\bar{p}} + \int_0^t dt' \, f(t') e^{-\gamma(t-t')} \tag{2.97}$$

We want to look at the variance of p, which is given as

$$\Delta p^2 = \overline{(p - \bar{p})^2} = \frac{D}{\gamma}(1 - e^{-2\gamma t}), \tag{2.98}$$

so for long times $\Delta p^2 = D/\gamma$, thus we have a temperature

$$k_B T = \frac{D}{M\gamma} = \frac{D}{\alpha} \tag{2.99}$$

Now for short times, $T_{int} \ll t \ll T_{ext}$, then by expanding the exponential

$$\Delta p^2 = 2Dt, \tag{2.100}$$

which allows us to consider the diffusion of photons. If during a time t, the atom scatters N photons, then

$$\Delta p^2 = \hbar^2 k^2, \tag{2.101}$$

since $\delta p = \hbar \vec{k}$. In one direction, we are interested in the projection of the three dimensional case on the axis, thus

$$\Delta p_z^2 = \frac{2\hbar^2 k^2}{5}, \tag{2.102}$$

where we have taken into account emission from a dipole.[17]

We know that for N photons, $N = (\pi_+ + \pi_-)\Gamma t$, which allows us to calculate the diffusion constant of the vacuum. When considering the atom laser interaction, we have already assumed the mean number, but really the number scattered is a random number with Poisson distribution and thus $\Delta N^2 = \overline{N}$. Thus

$$\Delta p^2 = 2Dt = \overline{N}\hbar^2 k_L^2 + \frac{2}{5}\bar{N}\hbar^2 k_L^2 \tag{2.103}$$

which leads to

$$D = \frac{\Gamma\Omega_1^2}{4\Delta^2 + \Gamma^2}\frac{7}{5}\hbar^2 k_L^2, \tag{2.104}$$

and thus our temperature

$$k_B T = \frac{D}{\alpha} = \hbar\Gamma\frac{7}{20}\frac{\Delta^2 + \Gamma^2/4}{|\Delta|\Gamma}, \tag{2.105}$$

and so the minimum temperature in 3D is given as

$$\frac{\hbar\Gamma}{2}, \tag{2.106}$$

which is interesting in that in the low saturation limit, it is not dependant on intensity. This is minimized when $|\Delta| = \Gamma/2$.

---

[17]The emission of a dipole is twice as large in one direction than the other. The emission value fraction is actually 2/5, not 1/3 as would be assumed isotropically

2.3.3   MOT as Non-Linear Object

So far we have made only single atom calculation and the consequence of this is that if one traps atoms and looks at the size of the cloud, it is a damped harmonic oscillator $\vec{F} = -\alpha\vec{v} - \kappa\vec{r}$. [18] We find that $\kappa\Delta r^2 = k_B T$. If we carry this out, we get a cloud of 10-100 μm.

However, we usually work with clouds of about 1mm. This means the model isn't well representing the size of the cloud. The actual MOT, is a Gaussian, with a flat top, meaning there is a maximum density. The missing element to our analysis is that in a one atom description does not account for the fact that the spontaneously emitted photon from one photon can interact with another atom. This multiple scattering occurs at high enough densities and this process is repulsive, but since the probability of absorption is perpendicular to the cross section, it falls off as $1/r^2$. This gives rise to a uniform density through the middle area of the MOT (would be completely uniform at $T = 0$).

This force can also give rise to non-linear effects since the force depends on the density and this gives rise to breathing in the MOT. This is similiar to Plasmas.

2.4   Lecture 4

2.4.1   Sub-Doppler Cooling

From our previous lecture, we found a minimum temperature, which gives a lower limit for Na of $T_{min} = 240\mu$K, but people working on Na at the time made some measurements using a technique called time of flight. This technique works by putting a sheet of light under the trap and turning off the cooling beams. As the atoms fall down, one can measure the absorption of the light as a function of time. There will be a profile which depends on the component of the velocity in the direction perpendicular to the beam. The spread of the profile allows one to extract the temperature.

In 1988, temperature was measured at 50 μK. Additionally, the temperature was going down with increased detuning. This violated the previous theory. in 1990, another violation was found as temperature increased with intensity.

The explanation for this is found by considering the fact that alkali atoms have many levels. Consider a system $J = 1/2 \to J' = 3/2$. The ground state has two levels and the excited state has four levels. We consider opposing laser of linear polarized light in x, y. The probability of absorption between different levels is proportional to the Clebsch-Gordon coefficients (also note only $\Delta J = \pm 1, 0$ are possible). We can

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[18]in a 3D MOT, there are six counter-propagating beams with correct propagation and a quadrupolar magnetic field given as $B = bx + by - 2bz$.

write the two fields as

$$\vec{E}_1 = \frac{\mathcal{E}}{2}\left(e^{-i\omega_L t + ikz}\vec{e}_x + c.c\right)$$

$$\vec{E}_2 = \frac{\mathcal{E}}{2}\left(e^{-i\omega_L t - ikz}\vec{e}_y + c.c\right)$$

$$\vec{E}_{tot} = \frac{\mathcal{E}}{2}\left(e^{-i\omega_L t}(e^{ikz}\vec{e}_x + e^{-ikz}i\vec{e}_y) + c.c\right)\left[e^{-i\omega_L t}(\cos kz(\vec{e}_x + i\vec{e}_y) + i\sin kz(\vec{e}_x - i\vec{e}_y)) + c.c\right]$$

(2.107)

So the coupling depends on the polarization and the position. So now we want to calculate the light-shifts in the ground state. The light-shift is the displacement of the energy level in the dressed state picture due to the interaction with light.

We will not do this for the general case, but in the case that $\Delta \gg \Gamma$ and low saturation $I \ll I_s$ and the population of the excited state is approximately zero, $\sigma_{ee} \approx 0$. We also note that σ_+ light couples $+1/2 \to 3/2$ and $-1/2 \to 1/2$ and the σ_- light couples $-1/2 \to -3/2$ and $1/2 \to -1/2$. This creates two independent three level systems. We can calculate the shift

$$u_+(z) = \frac{\hbar\Omega_1^2}{4\Delta}\left[\cos^2(kz) + \frac{1}{3}\sin^2(kz)\right]$$

$$u_-(z) = \frac{\hbar\Omega_1^2}{4\Delta}\left[\frac{1}{3}\cos^2(kz) + \sin^2(kz)\right],$$

(2.108)

and since we are still in the case that the Doppler cooling is working, we will consider $\Delta < 0$ which means the ground state is shifted down.

One can go to more complicated situations such as $J = 1 \to J' = 2$, which will give three separate three level systems.

Now we must consider the spontaneous emission from $|e, 1/2\rangle \to |g, -1/2\rangle, |g, 1/2\rangle$. At $z = 0$, there is σ_+ light which couples the $|g, -1/2\rangle$ state to $|e, 1/2\rangle$ which can emit to two states. In fact the decay is twice as likely to go to $|g, 1/2\rangle$, where it will then cycle between $|g, 1/2\rangle$ and $|e, 3/2\rangle$. This is called optical pumping, and will be the opposite for σ_- light. This means that the decay rate to the $1/2$ from the $-1/2$ is given as

$$\gamma_{-\to+} = \frac{2}{9}\Gamma\frac{\Omega_1^2/2}{\Delta^2 + \Gamma^2/4}\cos^2(kz).$$

(2.109)

So there is a correlation between the level shift and the optical pumping to other states. This is the cooling mechanism because atoms are optically pumped to the low energy contour of the opposite ground state whenever they reach high energy, losing potential energy in the process repeatedly.

While we are no longer in a regime where temperature is well defined by Boltzmann statistics, we can can get a temperature on order $\hbar\Omega_1^2/12\Delta$.

To make a more accurate calculation, we can write

$$F_\pm = -\nabla U_\pm,$$

(2.110)

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which implies that

$$\vec{F} = \pi_+(v)\vec{F}_+ + \pi_-(v)\vec{F}_-. \tag{2.111}$$

We are not going to do the calculation, but it turns out that

$$\vec{F} = \frac{-\alpha_s v}{1 + \frac{v^2}{v_c^2}}, \tag{2.112}$$

which is the normal friction force, but with an added capture range, so atoms that are too quick do not feel the effects of optical pumping. The friction coefficient can be calculated as

$$\alpha_s = 3\hbar k^2 \frac{|\Delta|}{\Gamma}, \tag{2.113}$$

and

$$kv_c = \frac{1}{9}\Gamma \frac{\Omega_1^2/2}{\Delta^2 + \Gamma^2/4}. \tag{2.114}$$

Comparing this with the Doppler cooling, we can also define a capture range since at high enough velocity, the atom is not resonant with either beam. So here the capture range is

$$v_c^{dop} = \frac{|\Delta|}{k}, \tag{2.115}$$

assuming large detuning.

So if we calculate the ratio of the Doppler cooling to the new mechanism (sisyphus cooling)

$$\frac{\alpha_d}{\alpha_s} \sim \frac{s\Gamma^2}{\Delta^2 + \Gamma^2/4} \ll 1 \tag{2.116}$$

we can see it has much larger cooling power. However, the capture range is much smaller.

The limiting temperature of this cooling mechanism is

$$k_B T \sim \frac{\hbar \Omega_1^2}{24\Delta}. \tag{2.117}$$

This explains how we get sub-Doppler temperatures.

2.4.2   Blue Sisyphus Cooling

Blue sisyphus cooling deals with two beams of the same polarization which are blue detuned. It requires large intensity, so it is not very useful.

3 Degenerate Gases (Dmitry Petrov)

3.1 Lecture 1

If we start with an $N = \infty$ ideal 3D uniform gas, we have no length scale except for the inter-particle spacing. There is some sort of universality related to this. We can break this by having short or long range interactions, go to lower dimensions, add a trap, or go to finite number. In practice we never have the ideal case.

Note that in these lectures $\hbar = m = k_B = 1$ and may be omitted.

We will consider a system with a discrete spectrum of single particle lectures and no interactions. We will consider the system in the grand canonical picture (connected to a bath of bosons with chemical potential μ). Equivalently, we can consider each level as a separate grand-canonical ensemble interacting with the bath of all other levels. We write the partition function as

$$Z_\nu = \sum_{n=0}^{\infty} e^{-(\epsilon_\nu n - \mu n)/T} = 1 + Z_\nu e^{-(\epsilon_\nu - \mu)/T} \implies Z_N = \frac{1}{1 - e^{-(\epsilon - \mu/T)}}, \tag{3.1}$$

and We can calculate the mean occupation of this level as

$$\begin{aligned} \langle N_\nu \rangle &= T \frac{\partial \ln Z}{\partial \mu}\Big|_{T \text{ constant}} \\ &= T \left(1 - e^{-(\epsilon - \mu)/T}\right)(-1)\frac{1}{T} e^{-(\epsilon - \mu)/T} \left(1 - e^{-(\epsilon - \mu)/T}\right)^{-2} \\ &= \frac{1}{e^{(\epsilon - \mu)/T} - 1}, \end{aligned} \tag{3.2}$$

which is the Bose-Einstein distribution. We want the nontrivial case of macroscopic ground state occupation, where $T \gg \epsilon_1 - \epsilon_0$. We can do the same to get the Fermi-Dirac distribution.

The total number of particles in the trap N, is given as

$$\sum_\nu \langle N_\nu \rangle = \sum_\nu \frac{1}{e^{(\epsilon_\nu - \mu)/T} - 1}. \tag{3.3}$$

We can now set $\epsilon_0 = 0$, which allows us to rewrite our state as

$$N = \frac{1}{e^{-\mu/T} - 1} + \sum_{\nu > 0} \langle N_\nu \rangle. \tag{3.4}$$

If the first term is large (denominator is small), then we can Taylor expand the exponential in the denominator if $\mu \ll T$ to get that

$$\frac{1}{e^{-\mu/T} - 1} \approx -\frac{T}{\mu}. \tag{3.5}$$

3.1.1 Harmonic Oscillator Example

Consider harmonic oscillators in 1,2,3 dimensions. For 1d, $\epsilon_n = \hbar\omega n$ (we have set ground state to zero). For 2d, $\epsilon_{n_x,n_y} = \hbar\omega(n_x + n_y) = \hbar\omega n$, which is degenerate by a factor of $g_n = n + 1$. For 3d $\epsilon = \hbar\omega n$, where the degeneracy is $(n+1)(n+2)/2$.

We have that

$$N = N_0 + \sum_{n=1}^{\infty} \frac{g_n}{e^{(\hbar\omega n - \mu)/T}}. \tag{3.6}$$

We know that the degeneracy is approximately n^2 and so for small n we have that

$$N \approx \sum_{n=1}^{T/\hbar\omega} \frac{n^2}{2} \frac{T}{n - \mu/\hbar\omega}, \tag{3.7}$$

and so the conclusion is that chemical potential is not important and the main contributions come from $n \approx T/\hbar\omega$. We can then integrate this equation to get N. For the two dimensional case, a similiar pattern emerges and we can also integrate. For the 1d case, we have a logarithmic divergence and we cannot integrate.

So for three dimensions

$$N = N_0 + \int_0^{\infty} \frac{n^2}{2\left(e^{\hbar\omega n/T} - 1\right)} \, dn = N_0 + \sum_{k=1}^{\infty} \int_0^{\infty} \frac{n^2}{2} e^{-\hbar\omega n/Tk} \, dn, \tag{3.8}$$

and if we define $x = \hbar\omega n/T$, then we can write

$$N = N_0 + \left(\frac{T}{\hbar\omega}\right)^3 \sum_{k=1}^{\infty} \frac{1}{k^3}, \tag{3.9}$$

and if we cna also note that $\sum_{k=1}^{\infty} \frac{1}{k^3} = \zeta(3) \approx 1.2$. We can write

$$N = N_0 + N\left(\frac{T}{T_c}\right)^3 \implies T_c = \hbar\omega\left(\frac{N}{\zeta(3)}\right)^{1/3} \tag{3.10}$$

which implies that

$$N_0 = N\left(1 - \left(\frac{T}{T_c}\right)^3\right). \tag{3.11}$$

This is a typical behavior for a BEC. In the 2d case,

$$N = N_0 + \int_0^{\infty} xe^{-x} \, dx \left(\frac{T}{\hbar\omega}\right)^2 \sum_{k=1}^{\infty} \frac{1}{k^2}, \tag{3.12}$$

which is also solvable, and $\sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{6}$. We have that

$$N = N_0 + N\left(\frac{T}{T_c}\right)^2, \tag{3.13}$$

and thus,

$$T_c = \hbar\omega\sqrt{\frac{N}{\zeta(2)}}. \tag{3.14}$$

This is all done in the limit $N \to \infty$, when N is finite, there is no longer a sharp transition at T_c. We would like to calculate the width of this region in 2d. We know that

$$N = N_0 + N\left(\frac{T}{T_c}\right)^2 + \sum_n \frac{g_n}{e^{(\hbar\omega n - \mu)/T} - 1} - \int_0^\infty \frac{n}{e^{\hbar\omega n/T} - 1}\, dn, \tag{3.15}$$

and we are interested in the correction term, which is the difference of the sum and the integral. We can cut off the sum at $T/\hbar\omega$, expand both terms and transform the integral into a sum as

$$\sum_n \frac{g_n}{e^{(\hbar\omega n - \mu)/T} - 1} - \int_0^\infty \frac{n}{e^{\hbar\omega n/T} - 1}\, dn = \sum_{n=1}^{T/\hbar\omega}\left[(n+1)\frac{T}{\hbar\omega(n - \mu/\hbar\omega)} - \frac{T}{\hbar\omega}\right]$$

$$= \frac{T}{\hbar\omega}\sum_{n=1}^{T/\hbar\omega}\left[\frac{n + 1 - n + \mu/\hbar\omega}{n - \frac{\mu}{\hbar\omega}}\right]$$

$$= \left(1 + \frac{\mu}{\hbar\omega}\right)\sum_{n=1}^{T/\hbar\omega}\frac{1}{n - \hbar\omega/\mu}$$

$$\approx \frac{T}{\hbar\omega}\left(1 + \frac{\mu}{\hbar\omega}\right)\ln\frac{T/\hbar\omega}{1 - \hbar\omega/\mu}, \tag{3.16}$$

which is the finite size correction (could be positive or negative).[19]

Now we can change $T \to T_c$ and we can estimate the correction as

$$\frac{N}{N_0}\ln\sqrt{N}. \tag{3.17}$$

So this gives tht

$$\frac{\Delta T}{T_c} \sim \frac{\ln N}{\sqrt{N}}. \tag{3.18}$$

Now by knowing the density of states, we can do this for real systems. This is given in a trap by

$$\rho(\epsilon) = \begin{cases} \frac{\epsilon^2}{(\hbar\omega)^2} & 3d \\ \frac{\epsilon}{(\hbar\omega)^2} & 2d \\ \frac{1}{\hbar\omega} & 1d \end{cases} \tag{3.19}$$

---

[19]This is just an estimate, but it is only off by corrections of $\ln(x)$ where x is small in the units of $\frac{T}{\hbar\omega}\left(1 + \frac{\mu}{\hbar\omega}\right)$.

For a box

$$\rho(\epsilon) \propto \begin{cases} \sqrt{\epsilon} & 3d \\ constant & 2d \\ \frac{1}{\sqrt{\epsilon}} & 1d \end{cases} \tag{3.20}$$

So in a 3d trap,

$$T_c = \hbar\omega \left(\frac{N}{\zeta(3)} \right)^{1/3}, \tag{3.21}$$

and for a 3d box

$$T_c = \frac{2\pi\hbar^2}{m} \left(\frac{N/V}{\zeta(3/2)} \right)^{2/3}. \tag{3.22}$$

So, we can get that $T \to T_c^{box}(n_0) = T_c^{trap}(N)$.

For the case of a 1d trap, we have that

$$N = N_0 + \sum_n \frac{1}{e^{(\hbar\omega n - \mu)/T} - 1} = N_0 + \frac{T}{\hbar\omega} \ln \left[\frac{T/\hbar\omega}{1 + (T/\hbar\omega N_0)} \right], \tag{3.23}$$

and if we neglect the term with $1/N_0$, we get

$$N_0 = N - \frac{T}{\hbar\omega} \ln \frac{T}{\hbar\omega}, \tag{3.24}$$

and the width of the crossover region is

$$\frac{\Delta T}{T_c} \sim \frac{1}{\ln N}. \tag{3.25}$$

This will be similar for a 2d box.

The conclusion of this lecture is that BEC is non-trivial for T larger than energy separation. For finite N, we have crossover regions.

3.2   Lecture 2

First we will clear up some peculiarities of a two dimensional finite BEC. We can define the degeneracy temperature in an $L \times L$ box with N particles,

$$T_d = \frac{\hbar^2 N}{mL^2} = \frac{\hbar^2 n}{m} \tag{3.26}$$

and the condensation temperature is given as

$$T_c = \frac{T_d}{\ln N}. \tag{3.27}$$

If we consider the difference in the lowest two energy states $\epsilon_1 - \epsilon_0 = \frac{\hbar^2}{mL^2} \sim 1/N$. If we keep n the same but send $L \to \infty$ and $n \to \infty$, we don't get condensation.

3.2.1   Perturbation Theory

Many potentials are hard to integrate[20] and thus we must develop some sort of theory to describe these potential. In practice, people integrate high order modes to create an effective potential.

For many purposes, all potentials with the same scattering length are equivalent. Take the case of a positive square well. Here the scattering length is positive, but smaller than the size of the well. So, consider a box of volume V, with a Hamiltonian for two particles neglecting interactions

$$H = -\frac{\hbar^2}{2m}(\nabla_1^2 + \nabla_2^2), \tag{3.28}$$

and We can consider the ground state wavefunction,

$$\psi_{0,0} = \frac{1}{\sqrt{V}}\frac{1}{\sqrt{V}}, \tag{3.29}$$

which is correctly normalized and has energy $E^{(0)} = 0$. We want to find the first correction with perturbation $U(r_1 - r - 2)$,

$$\Delta^{(1)} = \langle\psi_{0,0}|U|\psi_{0,0}\rangle = \int_v\int_V d^3r_1 d^3r_2 U(r_1 - r_2)\frac{1}{V^2} = \frac{1}{V}U(0), \tag{3.30}$$

where $U(0) = \int(U(r)d^3r$, where we have switched to relative coordinates $R = (r_1 + r_2)/2$ and $r = r_1 - r_2$. Now we can calculate the second order correction

$$\Delta^{(2)} = \sum_{k_1,k_2\neq 0,0}\frac{|\langle\psi_{k_1,k_2}|U|\psi_{0,0}\rangle|^2}{\epsilon_0 - \hbar^2 k_1^2/2m - \hbar^2 k_2^2/2m}. \tag{3.31}$$

We can write

$$\psi_{k_1,k_2} = \frac{1}{V\sqrt{2}}\left(e^{i\vec{k}_1\cdot\vec{r}_1}e^{i\vec{k}_2\cdot\vec{r}_2} + e^{i\vec{k}_2\cdot\vec{r}_1}e^{i\vec{k}_1\cdot\vec{r}_2}\right), \tag{3.32}$$

where we have symmetrized the wavefunction since we are using Bosons.

So now we can calculate

$$\langle\psi_{k_1,k_2}|u|\psi_{0,0}\rangle = \int\int d^3r_1 d^3r_2 \frac{1}{V\sqrt{2}}\left(e^{i\vec{k}_1\cdot\vec{r}_1}e^{i\vec{k}_2\cdot\vec{r}_2} + e^{i\vec{k}_2\cdot\vec{r}_1}e^{i\vec{k}_1\cdot\vec{r}_2}\right)u(r_1-r_2)\frac{1}{V}, \tag{3.33}$$

and by using $r_1 = R + R/2$ and $r_2 = R - r/2$, we have

$$\langle\psi_{k_1,k_2}|u|\psi_{0,0}\rangle = \frac{1}{\sqrt{2}V^2}\int d^3R d^3r e^{-i(\vec{k}_1+\vec{k}_2)R}\left[e^{-i(\vec{k}_1-\vec{k}_2)r/2} + c.c\right]u(r) \tag{3.34}$$

Now, we will let $\vec{k}_1 = \vec{k}_2 = \vec{q}$. This means that

$$\langle\psi_{k_1,k_2}|u|\psi_{0,0}\rangle = \frac{1}{\sqrt{2}V}U(\vec{q}) + u(-\vec{q}) = \frac{\sqrt{2}}{V}u(\vec{q}), \tag{3.35}$$

---

[20]The simplest example, the hard infinite wall, cannot be integrated in the Born Approximation.

which implies that

$$\Delta^{(2)} = \left(\frac{\sqrt{2}}{V}\right)^2 \sum_{q>0} \frac{|U(q)|^2}{-\hbar^2 q^2/m} = -\frac{1}{V^2}\frac{m}{\hbar^2}\sum_q \frac{U(q)^2}{q^2} \tag{3.36}$$

where we have set $\epsilon_0 = 0$. We can write the total change in energy to second order as

$$\Delta E = \frac{U(0)}{V} - \frac{1}{V^2}\frac{m}{\hbar^2}\sum_q \frac{U(q)^2}{q^2} \tag{3.37}$$

Now we impose a validity condition, which is that $U(0)/V \gg \Delta^{(1)}, \Delta^{(2)}$. If we note that

$$\sum_q = V \int \frac{d^3q}{(2\pi)^3}, \tag{3.38}$$

we can take a real potential and write $U(0) \sim U_c r_0^3$ (c stands for coordinate) and thus for $q \ll 1/r_0$

$$\sum_q \frac{1}{V}\frac{m}{\hbar^2}\frac{U^2}{q^2} = \frac{1}{V^2}\frac{m}{\hbar^2}U_c^2 r_0^5 V, \tag{3.39}$$

Thus the validity condition becomes

$$U_c \ll \frac{\hbar^2}{mr_0^2}, \tag{3.40}$$

which is the condition for application of the Born series. This condition is equivalent to $a \ll r_0$.

If we calculate $\Delta^{(1)}$ for the general state, we have

$$\Delta^{(1)} = \langle\psi_{k_1,k_2}|U|\psi_{k_1,k_2}\rangle = \int\int d^3R d^3r \frac{\left[e^{-i\vec{q}\cdot\vec{r}} + e^{i\vec{q}\cdot\vec{r}}\right]^2}{2V^2}U(\vec{r}) = \frac{1}{V}\frac{[U(2\vec{q}) + U(0)]}{V} \tag{3.41}$$

In this case of $q \ll 1/r_0$, we have

$$\Delta^1 = \frac{2U(0)}{V}. \tag{3.42}$$

So condensed atoms have half the energy shift of the non-condensed atoms.

If we only know the scattering length, but not the potential, we can still make some claims about the potential. To see this, we can calculate the correction to the wavefunction

$$\psi_{0,0}^{(1)} = \sum_{k_1,k_2} \frac{\langle\psi_{k_1,k_2}|U|\psi_{0,0}}{-\hbar^2 k_1^2/2m - \hbar^2 k_2^2/2m}|\psi_{k_1,k_2}\rangle = \sum_{q>0} \frac{\frac{\sqrt{2}}{V}U(\vec{q})}{-\hbar^2 q^2/2m} \tag{3.43}$$

and we are interested in the limit $r \gg r_0$. This allows us to simplify the integral and get that

$$\psi_{00} = \frac{1}{V}\left(1 - \frac{mU(0)}{4\pi\hbar^2}\right), \tag{3.44}$$

which means that to first order

$$a^{(0)} = \frac{mU(0)}{4\pi\hbar^2}E, \tag{3.45}$$

where E is the energy with corrections and higher terms are negligible. Additionally,

$$a^{(\infty)} = \frac{mV}{4\pi\hbar^2}E^{(\infty)} \tag{3.46}$$

3.2.2   Many Body Bosons, Second Quantization

We can write the many body Hamiltonian for N bosons with weak interaction as

$$H = \sum_i -\frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}\sum_{ij}u(r_i - r_j) + \frac{1}{3!}\sum_{ijk}u(r_i, r_j, r_k), \tag{3.47}$$

including three body interactions. Fortunately, Dirac created second quantization for Bosons. It was generalized one year later by Wigner and Jordan to fermions. In second quantization the state of the system is described by the number of the particles in each of the states $|n_0, n_1, \ldots\rangle$, and postulate an operator a_ν which takes

$$a_\nu |n_0, \ldots, n_\nu, \ldots\rangle = \sqrt{n_\nu}|n_0, \ldots, n_\nu - 1, \ldots\rangle, \tag{3.48}$$

and its Hermition conjugate $a_\nu^\dagger$, which operates by

$$a_\nu^\dagger |n_0, \ldots, n_\nu, \ldots\rangle = \sqrt{n_\nu + 1}|n_0, \ldots, n_\nu + 1, \ldots\rangle, \tag{3.49}$$

and these operators have the following properties

1. $a_\nu^\dagger a_\nu = n_\nu$.

2. $[a_\nu, a_\nu^\dagger] = a_\nu a_\nu^\dagger - a_\nu^\dagger a\nu = 1$.

3. $a_\nu a_\mu = a_\mu a_\nu$

We can write down the original Hamiltonian as

$$H = \sum_{\vec{k}} a_k^\dagger\left(-\frac{\hbar^2 k^2}{2m}\right)a_k + \frac{1}{2V}\sum_{k_1,k_2,q}a_{\vec{k}_1+\vec{q}}^\dagger a_{\vec{k}_2-\vec{q}}^\dagger U(q)a_{k_1}a_{k_2} + \text{higher order} \tag{3.50}$$

Now we can again calculate $\Delta^{(1)}$ for the ground state. Note that this corresponds to

$$\psi_{0,0} = |2, 0, 0, \ldots, 0\rangle. \tag{3.51}$$

Now, when we calculate this, we have three summed terms, but only terms where $q = k_1 = k_2 = 0$ contribute. Thus we will get

$$\Delta^{(1)} = \frac{U(0)}{V}, \tag{3.52}$$

exactly what we got before. We can also calculate the second order contribution. It is straightforward, but tedious and we will only quote the answer as

$$\Delta^{(2)} = \frac{1}{V}(U(k_1 - k_2) + U(0)), \tag{3.53}$$

which is also the same answer, thus this may be an easier framework to work in as it automatically accounts for symmetrization.

3.3 Lecture 3

3.3.1 Bogoliubov Theory

We will focus on Bogliubov theory which was the first theory to treat weakly inter-acting Bose gas. If we start with $T = 0$ and $U = 0$ with N_0 atoms in the ground state. We now note that $a_0 \sim \sqrt{N_0}$ and we can make the approximation $a_0^\dagger \sim \sqrt{N_0}$ since N_0 is large and if we ignore the quantum nature of the operator, we get

$$a_0 = a_0^\dagger = \sqrt{N_0}. \tag{3.54}$$

Thus the Hamiltonian becomes

$$H = \frac{N_0^2}{2V}U(0) + \sum_{k \neq 0} a_k^\dagger \left(-\frac{\hbar^2 k^2}{2m}\right) a_k + \frac{1}{2V} \sum_q \left[a_q^\dagger a_{-q}^\dagger U(q) + a_q a_{-q} U(q)\right]$$

$$+ \frac{N_0}{V} \sum_q \left[a_q^\dagger u(0) a_q + a_q^\dagger U(q) a_q\right], \tag{3.55}$$

where the factor of two in the second term comes from symmetry in k_1, k_2. There will also be higher order terms, but we will rewrite this Hamiltonian as

$$H = \frac{N_0^2}{2V}U(0) + \sum_q \left[\left(\frac{\hbar^2 q^2}{2m} + \frac{(U(0) + U(q))}{V}N_0\right)a_q^\dagger a_q + \sum_q \frac{N_0 U(q)}{2V}\left(a_q^\dagger a_{-q}^\dagger + a_q a_{-q}\right)\right], \tag{3.56}$$

where q is understood to be a vector. We know that we can take these two coupled operators and find normal modes. We want to get the Hamiltonian in the form $H = n + \sum_q \epsilon(q)\alpha_q^\dagger \alpha_q$, where n is a number. We introduce the Bogoliubov transformation

$$a_k = u_k \alpha_k + v_k \alpha_{-k}^\dagger, \tag{3.57}$$

where $u_k = u_{-k}$, $v_k = v_{-k}$ and are real numbers. Additionally, we require $[\alpha_k^\dagger, \alpha_k] = 1$, which yields the condition

$$u_q^2 - v_q^2 = 1. \tag{3.58}$$

If we substitute these into our Hamiltonian, we wind up with a formula giving rise to coupled non-linear differential equations. This is quite hard to solve in general for many coupled modes. Thus, we need another method.

We first note that $N_0 = N - \sum_q a_q^\dagger a_q$ and thus we can approximate $N = N_0$ except in the first term of the Hamiltonian as the first term is quadratic in N_0 and the other terms are linear in the operators. We get some cancellation in our Hamiltonian which now becomes

$$H = \frac{N^2 U(0)}{2V} - \frac{1}{2}\sum_q \left(\frac{\hbar^2 q^2}{2m} + \frac{NU(q)}{V}\right) + \frac{1}{2}\sum_q (a_q^\dagger, a_q)\begin{pmatrix} \frac{\hbar^2 q^2}{2m} + \frac{NU(q)}{V} & \frac{NU(q)}{V} \\ \frac{NU(q)}{V} & \frac{\hbar^2 q^2}{2m} + \frac{NU(q)}{V} \end{pmatrix}\begin{pmatrix} a_q \\ q_{-q}^\dagger \end{pmatrix}, \tag{3.59}$$

for a two component gas. The matrix will scale with the number of components. If we looks for the solution to the equation

$$\begin{pmatrix} A & B \\ B & A \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = \epsilon\begin{pmatrix} u \\ -v \end{pmatrix} \tag{3.60}$$

then $-\epsilon$ will also be a solution, in the sense that

$$\begin{pmatrix} A & B \\ B & A \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = -\epsilon\begin{pmatrix} u \\ -v \end{pmatrix} \tag{3.61}$$

which implies that

$$\begin{pmatrix} u & v \\ v & u \end{pmatrix}\begin{pmatrix} A & B \\ B & A \end{pmatrix}\begin{pmatrix} u & v \\ v & u \end{pmatrix} = \epsilon\begin{pmatrix} u^2 - v^2 & 0 \\ 0 & u^2 - v^2 \end{pmatrix} = \epsilon\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{3.62}$$

which means this is equivalent to diagonalizing the matrix

$$\begin{pmatrix} A & B \\ -A & -B \end{pmatrix}, \tag{3.63}$$

which gives the solution

$$\epsilon = \pm\sqrt{A^2 - B^2}, \tag{3.64}$$

and now going back to the matrix in the Hamiltonian, and making the change of variables

$$\begin{pmatrix} a_q \\ a_q^\dagger \end{pmatrix} = \begin{pmatrix} u & v \\ v & u \end{pmatrix}\begin{pmatrix} \alpha_q \\ \alpha_{-q}^\dagger \end{pmatrix}, \tag{3.65}$$

the Hamiltonian becomes

$$H = \frac{N^2 U(0)}{2V} - \sum_q \epsilon(q)(\alpha_q^\dagger, \alpha_{-q})\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}\begin{pmatrix} \alpha_q \\ \alpha_{-q}^\dagger \end{pmatrix} = \frac{N^2 U(0)}{2V} - \sum_q \frac{\epsilon_q}{2} + \sum_q \alpha_q^\dagger \alpha_q \tag{3.66}$$

which gives us that

$$\epsilon = \sqrt{\left(\frac{\hbar^2 k^2}{2m} + \frac{NU(k)}{V}\right)^2 - \left(\frac{NU(k)}{V}\right)^2}, \tag{3.67}$$

and if we $U(k) = U(0)$, then we can define characteristic momentum as

$$\frac{\hbar^2 k_c^2}{m} = \frac{NU(0)}{V}, \tag{3.68}$$

and we can introduce the healing length as $\zeta = 1/k_c$.

Now we return to the assumption we made that $U(k) = U(0)$, which is valid if $|U(k_c) - U(0)| \ll U(0)$. This is true if $1/r_0 \ll k_c = \sqrt{na}$. We can also define the Bogliubov sound as $c = \hbar k_c/m$.

3.3.2 Superfluidity

Suppose we have a gas and there is an impurity which interacts with the impurity

$$V = \frac{1}{V} \sum_{k_1,k_2,q} b_{k_1+q}^\dagger a_{k_2-q}^\dagger \tilde{U}(q) b_{k_1} a_{k_2} = \frac{N_0}{V} \tilde{U}(0) b_k^\dagger b_k + \frac{\sqrt{N_0}}{V} \sum_{k+1,q} b_{k_1+q}^\dagger a_{-q}^\dagger \tilde{U}(q) b_{k_1} \tag{3.69}$$

where the second equality is loose. So again switching coordinates to α, we have that

$$V \sim MF + \dots b_{k_1-q}^\dagger \alpha_q^\dagger \tilde{U} b_{k_1}, \tag{3.70}$$

where MF is the mean field interaction and this means that phonons can be excited with momentum $\vec{q}$ and energy $\epsilon(q)$. Then writing the intial energy as $E_i = Mv^2/2$, the final energy is given as

$$E_f = \epsilon(q) + (m\vec{v} - \vec{q})^2/2m = \frac{mv^2}{2} - \vec{v} \cdot \vec{q} + \frac{q^2}{2m} + \epsilon(q), \tag{3.71}$$

and since we have energy conservation, we have that

$$-\vec{v} \cdot \vec{q} + \frac{q^2}{2m} + \epsilon(q) = 0, \tag{3.72}$$

which is the condition for the allowable q for the phonons. If $M \ll m_i$ we can neglect the q^2 term, which implies that

$$\epsilon(q) = \vec{v} \cdot \vec{q} = vq\cos\theta. \tag{3.73}$$

The condition for superfluidity relates to the phonon speed being near the sound speed (NEED TO CLARIFY THIS)

Now we can look at the case where $U(k) \neq U(0)$, and we can write

$$\epsilon = \sqrt{\left(\frac{\hbar^2 k^2}{2m}\right)^2 + \frac{\hbar^2 k^2 NU(k)}{mV}} = \frac{\hbar k}{\sqrt{m}} \sqrt{\frac{NU(k)}{V} + \frac{\hbar^2 k^2}{4m}}, \tag{3.74}$$

and We can look at the case where this becomes zero, which we will denote as k_{rot}, as we can develop a roton. If we have a long range coordinate potential, which will give a potential that has k dependence in the Fourier transformed k space.

3.4   Lecture 4

3.4.1   Ground State Energy

We can write the ground state energy from before to first order

$$E_0 = \frac{N^2 U(0)}{2V} + \frac{1}{2} \sum_k i \left[\epsilon(k) - \frac{\hbar^2 k^2}{2m} - \frac{NU(k)}{V} \right] \tag{3.75}$$

where we can write in the limit $k \gg k_c$,

$$\epsilon(k) = \frac{\hbar^2 k^2}{2m} \sqrt{1 + \frac{4k_c^2}{k^2}} = \frac{\hbar^2 k^2}{2m} + \frac{NU(k)}{V} - \left(\frac{NU(k)}{V} \right)^2 \frac{m}{\hbar^2 k^2}, \tag{3.76}$$

and we can notice that this might be an issue since it depends on the choice of cutoff energy and we are dealing in perturbation theory. Thus, we must go to the next order. If we note that the expression for the corrections for the ground state given as

$$\frac{U(0)}{V} - \frac{m}{\hbar^2 V^2} \sum_k \frac{U(k)}{k^2} = \frac{4\pi \hbar^2 a}{mV} \tag{3.77}$$

Then we get can renormalize to get

$$E_0 = \frac{N^2}{2V} g + \frac{1}{2} \sum_k i \left[\epsilon(k) - \frac{\hbar^2 k^2}{2m} - \frac{NU(0)}{V} \right] + \frac{N^2}{2V^2} \frac{m}{\hbar^2} \sum_k \frac{U(0)}{k^2}, \tag{3.78}$$

where $4\pi \hbar^2 a/m$. We can calculate this as an integral

$$E_0 = \frac{N^2 g}{2V} + \frac{1}{2} \frac{\hbar^2 k_c^2}{m} V \int \frac{4\pi k^2 \, dk}{(2\pi)^3} \left(\sqrt{ \left(\frac{k}{k_c} \right)^2 + \frac{1}{4} \left(\frac{k}{k_c} \right)^4 } - \frac{k^2}{2k_c^2} + \left(\frac{k_c}{k} \right)^2 \right)$$

$$= \frac{Ng^2}{2V} + \frac{1}{2} \frac{4\pi}{(2\pi)^3} \frac{\hbar^2 k_c^5}{mV} \int_0^\infty x^2 \left(\sqrt{x^2 + \frac{x^4}{4}} - \frac{x^2}{2} - 1 + \frac{1}{x^2} \right), \tag{3.79}$$

where we changed variables $k/k_c \to x$. The main contribution to this momentum comes from $k \sim k_c$. Thus we are justified in replacing $k \to 0$ in our potential in the previous step as long as $k_c r_0 \ll 1$. This integral can be evaluated to get $32/15$ and writing

$$k_c = \sqrt{ \frac{mU(0)N}{V\hbar^2} } = \frac{\sqrt{mga}}{\hbar} \tag{3.80}$$

gives

$$E_0 = \frac{gN^2}{2V} \left(1 + \frac{128}{15} \sqrt{ \frac{a^3 N}{\pi V} } \right), \tag{3.81}$$

which was first calculated by Lee and Yang and called the LHY correction. It is a universal correction since it has no dependence on the short range. This comes only from phonons changing the vacuum.

The validity of this expansion is that $\sqrt{na^3} \ll 1$. An important interpretation is that if we calculate the number of atoms in a cube of size ζ, then

$$\zeta^3 n = \left(\frac{\hbar}{\sqrt{m\frac{4\pi a\hbar^2}{m}n}}\right)^3 n = \frac{1}{\sqrt{na^3}} \gg 1. \tag{3.82}$$

For multi-component systems or spinor systems, one can tune the leading mean field term to zero and have the leading order term be the LHY correction.

3.4.2   Inhomogeneous Condensate

Consider a box of length ζ, and introduce another length scale l such that

$$\frac{1}{n^{1/3}} \ll l \ll \zeta, \tag{3.83}$$

so there is still a large number of atoms in each box of length l^3. Now consider

$$\hat{\psi}(\vec{r}) = \sum_k \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}} a_k, \tag{3.84}$$

and a Hamiltonian

$$\hat{H} = \int d^3r \hat{\psi}^\dagger(\vec{r}) \left(-\frac{\hbar^2\nabla^2}{2m}\right) \hat{\psi}(\vec{r}) + \frac{1}{2}\int \hat{\psi}^\dagger(\vec{r}_1)\hat{\psi}^\dagger(\vec{r}_2)U(\vec{r}_1,\vec{r}_2)\hat{\psi}(\vec{r}_1)\hat{\psi}(\vec{r}_2), \tag{3.85}$$

and if we treat the wavefunctions as semi-classical, we get

$$E = \int d^3r \, \psi^*(\vec{r}) \left(-\frac{\hbar^2\nabla^2}{2m}\right) \psi(\vec{r}) + \frac{1}{2}\int \psi^*(\vec{r}_1)\psi^*(\vec{r}_2)U(\vec{r}_1,\vec{r}_2)\psi(\vec{r}_1)\psi(\vec{r}_2), \tag{3.86}$$

which we want to minimise with the constraint that $N = \int \psi^*\psi \, d^3r$ is constant. Which means that $E - \mu N$ must be minimized, which means that

$$\frac{\partial(E - \mu n)}{\partial \psi^*} = 0, \tag{3.87}$$

which is called the Gross-Pitaevskii equation. We do not need to consider higher order potentials, meaning we can write

$$\left[-\frac{\hbar^2\nabla^2}{2m} + V(r)\right]\psi + U(0)|\psi|^2\psi = \mu\psi, \tag{3.88}$$

which is also referred to as non-linear term. ψ is referred to as the wavefunction for the condensate since we have put all the many body dependence into this equation for a single complex function.

3.4.3   Gross-Pitaevskii Equation

We define the healing length

$$\xi = \frac{\hbar}{\sqrt{mgn}},\tag{3.89}$$

and we look at a condensate near a wall where $n_\infty = \psi_\infty^2$ and $\mu = U(0)n_\infty$. We can write the GP equation as

$$\psi'' = -U(0)(n_\infty - \psi^2)\psi\left(\frac{2m}{\hbar}\right) = \frac{-2m}{\hbar}U(0)\frac{d}{dx}\left(n_\infty\frac{\psi^2}{2} - \frac{\psi^4}{4}\right),\tag{3.90}$$

which we can write as

$$\psi' = \sqrt{\frac{4m}{\hbar^2}U(0)\left[\frac{n_\infty^2}{4} - \frac{n_\infty\psi^2}{2} + \frac{\psi^4}{4}\right]},\tag{3.91}$$

which we can integrate by separating variables as

$$\int_0^\infty dx = \int_0^\psi \frac{\hbar}{2\sqrt{mU(0)n_\infty}}\int_0^\psi \frac{ds}{\sqrt{n_\infty}\sqrt{\frac{1}{4} - \frac{s^2}{2n_\infty} + \frac{s^4}{4n_\infty^2}}} = \frac{\xi}{2}\int_0^{\frac{\psi}{\sqrt{n_\infty}}} \frac{dx}{\sqrt{\left(\frac{1}{2} - \frac{x^2}{2}\right)^2}},\tag{3.92}$$

which allows us to find that

$$\psi = \sqrt{n_\infty}\tanh\left(\frac{x}{\xi}\right).\tag{3.93}$$

This makes sense because we should find constant density at large distances. ξ characterizes the distances at which the condensate becomes constant.

3.4.4   Bogliubov-Degennes

The equation of motion for a classical field is

$$i\dot{\psi} = \frac{\partial H}{\partial \psi^*},\tag{3.94}$$

and

$$E - \int \psi^*\left(-\frac{\hbar^2\nabla^2}{2m} + V(r) - \mu\right)\psi + g\int \psi^*\psi^*\psi\psi,\tag{3.95}$$

which gives us a GP equation

$$i\dot{\psi} = \left(-\frac{\hbar^2\nabla^2}{2m} + V(r) - \mu\right)\psi + g|\psi|^2\psi,\tag{3.96}$$

which has a solution ψ_0. Now we let

$$\psi = \psi_0 + \chi_+e^{-i\epsilon t} + \chi_-e^{i\epsilon t},\tag{3.97}$$

and then if we substitute ψ into the GP equation and linearise around small ξ_+, ξ_- giving two equations

$$\epsilon\xi_+ = \left(-\frac{\hbar^2\nabla^2}{2m} + V - \mu\right)\chi_+ + g[\psi_0 e^{-i\epsilon t} + \chi_- e^{i\epsilon t}]^2[\psi_0 + \chi_+^* e^{i\epsilon t} + \chi_-^* e^{-i\epsilon t}]$$

$$= \left(-\frac{\hbar^2\nabla^2}{2m} + V - \mu\right)\chi_+ + g\psi_0^3 + 2g\psi_0^2\chi_+ + g\psi_0^2\chi_-^*, \tag{3.98}$$

$$-\epsilon\xi_- = \left(-\frac{\hbar^2\nabla^2}{2m} + V - \mu\right)\chi_- - g[\psi_0 e^{-i\epsilon t} + \chi_- e^{i\epsilon t}]^2[\psi_0 + \chi_+^* e^{i\epsilon t} + \chi_-^* e^{-i\epsilon t}]$$

$$= \left(-\frac{\hbar^2\nabla^2}{2m} + V - \mu\right)\chi_- + g\psi_0^3 + 2g\psi_0^2\chi_- + g\psi_0^2\chi_+^*, \tag{3.99}$$

$$\tag{3.100}$$

and if we put $V = 0$ we get $\mu = g\psi_0^2$, which gives

$$\epsilon_+ = \left(-\frac{\hbar^2\nabla^2}{2m} + g\psi_0^2\right)\chi_+ + g\psi_0^2\chi_-^* \tag{3.101}$$

$$-\epsilon\chi_- = \left(-\frac{\hbar^2\nabla^2}{2m} + g\psi_0^2\right)\chi_- + g\psi_0^2\chi_+^* \tag{3.102}$$

This is the case for constant density, but in a trap, we can solve the GP equation and plug this into the BG equations which are coupled differential equations which gives the spectrum inside the trap.

If we want to calculate the number of real atoms at momentum k

$$\langle N_k \rangle = \left\langle a_k^\dagger a_k \right\rangle$$

$$= \left\langle u_k\alpha_k^\dagger + v_k\alpha_{-k})(u(k)\alpha_k + v_k\alpha_{-k}^\dagger) \right\rangle$$

$$= u_k^2 \left\langle \alpha^\dagger\alpha \right\rangle + v_k^2 \left\langle \alpha\alpha^\dagger \right\rangle$$

$$= (u_k^2 + v_k^2) \left\langle \alpha_k^\dagger\alpha_k \right\rangle + v_k^2$$

$$\propto \frac{k_c T}{k\epsilon} + \frac{k_c}{k}, \tag{3.103}$$

in the limit $k \ll k_c$. Here we have noted that photons are bosons with chemical potential zero. It is important to note that

$$V \int_0^{k_c} \frac{k^2 dk}{(2\pi)^3} \left(\frac{T}{\hbar^2 k^2/m} + \frac{k_c}{k}\right), \tag{3.104}$$

converges, however, in 2D, finite temperatures becomes an issue and there would be a logarithmic divergence. We can replace the lower limit with $1/L$, where $L < \xi e^{T_d/T}$ where we can find this by integrating and ensuring total number.

4 Optical Lattices (Helene Perrin)

4.1 Lecture 1

4.1.1 Background and Applications

What will be described here are far off resonance optical lattices where spontaneous emission can be neglected. Atoms are placed in a periodic potential produced by the light shift of a standing wave. In a single dimension, the potential is of the form

$$V(x) = V_0 \sin^2(kx), \tag{4.1}$$

where k is a light wave vector. We will speak of the recoil energy, however, it is not the same as for the atom. We will define it here with respect to the wavelength of the light, so

$$E_{red} = \frac{\hbar^2 k^2}{2M}, \tag{4.2}$$

where M is the mass of the atom. So if we have two transverse lasers with a well defined phase and the same polarization, we have two cases, red-detuned, blue-detuned. In the red detuned case, the atoms are attracted to the maxima of the intensity, in the blue detuned case, the atoms are attracted to the minima.

For a red-detuned laser, heating is inefficient, although there are many scattered photons. For the blue-detuned laser, heating is efficient, but there are few scattered photons. Thus, the rates essentially cancel out. Red is slightly better.

Optical lattices are very broadly used in two situations. One situation is metrology. One can free the external degrees of freedom very well and thus measure the pure clock frequency in the system. This is used in such things as the Sr atomic clock, where they used the Lamb-Dicke regime, where

$$\Delta x \ll \frac{\lambda}{2\pi}, \tag{4.3}$$

which means no Doppler effect.

The other big application is optical lattices for quantum gases. The idea is to use these systems as a quantum simulator.

4.1.2 Bloch Functions

We first consider translation operators in a periodic potential, such that

$$V(\vec{r} + \vec{d}) = V(\vec{r}), \tag{4.4}$$

where $\vec{d} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3$. This means that the Hamiltonian is invariant under translation $\hat{T}_{\vec{a}_i}$, and

$$\hat{T}_{\vec{a}_i} = e^{-i\vec{a}_i \cdot \vec{p}/\hbar}, \tag{4.5}$$

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and since the Hamiltonian $P^2/2M + V(\vec{r})$ commutes with any $\hat{T}_{\vec{a}_i}$ and all the translation operators commute with each other, we can find a common basis.

Now we introduce the reciprocal lattice, another Bravais lattice, which is generated by $(\vec{b}_1, \vec{b}_2, \vec{b}_3)$ such that for all i, j

$$\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}, \tag{4.6}$$

and then we let $\vec{q}$ be

$$\vec{q} = \frac{1}{2\pi} \sum_j \theta_j \vec{b}_j. \tag{4.7}$$

and $\vec{q}$ is in some sense defined modulo the $\vec{b}_j$. We can compute

$$\vec{a}_i \cdot \vec{q} = \theta_i. \tag{4.8}$$

We introduce this $\vec{q}$ as it will label the eigensates of H. So if $\psi_{\vec{q}}$ is some eigenstate of H, it must be an eigenstate of all the translation operators, in the sense that

$$\hat{T}_{\vec{a}_i} \psi_{\vec{q}}(\vec{r}) = e^{-i\theta_i} \psi_{\vec{q}}(\vec{r}) = e^{-i\vec{q}\cdot\vec{a}_i} \psi_{\vec{q}}(\vec{r} - \vec{a}_i). \tag{4.9}$$

So if we define

$$u_{\vec{q}}(\vec{r}) = e^{-\vec{r}\cdot\vec{q}} \psi_{\vec{q}}(\vec{r}), \tag{4.10}$$

then we have that

$$u_{\vec{q}}(\vec{r} - \vec{a}_i) = e^{-i(\vec{r}-\vec{a}_i)\cdot\vec{q}} \psi_{\vec{q}}(\vec{r} - \vec{a}) = e^{-i\vec{r}\cdot\vec{q}} \psi_{\vec{q}}(\vec{r}) = u_{\vec{q}}(\vec{r}). \tag{4.11}$$

Thus, the eigenfunctions satisfy

$$\psi_{\vec{q}}(\vec{r}) = e^{i\vec{r}\cdot\vec{q}} u_{\vec{q}}(\vec{r}), \tag{4.12}$$

where $u_{\vec{q}}$ is periodic. This means that

$$\psi_{\vec{q}+\vec{b}_i}(\vec{r}) = e^{i\theta} \psi_{\vec{q}}(\vec{r}). \tag{4.13}$$

These functions are called the Bloch functions and they form an orthonormal basis. They are periodic up to a constant phase shift with each step.

4.1.3   Energy Bands

We will go back to the 1D case and use potential $V(x) = V_0 \sin^2(ka) = \frac{V_0}{2}(1 - \cos(2kx))$, thus the period is $\lambda/2 = \pi/k = a$. Since we have a periodic function, we can write it as a Fourier series

$$u_q(x) = \sum_j \alpha_j(q) e^{ij2kx}, \tag{4.14}$$

which implies that

$$\psi_q(x) = \sum_j \alpha_j(q) e^{i(q+2jk)x}.$$
(4.15)

Thus this is summation of plane waves with wave vector $q + 2jk$. We can write the Shrodinger equation

$$\sum_j \left[\alpha_j(q) \left(\frac{\hbar^2(p+2jk)^2}{2M} + \frac{V_0}{2} \right) - \frac{V_0}{4}\alpha_{j+1} - \frac{V_0}{4}\alpha_{j-1} \right] e^{i(q+j2k)x} = E \sum_j \alpha_j(q) e^{i(q+2jk)x},$$
(4.16)

which is a system of linear equations and can be solved numerically.

The eigenenergies organize in bands $E_n(q)$ with eigenstates $\psi_{nq}(x)$. Typically there are gaps in the allowed eigenstates corresponding to the bands.

Now we will look at the trivial case V_0. This should correspond to plane waves, $\phi(x) = e^{ipx/\hbar}$. If we apply the Bloch theorem, we know that with $q = p/\hbar - j2k$.

$$e^{ipx/\hbar} = e^{iqx} \sum_j \alpha_j e^{ij2kx},$$
(4.17)

with energy

$$E_j(q) = \frac{\hbar^2(q+2jk)^2}{2m} = \frac{p^2}{2m},$$
(4.18)

which implies that

$$p = \hbar q + 2\hbar jk,$$
(4.19)

thus

$$E_{j,q} = \frac{\hbar^2}{2m}(q + 2|j|k)^2.$$
(4.20)

4.2   Lecture 2

4.2.1   Wannier Functions

We can consider $V_0 \gg E_{rec}$ in which case ψ_{0q} are localized in the wells. We can restrict to the lowest band and for notational purposes, we have $\psi_{0q} \to \psi_q$. We can now use a different set of functions to describe these bands which are located on the different lattice sites, known as the Wannier functions.

These functions are localized and can be defined as

$$w_{n,j}(n) = \sqrt{\frac{a}{2\pi}} \int_{-\pi/a}^{\pi/a} \psi_{n,q}(x) e^{-ijaq} \, dq,$$
(4.21)

which is an integration over the wavefunctions weighted by a phase factor and n is the band number. These functions are orthogonal in the sense that

$$\int w_{n,j}(x) w_{n',j'}(x) \, dx = \delta_{n,n'} \delta_{j,j'},$$
(4.22)

and if we use the fact that $\psi_{n,q}(x - ja) = e^{-ijqa}\psi_{nq}(x)$ to get that

$$w_{n,j}(x) = \sqrt{\frac{a}{2\pi}} \int_{-\pi/a}^{\pi/a} \psi_{nq}(x - ja)\,dx = w_{n,0}(x - ja), \qquad (4.23)$$

so all functions are really just shifted versions of the one centered at 0. Also notice that

$$\sqrt{\frac{a}{2\pi}} \sum_n w_{n,j}(x)e^{ijqa} = \frac{a}{\pi} \int_{-\pi/a}^{\pi/a} dq'\, \psi_{n,q'}(x) \sum_j e^{ij(q-q')a} = \psi_{n,q}(x). \qquad (4.24)$$

We can compose

$$w_{n,0} = \sqrt{\frac{a}{2\pi}} \sum_n w_{n,0}(x - ja)e^{ijqa}. \qquad (4.25)$$

4.2.2 Hamiltonian with Wannier Functions

Now we can express the Hamiltonian in terms of Wannier functions using second-quantization. First we can write the Hamiltonian in terms of Bloch functions

$$H = \sum_n \int_{-\pi/a}^{\pi/a} dq\, E_n(q) \,|\psi_{n,q}\rangle \langle\psi_{n,q}|, \qquad (4.26)$$

and then going to the second quantization, we get

$$H = \sum_n \int_{-\pi/a}^{\pi/a} dq\, E_n(q) a_{n,q}^\dagger a_{n,q}. \qquad (4.27)$$

We are assuming for the moment that we have bosons which means that $[a_{n,q}, a_{n',q'}^\dagger] = \delta_{n,n'}\delta(q-q')$, and so for the Wannier states, we introduce $[b_{n,j}, b_{n',j'}] = \delta_{n,n'}\delta_{j,j'}$, where the operators are defined as

$$a_{n,q} = \sqrt{\frac{a}{2\pi}} \sum_j b_{n,j}e^{ijqa}, \qquad (4.28)$$

where the lowering operators are understood to be operators and different from the non-sub-scripted a. We can now write the Hamiltonian as

$$H = \sum_n \int_{-\pi/a}^{\pi/a} dq\, E_n(a)\frac{a}{2\pi} \sum_j \sum_{j'} e^{-ijqa}e^{ij'qa}b_{n,j}^\dagger b_{n,j'}, \qquad (4.29)$$

and we can do this q integral which gives some number depending on $j - j'$ which we will denote $J_n(j - j')$, allowing us to write

$$H = \sum_n \sum_j \sum_{j'} J_n(j - j')b_{n,j}^\dagger b_{n,j'}, \qquad (4.30)$$

where

$$J_n(\Delta j) = \frac{a}{2\pi} \int_{-\pi/a}^{\pi/a} E_n(q) e^{i\Delta jqa} \, dq, \tag{4.31}$$

then we can look at terms within the same band as

$$\langle w_{n,j}|H|w_{n,j'}\rangle = J_n(j - j'), \tag{4.32}$$

so the J_n function which describes the site to site hopping.

If we Fourier transform this equation, we get that

$$E_n(q) = \sum_j J_n(j) e^{-ijqa}. \tag{4.33}$$

Prior, we made the assumption that we had a deep lattice and our wavefunctions were localized so $J_n(j)$ is very small for $|j| > 1$. So this means that

$$E_n(a) \approx J_n(0) + J_n(n)(e^{-iqa} + e^{iqa}) = J_n(0) + 2J_n(1)\cos(qa) \tag{4.34}$$

and this is especially true for lower n. We can write $E_0(q) = J_0(0) + 2J_0(1)\cos(qa)$.[21] Now we will introduce $J = -J_0(1)$, which means that the height of the band (or width) is $4J$.

If we now neglect all $J_0(j)$ with $|j| > 1$, we can rewrite the Hamiltonian for the lowest band with $V_0 \ll E_{rec}$, keeping only $j' = j \pm 1$, as

$$H = -J \sum_j [b_{j+1}^\dagger b_j + h.c], \tag{4.35}$$

4.2.3   Bose-Hubbard Hamiltonian

The Bose-Hubbard model includes interactions of the form

$$H_{int} = \frac{g}{2} \int \hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x) \, dx, \tag{4.36}$$

where we write $\hat{\psi}(x)$ as

$$\hat{\psi}(x) = \sum_n \sum_j w_{n,j}(x) b_{n,j}, \tag{4.37}$$

and if we restrict to $n = 0$, we can write the interaction Hamiltonian as

$$H_{int,0} = \frac{g}{2} \sum_{i,j,l,m} b_i^\dagger b_j^\dagger b_l b_m \int dx \, w_i(x) w_j(x) w_l(x) w_m(x), \tag{4.38}$$

where we have noticed that w is real. We can write this as

$$H_{int,0} = \frac{g}{2} \sum_{i,j,l,m} b_i^\dagger b_j^\dagger b_l b_m \int dx \, w_0(x - ia) w_0(x - ja) w_0(x - la) w_0(x - ma), \tag{4.39}$$

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[21] $J_0(1) < 0$.

and we also know that unless all indexes will be the same, the contribution will be vanishingly small for large V_0 and We can write

$$H_{int,0} = \frac{g}{2} \sum_j b_j^\dagger b_j^\dagger b_j b_j \int dx \, w_0(x)^4 \tag{4.40}$$

and now we will define $U = g \int w_0(x)^4 \, dx \approx g/\sqrt{2\pi} a_{osc}$ where a_{osc} is the harmonic oscillator length which in one dimension is given as

$$a_{osc} = \sqrt{\frac{\hbar}{\pi\omega}} = k^{-1} \left(\frac{E_{rec}}{V_0}\right)^{1/4}, \tag{4.41}$$

and thus, we can write

$$H_{int,0} = \frac{U}{2} \sum_j n_j(n_j - 1), \tag{4.42}$$

where we have used operator identities for the b_j.[22] Now we write the full Bose-Hubbard Hamiltonian as

$$H = -J \sum_j [b_{j+1}^\dagger b_j + h.c + \frac{U}{2} \sum_j n_j(n_j - 1)]. \tag{4.43}$$

[23] The values of J, U can be estimated in 3D as

$$\frac{U}{E_{rec}} = \sqrt{\frac{8}{\pi}} k a_s \left(\frac{V_0}{E_{rec}}\right)^{3/4}, \tag{4.44}$$

and

$$\frac{J}{E_{rec}} \approx \frac{4}{\sqrt{\pi}} \left(\frac{V_0}{E_{rec}}\right)^{3/4} e^{-2\sqrt{\frac{V_0}{E_{rec}}}}, \tag{4.45}$$

which implies that

$$\frac{J}{U} \approx \frac{\sqrt{2} k a_s}{e}^{-2\sqrt{\frac{V_0}{E_{rec}}}}, \tag{4.46}$$

and this can be tuned with V_0 to control the model. This allows one to explore the Mott Insulator to superfluid phase transition, an example of a quantum phase transition.

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[22]This means that U is the interaction energy associated with having 2 particles at a single site.

[23]This Hamiltonian is only valid for bosons, however, a similar Hamiltonian can be written for Fermions.

5   Ultracold Fermi Gases in Optical Latices (Leticia Tarruell)

5.1   Lecture 1

We will first talk about non-interacting systems. We will then move into highly interacting systems. The goal of these systems is quantum systems. Often we want to simulate electrons in solids and we do that with fermions on optical lattices.

5.1.1   The non-interacting Fermi gas

Fermionic atoms have half integer spin, many have been cooled to quantum degeneracy including Alkali atoms, two-electron atoms, and dipolar atoms. To cool to quantum degeneracy one needs distinguishable atoms to get collisions for evaporative cooling: 2 spin-states or sympathetic cooling with another species. An exception is dipolar gases.[24]

To get notation set, we can define the fermionic distribution function

$$f(E) = \frac{1}{e^{\beta(E-\mu)} + 1} = \frac{1}{\frac{1}{\zeta}e^{\beta E} + 1}, \tag{5.1}$$

where $\zeta = e^{\beta\mu}$ is the fugacity and measures the level of degeneracy. The characteristic energy scale is the fermi energy E_F ($\mu = 0$ at $T = 0$). So $E_F = k_B T_F$, where $E_F = \hbar^2 k_F^2/2m$ and the Fermi momentum is

$$k_F = ((6\pi^2)n)^{1/3}, \tag{5.2}$$

where n is the density.

If we put the Fermi gas in a harmonic trap

$$V(x, y, z) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2), \tag{5.3}$$

and define $\bar{\omega} = (\omega_x \omega_y \omega_z)^{1/3}$, we can introduce a density of states $\rho(E) = E^2/(2(\hbar\omega)^3)$, which gives us that

$$N = \int_0^{E_F} dE\rho(E)f(E) \implies E_f = \hbar\bar{\omega}(6N)^{1/N}, \tag{5.4}$$

which gives a Fermi energy of tenths of kHz or hundreds of nK. In a Fermi gas, the energy per particle as $T \to 0$ does not go to zero. So there is a saturation energy that for the harmonic trap is $3/4E_F$.

---

[24]Diplar gases have interactions with identical fermions through the dipolar interaction

The density and momenum distribution can be derived using the Thomas-Fermi approximation where $H(\vec{r}, \vec{k}) = \frac{\hbar^2 k^2}{2m} + V(r)$ and define

$$w(\vec{r}, \vec{k}) = \frac{1}{(2\pi)^3} \frac{1}{\frac{1}{\zeta} e^{\beta H(\vec{r}, \vec{k})} + 1}, \tag{5.5}$$

which gives a dneisty profile

$$n(\vec{r})|_{T=0} \propto \left(1 - \frac{x^2}{R_{F,x}^2} + \frac{y^2}{R_{F,y}^2} + \frac{z^2}{R_{F,z}^2} \right)^{3/2}, \tag{5.6}$$

where $R_{F,i} = \sqrt{\frac{2E_F}{m\omega_i^2}}$, which is larger than the BEC distribution. The momentum distribution is given as

$$n(\vec{k})|_{T=0} \propto \left(1 - \frac{k^2}{k_F^2} \right)^{3/2}, \tag{5.7}$$

which at finite temperature depends on fugacity and gives

$$\frac{S}{N} \sim k_B \pi^2 \left(\frac{T}{T_f} \right) \tag{5.8}$$

5.1.2   Fundamental of Optical Lattices

We will now go over optical lattices. The Hamiltonian is given as

$$H = \frac{p^2}{2m} + V_0 \cos^2(kx), \tag{5.9}$$

where $k = 2\pi/\lambda$. The eigenenergies are energy bands with quasimomentum q and the eigenstates are Bloch functions

$$\psi_{n,q}(x) = e^{iqx} u_{n,q}(x), \tag{5.10}$$

and we will restrict to the first Brillouin zone, which is characterized by the recoil energy $E_r = \hbar^2 k^2 / 2m$. This is a good approximation for large lattice potential.

Atoms can tunnel from site to site. We can describe this in the convenient basis of the Wannier functions $w_{n,j}(x)$, and

$$t_n(j) = - \int w_{n,j}^*(x) \left(\frac{-\hbar^2}{2m} \nabla^2 + V_0 \cos^2(kx) \right) w_{n,0}(x) \, dx, \tag{5.11}$$

For deep lattices, only the nearest neighbor tunneling is significant, referred to as the tight-binding limit.[25]

---

[25]This is similar to the J introduced in Helene's lecture

We can write the Hamiltonian in this limit in second quantization as

$$H = -t \sum_{\langle i,j \rangle, \sigma} \left(c_{i\sigma}^\dagger c_{j\sigma} + h.c \right), \tag{5.12}$$

where the extra sum accounts for multiple spin states. If the energy scales of the system are much less than the band gas, only the lowest energy band is relevent. We can write the significant dispersion relation

$$E(q) = -2t \cos(dq), \tag{5.13}$$

which gives a bandwidth

$$W = 4t = 2zt, \tag{5.14}$$

where z is the connectivity. We can write

$$\frac{W}{E_R} \propto \left(\frac{V_0}{E_R} \right)^{3/4} \exp \left[-2 \left(\frac{V_0}{E_R} \right)^{1/2} \right], \tag{5.15}$$

so its clear as $V_0 \gg E_R$, then W/E_r is suppressed exponentially.

5.1.3   Experimental Aspects and Probes

One can use band-mapping, where the lattice is switched off slowly enough such that they adiabatically follow the wavefunction, which has the condition

$$\hbar \left| \left\langle \phi_n' \left| \frac{d}{dt} \right| \phi_n \right\rangle \right| \ll |E_{n'} - E_n|, \tag{5.16}$$

and thus q is mapped onto real momentum. So one can see the Fermi surface. This is important because almost all physics happens in the vicinity of the Fermi surface since excitations occur near the vicinity of the Fermi surface.

If we put the particle in a band structure, but apply a constant for, we can write the Hamiltonian as

$$H = \frac{p^2}{2m} + V_0 \sin(kx) - Fx, \tag{5.17}$$

and write the seimclassical eequation of motion, we get

$$h \frac{dq}{dt} = F, \tag{5.18}$$

has solution $q(t) = q(0) + Ft/\hbar$. Which means there are periodic oscillations in momentum space, known as *Bloch oscillations*, where

$$T = \frac{2\hbar k}{|F|}. \tag{5.19}$$

This allows one to move particles around the lattice.

5.1.4   Dirac points in a graphene lattice

Here the atoms are contained in a brick-wall lattice, which is similar to a square lattice, but every other site in an alternating pattern by columns are removed. This gives different physics because there is now a two site unit cell. It is sort of like two triangular lattices which are rotated with respect to each other.

The lattice vectors of a brick wall lattice are given as

$$\vec{a}_1 = d \begin{pmatrix} 1 \\ 1 \end{pmatrix} \; ; \; \vec{a}_2 = d \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \tag{5.20}$$

We can find the reciprocal lattice as

$$\vec{b}_1 = \frac{\pi}{d} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \; ; \; \vec{b}_2 = \frac{\pi}{d} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \tag{5.21}$$

which fulfill the condition

$$\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}. \tag{5.22}$$

The Brilloin zone is a square, but it is rotated by $\pi/2$ and smaller compared to the square lattice. It is inscribed within the Brilloin zone of the square lattice, meaning it intersections at π/d.

To obtain the energy spectrum, we will go to the tight-binding limit, and notate the hopping dx, dy for hopping in the x and y directions respectively. The wavefunction is a Bloch wavefunction, give as

$$\psi_{\vec{q}}(\vec{r}) = e^{i\vec{q}\cdot\vec{r}} u_{\vec{q}}(\vec{r}), \tag{5.23}$$

where $\vec{q}$ is the quasi-momentum. The periodic function is complicated by the two sublattices, thus

$$|u_{\vec{q}}\rangle = \alpha_{\vec{q}} \left(\sum_{\vec{j}} \left| w_{A,\vec{j}} \right\rangle \right) + \beta_{\vec{q}} \left(\sum_{\vec{j}} \left| w_{B,\vec{j}} \right\rangle \right), \tag{5.24}$$

which means the particles have some amplitude to be positioned at either A or B sites. Note that $\vec{j}$ is an index for the unit cells and we can write the full Bloch wavefunction as

$$|\psi_{\vec{q}}\rangle = \sum_{\vec{j}} e^{i\vec{q}\cdot\vec{r}_{\vec{j}}} \left(\alpha_{\vec{q}} \left| w_{A,\vec{j}} \right\rangle + \beta_{\vec{q}} \left| w_{B,\vec{j}} \right\rangle \right). \tag{5.25}$$

We can solve the Schrodinger equation $H |\psi_{\vec{q}}\rangle = E(\vec{q}) |\psi_{\vec{q}}\rangle$,

$$H(\vec{q}) \begin{pmatrix} \alpha_{\vec{q}} \\ \beta_{\vec{q}} \end{pmatrix} = E(\vec{q}) \begin{pmatrix} \alpha_{\vec{q}} \\ \beta_{\vec{q}} \end{pmatrix}, \tag{5.26}$$

and the problem simplifies since we will only consider nearest neighbor coupling. We can write the Hamiltonian by taking the A, B site energy to be the same and equally

0. We can always introduce a difference if we want. The coupling term $f(\vec{q})$ allows us to write the Hamiltonian as

$$H(\vec{q}) = \begin{pmatrix} 0 & f^*(\vec{q}) \\ f(\vec{q}) & 0 \end{pmatrix} \tag{5.27}$$

where the coupling function is given as

$$f(\vec{q}) = -t_x - t_y \left[e^{i\vec{q}\cdot\vec{a}_1} + e^{i\vec{q}\cdot\vec{a}_2} \right] = -t_x - 2t_y e^{iq_x d} \cos(dqy), \tag{5.28}$$

thus the eigennerges are

$$E(\vec{q}) = \pm |f(q)| = \pm\sqrt{(t_x + 2t_y \cos(q_x d)\cos(q_y d))^2 + 4t_y^2 \sin^2(q_x d)\cos^2(q_y d)}. \tag{5.29}$$

Thus, the condition for $f(\vec{q}) = 0$ corresponds to

$$\begin{cases} \sin(q_x d) & = 0 \\ \cos(q_x d)\cos(q_y d) & = -\frac{t_x}{2t_y} \end{cases} \tag{5.30}$$

and . This is where the bands will cross and has solutions where $q_x = 0$ and $\cos(q_y d) = -t_x/(2t_y)$ which has solutions when $t_x = 2t_y$ of $q_y = \pi/d$ and many other solutions where $t_x < 2t_y$ all of which are between π/d and $\pi/(2d)$. Some of points are called Dirac points.

Dirac points are where the dispersion relation touches in a linear way corresponding to $t_x = \sqrt{2}t_y$ which gives a solution

$$q_y^D = \pm\frac{3\pi}{4d} \implies \vec{q} = \begin{pmatrix} 0 \\ \pm\frac{3\pi}{4d} \end{pmatrix}, \tag{5.31}$$

which means that when $\vec{q} - \vec{q}_D = \delta\vec{q}$ for small $\delta\vec{q}$, then

$$E(\vec{q})|_{\delta\vec{q}} = \pm\sqrt{2}t_y d[\delta q_x + \delta q_y]. \tag{5.32}$$

This gives rise to a conical dispersion relation and thus they are called Dirac points because this is analogous to the dispersion relation of a relativistic particle $\hbar c|\vec{q} - \vec{q}_D|$, where c is the speed of light. This is seen in graphene.

5.2   Lecture 2

5.2.1   Dirac Points cont.

Returning to discussions from before, a lattice can be made using a set consisting of three lasers with two perpendicular $(X, \bar{X})$ to the other Y and the two parallel beams differing by a phase shift. This gives the potential as

$$V(x,y) = V_{\bar{X}} \cos^2\left(kx + \frac{\theta}{2}\right) + V_X \cos^2(kx) + V_Y \cos^2(ky) + 2\sqrt{V_x V_y} \cos(kx)\cos(ky). \tag{5.33}$$

A brick wall lattice can be made by using specific powers in the three beams.

In order to see the Dirac points, one can use Bloch oscillations induced by a magnetic field gradient and this allows observation of the quasi-momentum distribution. If not at a Dirac point, the atoms will oscillate back to their original energy, if passing through a Dirac point, the atom will transfer to the second band. Thus, by measuring the band populations, one can "see" these Dirac points.

If there is an offset in the A and B energy, then there are diagonal terms in the Hamiltonian

$$H = \begin{pmatrix} -\Delta/2 & f^*(\vec{q}) \\ f(\vec{q}) & \Delta/2 \end{pmatrix}, \tag{5.34}$$

wich gives energies of

$$E = \sqrt{\left(\frac{\Delta}{2}\right)^2 + |f(\vec{q})|^2}. \tag{5.35}$$

This can be realized experimentally by adjusting the detuning in the three beams making the lattice. This results in reduced transfer to the second band as the bands are further away.

The position of the Dirac points can also be changed by adjusting the laser intensities of $X, \bar{X}$. This affects the asymmetry of the cone. As the Dirac points come together, there is a topological transition. The wavefunction can acquire a Berry phase if closed loop encircling a Dirac point. Technically this is not really topological since these points have different chirality and there are two of them.

5.3   Lecture 3

5.3.1   Interactions in an optical lattice

In fermions interactions can only occur between opposite spins. The potential is modeled as

$$V_{int}(r) = \frac{4\pi\hbar^2 a}{m}\delta(r) = g\delta(r), \tag{5.36}$$

which gives the interaction term in the lattice

$$H_{int} = g \int d^3r \, \psi_\uparrow^\dagger(\vec{r})\psi_\downarrow^\dagger(\vec{r})\psi_\downarrow(\vec{r})\psi_\uparrow(\vec{r}). \tag{5.37}$$

In the single band (interaction energy $\ll$ band gap) and only on site interactions

$$H_{int} = g \int d^3r \, |w_0(\vec{r})|^4 \sum_i c_{\uparrow i}^\dagger c_{\downarrow i}^\dagger c_{\downarrow i} c_{\uparrow i} = U \sum_i n_{\uparrow i} n_{\downarrow i}, \tag{5.38}$$

where w_0 is the usual Wannier function. This implies the interactions can be tuned by changing the lattice depths, however, they can also be changed by altering g with the Feshbach resonance and adjusting the scattering length. Feshbach resonances in a lattice are somewhat more complicated since relative motion and central of mass motion cannot be separated in a lattice. The solution will impose a range of scattering length in which the single band regime approximation is valid.

5.3.2   The Fermi-Hubbard Hamiltonian

The Fermi-Hubbard Hamiltonian can be written as

$$
H_{F-H} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + h.c) + U \sum_i n_{i\uparrow} n_{i\downarrow},
\tag{5.39}
$$

which can be controlled by:

- tunneling through lattice depth

- the lattice geometry

- the filling by changing atom number

- the spin by choosing internal states

- interactions through Feshbach resonances

This model is very difficult to solve and only has analytic solutions for limiting cases.

In a very simple case, consider two fermions in a double well where we denote the wells by l, r. The Hamiltonian then becomes

$$
H = -t_d \sum_{\sigma} (c_{l,\sigma}^{\dagger} c_{r,\sigma} + c_{l,\sigma} c_{r,\sigma}^{\dagger}) + U(n_{l,\uparrow} n_{l,\downarrow} + n_{r,\uparrow} n_{r,\downarrow}),
\tag{5.40}
$$

which can be solved by noting that

$$
c_{l,\sigma} c_{r,\sigma}^{\dagger} = -c_{r,\sigma}^{\dagger} c_{l,\sigma},
\tag{5.41}
$$

which allows the matrix to be written in basis $|\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle, |\uparrow\downarrow, 0\rangle, |0, \uparrow\downarrow\rangle$ as

$$
H = \begin{pmatrix} 0 & 0 & -t_d & -t_d \\ 0 & 0 & t_d & t_d \\ -t_d & t_d & U & 0 \\ -t_d & t_d & 0 & U \end{pmatrix},
\tag{5.42}
$$

which can be solved exactly. For $U = 0$, the lowest energy state is given as

$$
\frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle + |\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle}{2},
\tag{5.43}
$$

and for very strong interactions $U \gg 0$, the lowest two states are the symmetric and anti-symmetric combinations of the single filled wells,

$$
\frac{1}{\sqrt{2}}(|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) \, ; \, \frac{1}{\sqrt{2}}(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle)
\tag{5.44}
$$

In a larger lattice with one atom per site, the interactions will tend to suppress doubly filled sites. There is a continuous transition as a function of the interaction strength

between a metal and a Mott insulator.[26] The transition relies on an interplay between kinetic energy and interaction energy.

For negative U, but still strong, $U \ll 0$, then the lowest energies are high double occupancy

$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle)\,;\; \frac{1}{\sqrt{2}}(|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle), \qquad (5.45)$$

and there is a transition into state with preformed pairs and also a transition into a superfluid which is sometimes called the BEC-BCS crossover in a lattice at low enough temperatures, but only in the preformed pairs state, except possibly in the limit of zero temperature.

The model is symmetric between superfluidity for attractive interactions and magnetism for repulsive interactions. in the middle, the gas behaves as a metal.

This is model may contain high temperature superconductivity, however, it requires quite low temperatures and it has not been experimentally accessed at this point.

5.3.3   Limits of Fermi-Hubbard Model

For non-single site filling, we can add a term depending on chemical potential to write

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + h.c) + U \sum_i n_{i\uparrow} n_{i\downarrow} - \sum_{i,\sigma} \mu n_{i,\sigma}, \qquad (5.46)$$

and in the atomic limit ($t = 0$), then the first term is zero. to know the thermodynamics, we can write the partition function as

$$Z = T[\exp(-\beta H)] = Z_1^N, \qquad (5.47)$$

since the sites are no longer coupled. So we compute the single site partition function by summing over all the configurations (no atoms, up atom, down atom, two atoms). So

$$Z_1 = 1 + 2e^{\beta\mu} + e^{2\beta\mu - \beta U}, \qquad (5.48)$$

and now the thermodynamics can be derived from the grand canonical potential

$$\Omega = -\frac{\ln Z}{\beta}$$
$$= -N\frac{\ln Z_1}{\beta}, \qquad (5.49)$$

which allows computation of any particular quantity that one wants to study. This can be extended perturbatively to included tunneling.

---

[26]This is not a phase transition as it is a gradual and continuous change. There is a phase transition into a magnetically ordered anti-ferromagnetic state.

5.4   Lecture 4

5.4.1   Characterstics of Mott insulator

To distinguish between a metal and a Mott insulator, are

- Metals are compressible, Mott insulators are not

- Metals have large number fluctuations, Mott insulators have reduced number fluctuations

- Metals have no gap in energy spectrum, Mott insulators have a gapped energy spectrum.

5.4.2   Super-exchange and the Heisenberg model

Returning to the two fermions in a double well model (eq. (5.40)), we can look at the singlet and triplet state $|s\rangle$ and $|t_0\rangle$ respectively, and also $|t_{+1}\rangle = |\uparrow, \uparrow\rangle$ and $|t_{-1}\rangle = |\downarrow, \downarrow\rangle$. To first order in the Hamiltonian, these four states are all degenerate. If we apply the interaction to these states, we break the degeneracy. For example

$$H_{int} |\uparrow, \downarrow\rangle = -t |0, \uparrow\downarrow\rangle - t |\uparrow\downarrow, 0\rangle$$
$$H_{int} |\downarrow, \uparrow\rangle = t |0, \uparrow\downarrow\rangle + t |\uparrow\downarrow, 0\rangle$$
$$H_{int} |\uparrow, \uparrow\rangle = H_{int} |\downarrow, \downarrow\rangle = 0, \tag{5.50}$$

thus we need to go to second order. Then we can compute the energy shift using perturbation theory as

$$\Delta E = \sum_n \frac{\langle \eta | H_{kin} | n \rangle \, \langle n | H_{kin} | \eta \rangle}{E_\eta - E_n}, \tag{5.51}$$

for state η. The results are

$$\Delta E_s^{(2)} = -\frac{4t^2}{U}$$
$$\Delta E_{t_0}^{(2)} = 0$$
$$\Delta E_{+1}^{(2)} = \Delta_{-1}^{(2)} = 0. \tag{5.52}$$

This is the energy spectrum of the Heisenberg model which is given as

$$H = J\vec{S}_l \cdot \vec{S}_r = J \left(S_l^z S_r^z + \frac{1}{2} \left[S_l^+ S_r^- + S_l^- S_r^+ \right] \right), \tag{5.53}$$

where l, r stand for the left and right well respectively and J is anti-ferromagnetic since it tends to anti-align the spin to minimize the energy.[27]

---

[27] We define $\vec{S}_l = (S_l^x, S_l^y, S_l^z)$ and we can define the raising and lowering operators as normal $S_l^{\pm} = \frac{1}{\sqrt{2}}(S_l^x \pm iS_l^y)$. In this case $S_i^z = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$ and $S_i^{+(-)} = c_{i\uparrow(\downarrow)}^\dagger c_{i\downarrow(\uparrow)}$

Computing this energy spectrum, we get three states with energy $J/4$, the triplet states, and a singlet state $-3J/4$. So if we set $J = 4t^2/U$ then the Hubbard model becomes the Heisenberg model. This is called super-exchange since it comes from second order hopping processes. This generalizes in a straightforward way to the full Heisenberg Hamiltonian

$$H = J\sum_i \vec{S}_i\vec{S}_{i+1}. \tag{5.54}$$

Nobody has seen long range magnetic order because of the low temperatures necessary to see magnetic ordering. However, one can observer precursors to long range order.

6 Quantum Interference in Scattering (Jook Walraven)

6.1 Lecture 1

If we have identical atoms, we need to symmetrize or anti-symmetrize the wavefunctions to get the scattering wavefunction.[28]

6.1.1 Colliding Atom Clouds

In order to collide atoms, one can move to the center of mass frame which is convenient in the sense that the measurement is already made in the center of mass frame (as opposed to scattering off a target). The way in which this is done in practice is to prepare the two clouds in a trap with two wells in the axial direction and one in the radial direction. The axial trap is then changed to a single harmonic trap and a magnetic field is applied to collide the atoms.

To do tomography, we can rely on axial symmetry and therefore only one picture is needed. We can analyze the optical density as

$$n(\rho, z) = \frac{1}{4\pi} \int_{-\infty}^{\infty} \tilde{n}_2(\kappa_x, z) J_0(\kappa_x \rho) |\kappa_x| \, d\kappa_x, \tag{6.1}$$

where $n(\rho, z)$ is the real 3D density. The $\bar{n}_2$ is the optical density. [29]

Now restricting to bosons (fermions are similar with different l parity), Theory gives that

$$\sigma(\theta) = 2\pi |f(\theta + f(\pi - \theta)|^2, \tag{6.2}$$

and we can substitute the partial wave expansion

$$\sigma(\theta) = 2\pi \left| \frac{2}{k} \sum_{l = \text{even}} (2l + 1) P_l(\cos\theta) e^{i\eta_l} \sin\eta_l \right|^2$$

$$= \frac{8\pi}{k^2} \left| e^{i\eta_0} \sin\eta_0 + \frac{5}{2}(3\cos\theta - 1) e^{i\eta_2} \sin\eta_2 \right|^2, \tag{6.3}$$

and interference terms will come from the cross terms. One can then fit the scattering from collision experiments to these formulas and extract a triplet potential.

We can find the cross section for identical particles as

$$\sigma_{\pm} = \frac{8\pi}{k^2} \sum_{l = \text{even/odd}} (2l + 1) \sin^2\eta_l \implies \theta_0 = \frac{8\pi}{k^2} \sin^2\eta_0, \tag{6.4}$$

and in the low energy limit $\eta_0 = -ka$. In terms out that there is a d-wave resonance near the first Ramsauer-Townnsend minimum of the s-wave scattering. So in this way interference can tell us something about collisions.

---

[28]See Jook Walraven's previous lecture on identical particle scattering
[29]More references in M.Born and E. Wolf, Principles of Optics

6.1.2   Many particle scattering

We now need to consider scattering with many particles. Consider a spherical volume with the scattering center in the center of the sphere. The wavefunction is given as

$$\psi_{nlm} = c_{nlm} Y_l^m(\theta, \phi) R_{nl}(r), \tag{6.5}$$

and we will go to ultra-cold temperatures where we are only concerned with s-wave scattering. We can write in the non-interacting situation

$$R_0^{(0)} = c_m \frac{\sin(k_m r)}{r}, \tag{6.6}$$

and there is no phase-shift due to no interaction. The boundary condition here is that $\sin(k_m R) = 0$ (R is the radius of the sphere) , which quantizes k as $k_m = m\pi/R$. We can normalize to find that $c_m = \sqrt{2/R}$.

Now we move to the interacting case. Our wavefunction for $r > r_0$ is now

$$R_0^{(0)}(k_m', r) = c_m' \frac{\sin(k_m' r + \eta_0(k_m'))}{r} \tag{6.7}$$

and so we can impose the boundary condition at the first zero as

$$\sin(k_m' R + \eta_0(k_m')) = 0 \implies k_m' = m \frac{\pi}{(R-a)}, \tag{6.8}$$

in the limit that $k_m' \to 0$, thus the energy levels shift which we can calculate as

$$
\begin{aligned}
\delta\epsilon = k'^2 - k^2 &= \left(\frac{\pi}{R-a}\right)^2 - \left(\frac{\pi}{a}\right)^2 \\
&= \left(\frac{\pi}{R}\right)^2 \left[\frac{1}{(1-a/R)^2} - 1\right] \\
&\approx \left(\frac{\pi}{R}\right)^2 \left[1 + 2\frac{a}{R} + \cdots - 1\right] \\
&= 2\pi^2 \frac{a}{R^3} \tag{6.9}
\end{aligned}
$$

where we are working in the wavenumber representation (scaled by units of $\hbar^2/2m$ and have expanded using the fact that $|a| \ll R$. So the energy change is linear in the scattering length. This means the sign of the scattering length determines whether the system is effectively attractive or repulsive.

6.1.3   Chemical potential

We will give now a pedestrian approach to the chemical potential μ for interacting bosons. Consider N bosons in the ground state. We take a sphere with volume

$4\pi R^3/3$. The wavefunction is not homogeneous and so we can calculate the density in the center of the trap. The norm is given as

$$\int |\psi_0(\vec{r})|^2 \, d\vec{r} = |\psi_0(0)|^2 \underbrace{\int \frac{|\psi_0(\vec{r})|^2}{|\psi_0(0)|^2} \, d\vec{r}}_{V_{eff}} \tag{6.10}$$

where V_{eff} is an effective volume given as $\frac{2}{\pi} R^3$ and thus

$$\delta\epsilon = \frac{\hbar^2}{m} 2\pi^2 \frac{a}{R^3} = \frac{4\pi\hbar^2}{m} \frac{a}{V_{eff}}, \tag{6.11}$$

which is the energy shift for one pair and so for N particles, there are $N(N-1)/2 \approx N^2/2$ pairs. Thus, the energy of the gas is given as

$$E = \delta\epsilon \frac{N^2}{2} = \frac{2\pi\hbar^2}{m} \frac{aN^2}{V_{eff}}, \tag{6.12}$$

and knowing that $\mu = \frac{\partial E}{\partial N}$, we can calculate

$$\mu = \frac{4\pi\hbar^2}{m} an = g_0 n, \tag{6.13}$$

where n is the density. The difficulty in this calculation is we assumed the center of mass of all the pairs in the center of the sphere which is an approximation.

Now we can do this for fermions which was first done by P.W. Anderson in 1967. Fermions have the same single particle energy levels as bosons, it is only the occupation that is different. For s-wave,

$$\epsilon_F = k_F^2 = n_F^2 \left(\frac{\pi}{R}\right)^2, \tag{6.14}$$

Since identical fermions cannot scatter each other, consider a single fermion of a different state (different isotope or spin state) located at the center of the sphere. [30]

Substituing this into the equation for Fermi energy

$$\epsilon_F = (6\pi^2 n_s)^{2/3} = \left(\frac{g\pi}{2} \frac{N}{R^3}\right)^{2/3}, \tag{6.15}$$

where $n_s = N/V_{eff}$. The number of particles scattered can be computed in

$$n_F \approx N^{1/3}. \tag{6.16}$$

To get an appreciation of this, for a million fermions in a box, only 100 will interact with the *impurity* embedded.

---

[30]This infinite mass approximation is good for a mixture of Li and K since K is so much heavier

The overlap of the perturbed gas of level j of the pertubed system with state of level i of the unperturbed system

$$\langle\alpha_i|\beta_j\rangle = \frac{2}{R}\int_0^R dr\,\sin(k_i r)\sin(k'_J r + \eta_0(k'_j)),\qquad(6.17)$$

and if $i = j$, then in the limit that the phase shift goes to zero, this must be unity. So we expect for small phase shifts and $i = j$, only small corrections. In fact

$$\langle\alpha_i|\beta_j\rangle = \frac{\sin\eta_0(k_j)}{(i-j)\pi + \eta_0(k_j)},\qquad(6.18)$$

which behaves properly if $i = j$ and $\eta_0 \to 0$ and if $i \neq j$, then the overlap becomes very small although non-zero since the interactions couple the particles.

With a shift in only $N^{1/3}$ levels, we want to know how the overall many body wavefunction changes. To shift the phase, we use a Feshbach resonance, which allows one to write

$$a(k) + a_s + \frac{1}{k}\arctan\left[\frac{ka_{res}}{1 + k^2 R^* a_{res}}\right],\qquad(6.19)$$

and now writing the Slater determinant

$$|\psi_\alpha\rangle = |\alpha_1, \alpha_2, \ldots, \alpha_N\rangle = \frac{1}{\sqrt{N!}}\sum_{P_\alpha}(-1)^{P_\alpha}P_\alpha\,|\alpha_1\rangle\otimes|\alpha_2\rangle\otimes\cdots\otimes|\alpha_N\rangle,\qquad(6.20)$$

which can also be written in the usual matrix form. So this allows us to find

$$\langle\psi_\alpha|\psi_\beta\rangle = \begin{vmatrix} \langle\alpha_1|\beta_1\rangle & \cdots & \langle\alpha_1|\beta_N\rangle \\ \vdots & \ddots & \vdots \\ \langle\alpha_N|\beta_1\rangle & \cdots & \langle\alpha_N|\beta_N\rangle \end{vmatrix},\qquad(6.21)$$

and this overlap for weak interactions is 0 although it might be expected to be perturbative.[31]

6.2　Lecture 2

6.2.1　Impurities in a Fermi Gas

We will study the experiment in the Grimm group where an impurity of ^{40}K was in a Fermi gas of 10^6 atoms of ^{6}Li. The wavefunctions were derived in the last lecture. In some limits this particle becomes a polaron. For the single particle state the overlap between interacting particles is perturbative, whereas the many particle state overlap is not perturbative and is zero in the thermodynamic limit.

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[31]This was the finding by Anderson in the thermodynamic limit. The Demler group then showed that a time dependent interferometric method can see this experimentally using a quench.

Experimental realizations of this can be performed using Feshbach Resonances. The signal is then observed using Ramsey spectroscopy.

To understand this we will look at the Loschmidt echo. Consider a superposition after the first $\pi/2$ pulse

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|\downarrow\rangle + |\uparrow\rangle)|\phi_\alpha\rangle, \tag{6.22}$$

and then the system evolves as

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}(e^{iH_0t/\hbar}|\downarrow\rangle|\phi_\alpha\rangle + e^{iH_1t/\hbar}|\uparrow\rangle|\phi_\alpha\rangle), \tag{6.23}$$

and applying an S_x operator, gives

$$S_x|\psi(t)\rangle = \frac{1}{2\sqrt{2}}(e^{iH_0t/\hbar}|\uparrow\rangle|\phi_\alpha\rangle + e^{iH_1t/\hbar}|\downarrow\rangle|\phi_\alpha\rangle), \tag{6.24}$$

and then we can calculate

$$\begin{aligned}
S(t) &= \langle S_x\rangle \\
&= \frac{1}{4}\langle\phi_\alpha|e^{iH_0t/\hbar}e^{-iH_1t/\hbar} + e^{-iH_0t/\hbar}e^{iH_1t/\hbar}|\phi_\alpha\rangle \\
&= \frac{1}{2}Re\left[\langle\phi_\alpha|e^{iH_0t/\hbar}e^{-iH_1t/\hbar}|\phi_\alpha\rangle\right] \\
&= \frac{1}{2}Re\left[\langle\phi_\alpha(t)|\psi_\beta(t)\rangle\right],
\end{aligned} \tag{6.25}$$

which is what was being sought to measure.
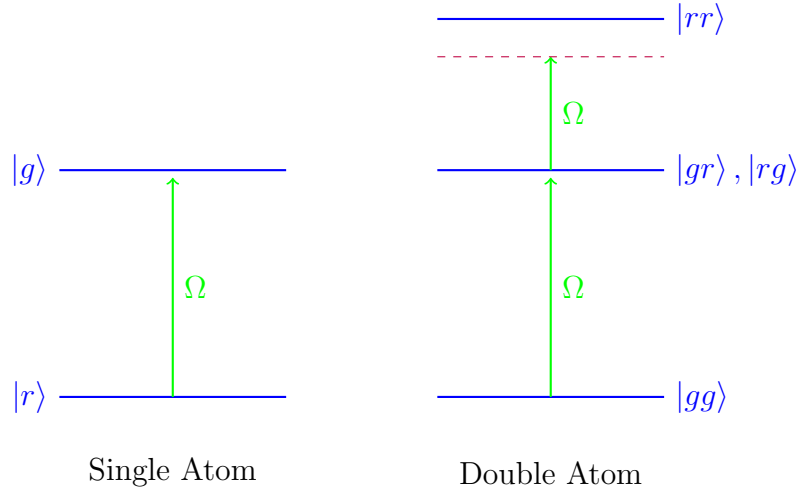
Figure 7: The doubly excited state in the double atom picture is never populated and thus there is enhanced coupling between $|gg\rangle$ and $(|gr\rangle + |rg\rangle)/\sqrt{2}$ as long as $U_{vdW} \gg \hbar\Omega$

7 Cold Rydberg Atoms (Thierry Lahaye)

7.1 Lecture 1

7.1.1 General introduction to Rydberg Atoms

Rydberg atoms are atoms in a state with a very large principal quantum number n. These atoms have exaggerated properties:

- Large size, long lifetime

- Strong interactions with external fields

- Strong interactions between atoms

Rydberg atoms were originally used a probe to study the first formulations of quantum mechanics. In the 1970's, the advent of tunable lasers fermented a new wave of study on atom-light interactions with Rydberg atoms. The recent studies deal with cold Rydberg atoms and are mainly used to probe interactions. These interactions can be used to do quantum state engineering. These often take advantage of the dipole dipole interaction in Rydberg atoms.

The idea behind a quantum gate proposal is a Rydberg blockade and is shown if 7.

We can write the one atom Hamiltonian as

$$H = \frac{\hbar\Omega}{2}(|r\rangle \langle g| + |g\rangle \langle r|), \tag{7.1}$$

Input	Output
$\lvert 00 \rangle$	$\lvert 00 \rangle$
$\lvert 01 \rangle$	$-\lvert 01 \rangle$
$\lvert 10 \rangle$	$-\lvert 10 \rangle$
$\lvert 11 \rangle$	$-\lvert 11 \rangle$

Table 1: Truth table of the 2 qubit gate proposal by Jacksh *et al.* PRL 2000. The last element is the blockade.

and if we write this in the basis $(\lvert gg \rangle, \lvert gr \rangle, \lvert rg \rangle, \lvert rr \rangle)$, then the matrix form of the Hamiltonian is given as

$$H = \frac{\hbar}{2} \begin{pmatrix} 0 & \Omega & \Omega & 0 \\ \Omega & 0 & 0 & \Omega \\ \Omega & 0 & 0 & \Omega \\ 0 & \Omega & \Omega & V_{vdW} \end{pmatrix} \tag{7.2}$$

and if we make the approximation $U_{dW} \gg \hbar\omega$, the blockade condition then only the top left 3x3 matrix is relevent. Transforming basis to the linear combinations of $\lvert rg \rangle$ and $\lvert gr \rangle$ states

$$\lvert \psi_{\pm} \rangle = \frac{\lvert rg \rangle \pm \lvert gr \rangle}{\sqrt{2}}, \tag{7.3}$$

then it can be computed that

$$H \lvert \psi_{+} \rangle = \frac{\hbar\Omega\sqrt{2}}{2} \lvert gg \rangle, \tag{7.4}$$

and $H \lvert \psi_{-} \rangle = 0$. This mechanism was used to couple the qubit states to $\lvert r \rangle$ with different frequencies. The idea was to send a π pulse on the first atom, a 2π pulse on the second atom and a π pulse on the third atom. The truth table is given in Table 1. This proposal generated an effort to observe this blockade. The recent developments are still motivated by these ideas.

7.1.2   Energy Levels

Consider Rydberg atoms with high principle quantum number $n \gg 1$. Classically the corresponds to an ionic core with charge $+q$ and a single electron at a far distance. This is reminiscent of the hydrogen atom which we can solve exactly and the energy levels are given as

$$E_n = \frac{-R_y}{n^2}, \tag{7.5}$$

which depend only on the principle quantum number and R_y is the Rydberg number which is approximately 13.6 eV. Rydberg noticed that for other atoms

$$E_{n,l} = \frac{-R_y}{(n - \delta_l)^2}, \tag{7.6}$$

where δ_l depends on the angular momentum quantum number and is usually referred to as the quantum defect. This makes sense because at high values of l, classically we expect the charge from the nucleus to be equivalent to a point source by Gauss' theorem. This implies that $\delta_l = 0$.

If we instead take $l = 0$, the electron follows a straight line to the nucleus in which case the potential of the ionic core, thus the potential matters. In the limit of short distance from the core, the charge goes as Zq. In this case $\delta_l > 0$. Higher l are between these two limits.

One can obtain a model for the Schrodinger equation and calculate the quantum defect, however, it is easier to perform spectroscopy and fit the quantum defects to the observations. This is often more accurate than *ab initio* calculations. In practice, other effects such as fine structure are also included in the quantum defect which introduces some dependence on the total angular momentum J.

One can also expand out the quantum defect in a power series to include some n dependence, which we can write as

$$\delta_{n,l,j} = \delta_0(l,j) + \frac{\delta_2(l,j)}{(n - \delta_0(l,j))^2} + \frac{\delta_4(l,j)}{(n - \delta_0(l,j))^4} + \dots \qquad (7.7)$$

which is an effective expansion in the energy of the electron.

We can easily calculate the scaling of the difference in energy as

$$E_{n+1} - E_n \sim \frac{R_y}{2n^3}, \qquad (7.8)$$

which implies that for $n \approx 50$, then the splitting is in the microwave domain on the order of tens of GHz.[32]

7.1.3   Wavefunctions of Rydberg Atoms

If we neglect spin, we can write the wavefunction as a radial part and an angular part

$$\psi_{n,l,m}(r,\theta,\phi) = R_{n,l}Y_l^m(\theta,\phi). \qquad (7.9)$$

Due to the central symmetry of the problem the angular part is given by the normal spherical harmonics, all we need to calcuate is the radial part.

For l large the radial wavefunctions must be the same as for a hydrogenic atom. But for l small corresponding to non-zero quantum defect, one can numerically derive the radial wavefunction. So we need to solve the Schrodinger equation, however, we already know the eigenenergies, thus the problem is simplified. So we need to integrate the radial Shrodinger equation simplified in the form $u_{n,l}(r) = rR_{n,l}(r)$ as

$$-\frac{\hbar^2}{2m}u''_{n,l} + \frac{\hbar^2}{2m}\left(\frac{l(l+1)}{r^2} - V(r) - E\right)u_{n,l} = 0, \qquad (7.10)$$

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[32]This is nice because microwaves can be easily generated with great precision.

and for Rydberg states, we can calculate the correct wavefunction by knowing the potential close to the origin and far away.

For large r, the potential is $V = -e^2/r$, the normal Couloumb potential. Close the the origin $r \to 0$ $V(r) = -Ze^2/r$. So one in practice solves the equation with $V(r) = eZe^2/r$ for $r \gg n^2 a_0$ starting at large radius.[33] The solution will give a wavefunction with increasingly rapid oscillations close to the a_0, and then a region is reached where the numerical integration cannot proceed. This is the correct wavefunction for large r. One also needs to specify $u(r_0)$ and $u'(r_0)$ for the integration to proceed. For the value of the wavefunction, it will come in as only a scaling and the wavefunction can be normalized at the end of the calculation. However, the derivative may be important, yet any value for the derivative will work. This is because an incorrect derivative gives a decaying exponential and a diverging integration, however there is an exponential damping of the incorrect part and so the correct wavefunction is still obtained. The peak of the probability is located about $3/2n^2 a_0$.

7.1.4   Dipole Matrix Elements

Now we seek to calculate matrix element of the dipole operator

$$\hat{d} = q_e \vec{r}, \tag{7.11}$$

and we know that $\left\langle \hat{d} \right\rangle = 0$ since the alkali atoms have a Hamiltonian which commute with the parity operator, thus the eigenfunctions have a definite parity and no dipole moment. But, the matrix element between two states is not zero. We can write

$$\left\langle n, L, m | \hat{d} | n', L \pm 1, m \right\rangle = \underbrace{\int_0^\infty R_{n',L\pm1}^* \vec{r} R_{n,l}(n) r^2 \, dr}_{\text{angular part}} \times (\text{radial part}), \tag{7.12}$$

The dipole moment will scale as n^2. This large dipole moment is what gives Rydberg atoms exaggerated properties.

Now we look at the dipole matrix element connecting low level states to the Rydberg states. For example, consider the $5s$ ground state of Rubidium which is the ground state and nP, which gives

$$\langle 5s | d | nP \rangle \sim \frac{1}{n^{3/2}}, \tag{7.13}$$

which can be seen by considering how the normalization of the wavefunctions are effected by n. This implies that it is difficult to excite atoms from ground states to Rydberg states. In practice, people use a two photon exitation. In the limit when the detuning from the middle state is large as compared to either Rabi frequency, this can be mapped onto a two level system with an effective two-photon Rabi frequency of

$$\Omega_{eff} = \frac{\Omega_R \Sigma_B}{2\Omega}. \tag{7.14}$$

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[33]The wavefunction is nonzero on the order of $n^2 a_0$.

7.2   Lecture 2

7.2.1   Lifetimes of Rydberg States

Assume we have a two level system $|a\rangle, |b\rangle$, where $|a\rangle$ is the ground state. The state $|b\rangle$ will decay to state $|a\rangle$ due to coupling with the vaccum field. The decay rate is given as

$$\Gamma_{b\to a} = \frac{d_{ab}^2 \omega_{ab}^3}{3\pi\epsilon_0 \hbar c^3}, \tag{7.15}$$

which we can use to compute lifetimes of a Rydberg state.

Consider a 50s state, then there exists many states which will directly couple to this state such as those of the form $|n'p\rangle$. The decay rate is given as the sum of the decay rate to all of these states. Define decay rate γ_{ns} as

$$\gamma_{ns} = \sum_{n'=5}^{n-2} \gamma_{ns\to n'p}. \tag{7.16}$$

We can break up the contributions between nearby states and far states. For nearby states $n' \approx n$ and thus

$$\gamma_{n\to n'} \propto n^4 n^{-9} = n^{-5}, \tag{7.17}$$

For low lying state $n' \approx 1$, then

$$\gamma_{n\to n'} \propto n^{-3} n^0 = n^{-3}, \tag{7.18}$$

which implies that when n is large the decay mechanism to the low lying states dominates. So the lifetime is inversely proportional to γ and thus $\tau \propto n^3$, and for $n = 50$, the lifetime is on the order of $200\mu s$. Since the dynamics we care about occur on nanosecond time scales, this lifetime is negligible in most experimental contexts.

If one prepares a state $|n, L = n - 1, m = L\rangle$, the so-called *circular Rydberg states*, the lifetime scales as n^5 as transitions to low lying states is not allowed. These lifetimes can reach 30ms.

Another contribution to the lifetime is blackbody radiation which lowers the lifetimes as it transfers populations to nearby states. Including this contribution, the depopulation rate due to blackbody radiation is given as

$$\gamma_{BBR} = \sum_{r\to r'} \gamma_{r\to r'} \bar{N}_{bbr}(\omega_{r\to r'}), \tag{7.19}$$

where the average number of photons is given by Planck's law

$$\bar{N}_{bbr}(k) = \frac{1}{e^{\hbar\omega k_B T} - 1}, \tag{7.20}$$

which for 300K is about 150. So this greatly decreases the lifetime, but is usually only on the order of the lifetime, so $200\mu s \to 100\mu s$. This is still long enough to do experiments.

One can understand all of this scaling through semi-classical arguments. Imagine an elliptic orbit of the electron around the ion. The period of this orbit scales as n^3, which can be found from Kepler's laws. In the classical picture, an accelerating charge emits radiation and lose energy with a power proportional to the square of the acceleration. The acceleration in this picture is only large near the ion. For the n^5 scaling, there is a different classical argument.

7.2.2   Stark effect in Rydberg Atoms

We can write electric field $\vec{F}$ as

$$\vec{F} = F\vec{u}_z, \tag{7.21}$$

and thus we get the Stark Hamiltonian

$$H_s = qFz = -\vec{d} \cdot \vec{F}. \tag{7.22}$$

to solve this, we can use perturbation theory. For the Hydrogen atom, we have degenerate states of opposite parity which gives rise to a linear dependence on electric field magnitude. This can be derived through degenerate perturbation theory to first order.

For an alkali atom, the states are no longer degenerate in n, thus we can use non-degenerate perturbation theory. The first order effect is always zero as there is no dipole transition between the same state. So we go to second order which means the shift will be quadratic in F and can be written as

$$\Delta E \frac{1}{2}\alpha F^2, \tag{7.23}$$

where α is the polarizability given as

$$\alpha_{ns} = \sum_{n'p} \frac{|\langle ns|d|n'p\rangle|^2}{E_{ns} - E_{n'p}}. \tag{7.24}$$

We can look at the polarizability scaling with n and using our previous results, we get $n \propto n^4/n^{-3} = n^7$. In the lab, this means that atoms are extremely sensitive to electric fields. for $n = 50$, $\alpha = 300\text{MHz}/(\text{V/cm})^2$.

Rydberg atoms can be ionized with electric fields, this allows state selective ionizaton to detect populations in the states.

7.2.3   Interactions between Rydberg atoms

The basic interaction is the dipole-dipole interaction, which can be written as

$$V_{dd} = \frac{1}{4\pi\epsilon_0 R^3} \left[\vec{d}_1 \cdot \vec{d}_2 - 3(\vec{d}_1 \cdot \vec{n})(\vec{d}_2 \cdot \vec{n}) \right], \tag{7.25}$$

where $\vec{n}$ is the unit vector defined as $\vec{n} = \vec{R}/R$. We can treat this in the context of perturbation theory. We can write the states as $|\alpha, \beta\rangle$, which corresponds to the

pair states of two atoms and contain all the quantum numbers for two atoms. The pair state energy is $E_\alpha + E_\beta$. We will use these as our unperturbed basis. To first order we calculate

$$\Delta^{(1)} = \langle \alpha | V_{dd} | \beta \rangle = 0, \tag{7.26}$$

for most states. So we must go to second order. If we consider for simplicity that the two atoms are in the same state $|\alpha, \alpha\rangle$, we can calculate the interaction as

$$\Delta E^{(2)} = \sum_{|\beta,\gamma\rangle} \frac{|\langle \alpha, \alpha | V_{dd} | \beta, \gamma \rangle|^2}{2E_\alpha - E_\beta - E_\gamma} = \frac{C_6}{R^6}, \tag{7.27}$$

which is the van der Waals-London interaction coefficient. We can look at how this interaction scales with the principle quantum number by

$$C_6 \sim \frac{n^6}{n^{-3}} = n^{11}, \tag{7.28}$$

so this interaction becomes very strong with large quantum numbers. As always, the perturbation theory is only valid for small shifts relative to the energy spacing of the unperturbed states. Sometimes for particular states, quasi-degeneracies exist between pair states.[34] Here the perturbation theory is not valid and we use degenerate perturbation theory only in the basis of the quasi-degenerate states.

The non-degenerate Hamiltonian is given as

$$H_0 = \begin{pmatrix} 0 & 0 \\ 0 & \delta \end{pmatrix}, \tag{7.29}$$

and the perturbation is given as

$$V_{dd} = \begin{pmatrix} 0 & \frac{C_6}{R^3} \\ \frac{C_6}{R^3} & 0 \end{pmatrix}, \tag{7.30}$$

and if we diagonalize $H_0 + V$, we get the perturbed eigenstates and eigenvalues. This will result in an avoided crossing at $\delta = 0$ which eigenstates of the symmetric and antisymmetric combinations of the pair states.[35] This is called the Forster resonance.

If we have calculate the interaction between states which are not the same, for example 50S and 50P, then dipole-dipole interaction couples the pair states which exchange the two states

$$|\alpha, \beta\rangle \leftrightarrow |\beta, \alpha\rangle, \tag{7.31}$$

and the eigenenergies are as before $E_\pm = \pm C_3/R^3$ and the eigenstates are the symmetric and antisymmetric combinations of the pair states. The term C^3/R^3 scales as n^4/R^3.

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[34]For Rb states $\alpha = |59D_{3/2}, m_j = 3/2\rangle$, $\beta = |57F_{5/2}, m_j = 5/2\rangle$, and $\gamma = |61P_{1/2}, m_j = 1/2\rangle$, the pair states $|\alpha, \alpha\rangle$ and $|\beta, \gamma\rangle$ differ in energy by only 8MHz.

[35]$|\psi_\pm\rangle = \frac{1}{\sqrt{2}}(|\alpha, \alpha\rangle \pm |\beta, \gamma\rangle)$

7.3 Lecture 3

7.3.1 Interactions cont.

Consider two states such that $\left\langle \uparrow |\hat{d}_q| \downarrow \right\rangle \neq 0$, the basis $\{|\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\}$ V_{ddi} reads

$$V_{ddi} = \frac{C_3}{R^3} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{C_3}{R^3}(\sigma_+^1 \sigma_-^2 + \sigma_-^1 \sigma_+^2). \tag{7.32}$$

Since these are not eigenstates, the populations should oscillate between the two states.

7.3.2 Rydberg Blockade

The idea for N atoms which will then undergo Rydberg, in the sense that all atoms have a strong interaction compared to the Rabi frequency. The maximum size is defined as the Blockade radius R_b and is when the interaction energy of two atoms is equal to the Rabi frequency,

$$\frac{C_6}{R_b^6} = \hbar\omega \implies R_b = \left(\frac{C_6}{\hbar\omega}\right)^{1/6}, \tag{7.33}$$

which can range from 5μm to 15μm. These sizes are hard to accomplish. In principle there should only be one Rydberg excitation, however this is also hard to detect.

7.3.3 Beyond Blockade

Three relevant spin Hamiltonians to beyond blockade dynamics are

$$H_1 = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_J \text{ (Heisenberg)}$$

$$H_2 = \sum_{i,j} J_{ij} S_i^z S_j^z \text{ (Ising)}$$

$$H_2 = \sum_{i,j} J_{ij} S_i^+ S)j^- + h.c. \text{ (XY)} \tag{7.34}$$

Writing the Hamiltonian for the Rydberg blockade as

$$H = \Omega \underbrace{\sum_{i=1}^{n}(|g_i\rangle \langle r_i| + |r_i\rangle \langle g_i|)}_{\text{Laser Driving}} + \underbrace{\sum_{i,j} \frac{c_6}{|\vec{r}_i - \vec{r}_j|^6} |r_i r_j\rangle \langle r_i r_j|}_{\text{Interaction}}, \tag{7.35}$$

and if we let $|g\rangle \to |\downarrow\rangle$ and $|r\rangle \to |\uparrow\rangle$, we can set the laser driving term to σ_x^i and the interaction term can be written as an Ising term plus signle particle terms giving rise to a Hamiltonian of

$$H = \Omega \sum_i \sigma_x^i + \sum_{i,j} J_{ij} \sigma_z^i \sigma_z^j + \sum_i B_i \sigma_z^i, \tag{7.36}$$

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which allows one to map the Rydberg system to quantum magnetism.[36]

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[36]One can absorb the offset terms by carefully choosing the detuning. One can see this by going to the rotating wave approximation in the dressed state picture.

8 Dipolar Gases (Bruno Laburthe-Tolra)

8.1 Lecture 1

8.1.1 Diplar Systems

There are two kinds of dipole systems, magnetic and electric. Consider first electric dipoles. There are no permanent electric dipole moments known, however, an electric dipole moment can be made by separating two opposite charges. The dipole moment operator is given as

$$D = \sum_i e_i \vec{r}_i, \tag{8.1}$$

and gives rise to an energy with electric field $\mathcal{E}$,

$$E = -D \cdot \mathcal{E}, \tag{8.2}$$

however $\langle S | e \cdot \vec{r} | S \rangle = 0$, because there is no dipole moment between states of the same parity. In molecules, these dipole interactions will couple rotational states and can be coupled by an electric field with energies typically scaling linearly in electric field. To study this, people have been using heteronuclear molecules. This is because rotation will be induced by an electric field. A homonuclear system will not work in this way.

The second dipolar system is magnetic atoms which has a permanent magnetic dipole moment which can be associated to either spin or angular momentum. The important difference between these atoms and molecules is that in the ground state $|S, m - S\rangle$ the energies go linearly in the magnetic field. However, at vanishingly small magnetic field, the levels are all degenerate, which is different than the molecular case.

Some typical atoms are Cr, which has $\mu = 6\mu_B$, Er, $\mu = 7\mu_B$, and Dy, $\mu = 10\mu_B$, whereas a typical alkali atom has $\mu = 1\mu_B$. The most common heteronuclear molecules are KRb, and NaK.

8.1.2 Diple-Dipole Interaction characteristics

The potential of the dipole-dipole interactions is given for magnetic dipoles as

$$V_{dd}^M = \frac{\mu_0}{4\pi}(g_s\mu_B)^2 \left[r^2\vec{S}_1 \cdot \vec{S}_2 - 3(\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r}) \right], \tag{8.3}$$

and for electric diples as

$$V_{dd}^E = \frac{1}{4\pi\epsilon_0 r^5} \left[r^2\vec{d}_1 \cdot \vec{d}_2 - 3(\vec{d}_1 \cdot \vec{r})(\vec{d}_2 \cdot \vec{r}) \right], \tag{8.4}$$

and we can normally write the ratio of magnetic to electric dipole as

$$\frac{V_{dd}^M}{V_{dd}^E} = \frac{\alpha^2}{4}, \tag{8.5}$$

thus the realm of magnetic dipoles is small interactions and electric dipoles can potentially have large interactions.

Dipole interactions have several useful properties which are often mentioned. First, they are considered *long range*. To see this, note that the phase shift of a partial wave scales as

$$\delta_l(k) \propto \begin{cases} k^{2l+1} & \text{if } l < (n-3)/2 \\ k^{n-1} & \text{else,} \end{cases} \tag{8.6}$$

which means that for dipolar gases, the scattering phase shift have contributions from all partial waves. In addition, this means that fermions collide even at low temperatures and when they are polarized.

The question of long range or short range depends on the type of physics one is examining. It is long range in the sense of all partial waves contributing, we can also calculate

$$A = \int d^D r V(r), \tag{8.7}$$

which converges only when $D > m$, where m is the power of interaction. So from this point of view the long rangeness of the interaction depends on the dimensionality. So in 3D, the dipole diple interaction is long range, but it is short range in 2D or 1D. This has the consequence that if there are two subsystems A and B, then

$$E(A \cup B) \neq E(A) + E(B). \tag{8.8}$$

now we consider the anisotropy of the interaction, by rewriting the interaction as

$$V = \frac{d^2}{r^3}(1 - 3\cos^2\theta), \tag{8.9}$$

which has many consequences, however, the main one is that this is not a central potential. As a consequence, the partial wave l is not a good quantum number. So different partial waves are coupled by the potential and angular momentum of rotation can change in time.

8.1.3 Two Body collisions

It is often useful to rewrite the operator part of the interaction in terms of ladder operators

$$S^+ = \frac{S^x + iS^y}{\sqrt{2}}; \; S_- = \frac{S^x - iS^y}{\sqrt{2}}, \tag{8.10}$$

and $r_+ = x + iy$ and $r^- x - iy$ as

$$\begin{aligned} \left[r^2 \vec{S}_1 \cdot \vec{S}_2 - 3(\vec{S}_1 \cdot \vec{r})(\vec{S}_2 \cdot \vec{r})\right] &= S_1^z S_2^z + \frac{1}{2}(S_1^+ S_2^- + S_1^- S_2^+) \\ &\quad - \frac{3}{4}\Big[(2zS_1^z + r^- S_1^+ + r^+ S_1^-) \\ &\quad \times (2zS_2^z + r^- S_2 + +r^+ S_1^-)\Big], \end{aligned} \tag{8.11}$$

which we can separate into the Ising term

$$S_1^z S_2^z (1 - 3\cos^2\theta),\tag{8.12}$$

which is the most studied term and the excgange interaction

$$-\frac{1}{2}(S_1^+ S_2^- + S_1^- S_2^+).\tag{8.13}$$

Therms like $zr^+ S_1^z S_2^-$ which is a collision between two atoms where one stays in the same spin state, and one spin state is lowered. This is known as diplar relaxation. We can write the two channels for this as

$$|m_s, m_s\rangle \to |m_s, m_s - 1\rangle$$
$$|m_s, m_s\rangle \to |m_s - 1, m_s - 1\rangle.\tag{8.14}$$

There is some interesting physics coming from this interaction if we note that

$$E(m_s) = m_s \mu_B B,\tag{8.15}$$

so there can be a change in energy of $2E(m_s)$ in the dipolar relaxation and since total angular momentum should be conserved, there must be an increase in orbital angular momentum $\Delta l = 2$. For normal magnetic fields, this energy is on order of MHz, however, for small magnetic fields $B \to 0$, there may be resonances from this interaction. This can only be achieved with magnetic atoms, since molecules do not go towards degeneracy at low B.

8.1.4   Strength of Dipole-Dipole Interaction

To calculate the strength of a dipole-dipole interaction, we first perform a back of the envelope calculations while thinking in terms of scattering. Typically the interaction is proportional to C_{dd}/r^3 and the cost of the scattering is on order $\hbar^2/mr_0^3$, and thus, we can define a dipolar length

$$r_0 = \frac{mC_{dd}}{\hbar^2},\tag{8.16}$$

and thus $\sigma = \pi r_0^2$. This is correct up to numerical factors. For atoms like Cr, r_0 is on order of the typical scattering length of the experiments.

To be more quantitative, one needs to do a full scattering calculation to get a Fermi Golden rule

$$dw = \frac{2\pi}{\hbar}|V_{k_0,k_f}|\delta(E_f - E_0)\delta^3(k_f),\tag{8.17}$$

which says that $\Gamma \propto V_{dd}^2 \rho(\epsilon_f)$, where ρ is the density of states at a certain energy. This will give quite different results for the different parts of the dipole-dipole interaction. The result of this calculation is that for the Ising interaction

$$\sigma_0 = \frac{16\pi}{4S}S^4 f^2(1 \pm h(1)),\tag{8.18}$$

and the diplar relaxation gives a result

$$\sigma_1^{(\Delta m=1)} = \frac{8\pi}{15} S^3 f^2 \left(1 \pm h\left(\frac{kf}{k_0}\right)\right) \frac{k_f}{k_0}, \tag{8.19}$$

where

$$f = \frac{\mu_0}{4\pi} \frac{(g_s \mu_B)^2 m}{\hbar^2}, \tag{8.20}$$

and $h(k)$ is some complicated analytic formula which is different for bosons and fermions.

8.1.5   Molecular Physics View

The diplar relaxation couples

$$|m_s, m_s\rangle |l = 0\rangle \leftrightarrow |m_s, m_s - 1\rangle |l = 1, m_l = 1\rangle, \tag{8.21}$$

which an energy difference of $g\mu_B B$. Now considering the centrifugal barrier

$$\frac{l(l+1)}{mR^2} \hbar^2, \tag{8.22}$$

there will be an avoided crossing with the potential at a difference such that

$$\frac{l(l+1)}{mR_c^2} = g\mu_B B \implies R_c \sim \frac{1}{\sqrt{B}}, \tag{8.23}$$

which gives large contributions for far distances at low magnetic fields.

The initial wavefunction for vanishingly low energy is given as

$$\psi_{in} = \left(1 - \frac{a}{R}\right) \tag{8.24}$$

and ψ_{out} is very oscillatory at long distance, however, at short distance, they both vary slowly, which gives the results

$$|\langle \psi_{in}|V_{dd}(R)|\psi_{out}\rangle|^2 \propto |\psi_{in}(R_c)|^2, \tag{8.25}$$

which says this interaction is only long range for small magnetic fields in some sense. Now we note that for large B,

$$|\langle \psi_{l=2}|V(R)|\psi_{l=4}\rangle|^2 \approx 0, \tag{8.26}$$

but for zero magnetic field

$$|\langle \psi_{l=2}|V(R)|\psi_{l=4}\rangle|^2 \neq 0. \tag{8.27}$$

8.1.6　Fourier Transform

It is useful to remember that the Fourier transform of a contact interaction is independent of k. One can prove that the Fourier transform of the dipole-dipole interaction in three dimensions is

$$V_dd(k) = \frac{C_{dd}}{3}(3\cos^2\theta_k - 1),\tag{8.28}$$

where θ_k is the angle between the wavevector and the magnetic field. Thus the Fourier transform is independent of the modulus of $\vec{k}$, but does depend on the angle. In 2D, $V_{dd}(k) \propto k$ for $k \to 0$. So in 2D, there will be a tendency of the gas to develop structure.

8.2　Lecture 2

8.2.1　Mean field

We can write down the time dependence of a quantum operator as

$$\frac{d\hat{S}}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{S}],\tag{8.29}$$

and if we consider the interaction of a spin with a magnetic field, we have the Hamiltonian for a magnetic field along the $\hat{z}$ direction

$$H = gB_zS_z,\tag{8.30}$$

which gives rise to the relation

$$\frac{dS_x}{dt} = \frac{i}{\hbar}B_z(S_zS_x - S_xS_z = \alpha LS_y, \implies \frac{d\hat{S}}{dt} = \gamma\hat{S} \times \vec{B},\tag{8.31}$$

which is an equation of precession. Now if there are two atoms, one atom will precess around the atom created by the other atom.

For many spins, we can consider the spin of one atom precessing in a mean field created by all the other spins. So a single spin of atom 1

$$\frac{d\vec{S_1}}{dt} = \gamma\vec{S_1} \times (\vec{B} + \sum_j \vec{B_j}(\vec{r})),\tag{8.32}$$

and thus, if a measurement should be made then

$$\frac{\langle dS_1\rangle}{dt} = \gamma\left\langle \vec{S_1} \otimes (\vec{B} + \sum_j \vec{B_j}(\vec{r}))\right\rangle \approx \gamma\langle S_1\rangle \otimes (\vec{B} + \left\langle\sum_j \vec{B_j}(\vec{r})\right\rangle),\tag{8.33}$$

where in the last equality we have made an assumption to ignore correlations, the mean field approximation. We can write it down in a more complicated way for a spin one particle

$$i\hbar\dot{\psi}_j(r) = H_{ij}^{dd}(r)\psi_j(r),\tag{8.34}$$

where

$$H_{ij}^{dd}(r) = \int d^3r' \psi_k^*(r') V_{jkl}^{dd}(r - r') \psi_l(r'), \tag{8.35}$$

and the interaction is written as

$$V_{jkl} = \frac{\mu^2}{|r - r'|^3} \hat{S}_{ij} \hat{S}_{kl} - \frac{3\mu^2}{|r - r'|^5}(S_{ij} \cdot (r - r'))(S_{kl} \cdot (r - r')), \tag{8.36}$$

which we can also write as

$$\phi(r) = \int d^3r' n(r) V_{dd}(r - r') n(r'), \tag{8.37}$$

which is not completely correct in some regimes since it is mean field. Certainly in the case of Fermions, this cannot be true since it allows for particles to be at the same place.

An example where this is wrong is a lattice in three dimensions with spin 1 particles. The intial state is given as

$$|\psi_0\rangle = |0, 0, \ldots, 0\rangle, \tag{8.38}$$

which indexes the spins at each site, all are $m_s = 0$. So the dipole-dipole interaction is

$$V_{dd} = \sum_{i,j} V_{ij}^{dd} = \sum_{i,j}(S_i^+ S_j^- + S_i^- S_j^+), \tag{8.39}$$

which is the part relevant here. So we have that

$$|\psi_1\rangle = \sum_{i,j} V_{ij} |0, \ldots, 1, \ldots, -1, \ldots, 0\rangle \times \frac{1}{\sqrt{\sum V_{ij}^2}}, \tag{8.40}$$

where the 1 is in the i location and the -1 is in the j location. The rate at which this occurs is given as

$$\Gamma = \frac{1}{\hbar} \left\langle \psi_0 \left| \sum_{ij} V_{ij}^{dd} \right| \psi_1 \right\rangle = \frac{1}{\hbar} \sqrt{\sum_{ij} V_{ij}^2}, \tag{8.41}$$

which can be derived from second order perturbation theory. There may be additional terms in fourth order. This is very different from the mean field description as in the mean field description a homogeneous system gives rise to a mean field interaction of zero. In the simple system we have enumerated, this is not true. The difference comes down to entanglement and correlations, which we ignore in mean field.

8.2.2 Correlations in mean field

The mean field equation does not work in some important regimes, but we can rework it to include some correlations. So consider a many body state

$$E = \int d^3 r_i \psi^*(r_1, r_2, \ldots, r_N) \sum_{i,j} V_{dd}(r_i - r_j) \psi(r_1, r_2, \ldots, r_N)$$

$$= \frac{N(N-1)}{2} V_{dd}(r_1 - r_2) \int d^3 r_1 d^3 r_2 \int d^3 r_3 \cdots d^3 r_N \psi^*(r_1, \ldots, r_N) \psi(r_1, \ldots r_N)$$

$$\frac{1}{2} \int dr_1 dr_2 V_{dd}(r_1 - r_2) \rho^{(2)}(r_1, r_2, r_1, r_2), \tag{8.42}$$

where we have used symmetry arguments and made no approximations. We can write the two body density matrix as

$$\rho^{(2)}(r_1, r_2, r_1', r_2') = N(N-1) \int d^3 r_3 \cdots d^3 r_N \psi(r_1, \ldots, r_N) \psi^*(r_1, \ldots, r_N). \tag{8.43}$$

One can derive the two body density matrix for Fermions and Bosons using only the commutation relations although we will simply state the results here.

For Fermions, one assumes the wavefunction is described by a modified Slater determinant where the one body wavefunctions used are dressed by interactions. Then

$$\rho^{(2)}(r_1, r_2, r_1', r_2') = \rho^{(1)}(r_1, r_1') \rho^{(1)}(r_2, r_2') - \rho^{(1)}(r_1, r_2') \rho^{(1)}(r_2, r_1'), \tag{8.44}$$

and thus the energy will consist of two terms

$$E = E_{dd}^{direct} + E_{dd}^{exchange}, \tag{8.45}$$

where

$$E_{dd}^{direct} = \frac{1}{2} \int dr_1 dr_2 \, n(r_1) n(r_2) V_{dd}(r_1 - r_2)$$

$$E_{dd}^{exchange} = \frac{1}{2} \int dr_1 dr_2 \, \rho^{(1)}(r_1, r_2) \rho^{(1)}(r_2, r_1) V_{dd}(r_1 - r_2), \tag{8.46}$$

where $n(r)$ is the density function.

For a BEC where there are no correlations,

$$\psi(r_1, \ldots, r_N) = \prod_i \phi(r_i), \tag{8.47}$$

and so

$$\rho^{(2)}(r_1, \ldots, r_N) = \int dr_3 dr_N \psi^*(r_1, \ldots, r_N) \psi(r_1, \ldots, r_N)$$

$$= \phi^*(r_1) \phi^*(r_2) \phi(r_1) \phi(r_2)$$

$$= n(r_1) n(r_2), \tag{8.48}$$

since the integral over all other degrees of freedom the normalized integral just gives 1. This validates the mean field approach.

8.2.3   Gross-Pitaevskii equation

For a weakly interacting BEC, we again have the GP equation given as

$$\frac{\hbar^2}{2m}\nabla\phi + (g|\phi|^2 + V + \Phi(r))\phi = \mu\phi, \tag{8.49}$$

where $g = 4\pi\hbar^2 a/m$ which represents the contact interaction and

$$\Phi(r) = \int n(r')V_{dd}(r - r')d^3r'. \tag{8.50}$$

We can write this equation in momentum space by writing

$$\phi(r) = \int dk\,\alpha_R e^{ikr}, \tag{8.51}$$

and so substituting this and writing $r - r' = r''$,

$$V_{dd}(r - r')|\phi(r')|^2 d^3r' = \int dr_2 dr_2 \int V_{dd}(r - r')e^{i(k_2 - k_2)r'}\alpha_{k_1}^*\alpha_{k_2}\,dr'$$

$$= \int dk_1 dk_2\,\alpha_{k_1}^*\alpha_{k_2}e^{i(k_2 - k_1)r}\tilde{V}_{dd}(k_1 - k_2), \tag{8.52}$$

where a tilde stands for a Fourier transform and substituting this into the GP equation,

$$i\hbar\dot{\alpha}_0 = \int dk_1 dk_2 dk_3 \alpha_{k_1}^*\alpha_{k_2}\alpha_{k_3}\tilde{V}_{dd}(k_1 - k_2)\delta(k_1 + k_2 = k_3 + k_2), \tag{8.53}$$

which can be thought of as four wave mixing or collisions.

8.2.4   Shape of Dipolar BEC

With contact interactions, a harmonic trap leads to a parabolic density profile. In the dipolar case, this is also true, but it is quite complicated. We will show this in this section.

We can write the dipole-dipole interaction as

$$V_{dd} = \frac{c_{dd}}{4\pi}\hat{e}_i\hat{e}_j\frac{[\delta_{ij} - 3r_ir_j]}{r^3} \implies \phi_{dd} = c_{dd}(e_j\nabla_i\nabla_j\chi(r) + \frac{1}{3}n(r)), \tag{8.54}$$

where

$$\chi = \int \frac{n(r_i)}{4\pi(r - r')}d^3r_1, \tag{8.55}$$

and thus

$$\nabla\chi = -n(r). \tag{8.56}$$

There are analytical solutions, but they are too complicated to give any insight and can be found in the literature. In general, the cloud will be distorted along the dipolar axis, this is known as magnetostriction.

8.2.5   Stability of dipolar BEC

There could be instability in the BEC arising from the attractive part of the dipole dipole interactions, similar to the implosion of a BEC with atoms of negative scattering length. In a harmonic trap of angular frequency ω and spherical cloud size x, there will be energy per particles of magnitude

$$E_{trap} = \frac{1}{2}m\omega^2 x^2$$

$$E_{quantum} = \frac{\hbar^2}{mx^2}$$

$$E_{dd} = N\frac{C_{dd}}{x^3}$$

$$E_{contact} = \frac{4\pi\hbar^2}{m}\left(\frac{N}{x^3}a_s\right), \tag{8.57}$$

and one can sum these energies and minimize them as a function of x. Adding atoms with contact interactions will typically displace atoms to the right. Adding in the dipole-dipole interactions depends on the sign of C_{dd}. If C_{dd} is negative, there can be instability with many particles. This will depend on the ratio of

$$\epsilon_{dd} = \frac{E_{dd}}{E_{contact}} = \frac{c_{dd}m}{4\pi\hbar^2 a_s}, \tag{8.58}$$

which is usually written as

$$\epsilon_{dd} = \frac{\mu_0\mu_m^2 m}{12\pi\hbar^2 a_s} = \frac{a_{dd}}{a_s}, \tag{8.59}$$

and the gas is stable $\epsilon_{dd} < 1$.

If we define

$$\lambda = \frac{w_z}{w_p}, \tag{8.60}$$

and if $\lambda \gg 1$, we have an oblate trap, which is quite stable, and if $\lambda \ll 1$, the BEC is less stable. We can assume the wavefunction is a Gaussian

$$\psi(r, z) = \sqrt{\frac{N}{\pi^{3/2}\omega_p^2\omega_z a_\perp^3}}\exp\left[-\frac{1}{2a_\perp^2}\left(\frac{z^2}{\omega_z^2} + \frac{r^2}{\omega_p^2}\right)\right], \tag{8.61}$$

and we can write the dipolar energy as

$$-\frac{N^2}{\sqrt{2\pi}}\frac{\hbar\bar{\omega}a_{dd}}{a_\perp\omega_p^2\omega_z}f(k), \tag{8.62}$$

where f is some complicated function which is known.

8.2.6 3D Bogoliubov Excitations

Due to interactions a BEC with mostly $k = 0$ atoms, interactions can created $\pm k$ quasiparticles. The Hamiltonian is given as

$$H = \sum_k \omega(k) b_k^\dagger b_k, \tag{8.63}$$

where

$$\omega(k) = \sqrt{\epsilon_k(\epsilon_k + 2gn)} = \sqrt{\epsilon_k(\epsilon_k + 2\tilde{V}(k)n)}, \tag{8.64}$$

where $\tilde{V}$ is the Fourier transform of the dipole-dipole interaction. We can rewrite this as

$$\omega(k) = \sqrt{\epsilon_k(\epsilon_k + 2gn(1 + \epsilon_{dd}(3\cos^2\theta_k - 1)))}, \tag{8.65}$$

which depends on the contact interaction a correction depending on the dipole-dipole interaction. If the dipole-dipole interactions are too strong $\Omega(k)$ becomes imaginary and then the BEC is unstable.

8.2.7 2D Bogoliubov Excitations

In two dimensions $\tilde{V}_{dd}(k) \propto k$ as $k \to 0$ and the Bogoliubov excitations will be given by a similiar expression

$$\omega(k) = \sqrt{\epsilon(\epsilon_k + 2gm(1 + \alpha k))}, \tag{8.66}$$

which means that structures could form under the correct conditions.

8.3 Lecture 3

8.3.1 Extended Bose-Hubbard Model

We can write the Hamiltonian as

$$H = -J\sum_{\langle i,j\rangle} a_i^\dagger a_j + \sum_i U\frac{n_i(n_i - 1)}{2}, \tag{8.67}$$

and if we consider a three site model with three atoms, they will go to the three wells, since this is the lower energy. For two atoms in three wells, there is a triply degenerate ground state. If we assume the atoms are both spin up and we add the dipole-dipole interaction, then they would go to the two out wells and it would be an insulating phase.

   To add the dipole-dipole interaction, we have the Hamiltonian

$$H = -\sum_{ij} a_i^\dagger a_j(J + \Delta_{ij}(n_i + n_j - 1)) + \frac{U}{2}\sum_i n_i(n_i - 1) + \sum_{i,j} V_{ij}^{dd} n_i n_j, \tag{8.68}$$

and note there is a modification of tunneling (term with Δ_{ij}) as well as the dipole-dipole interaction.[37] Thus, one is studying the extended Bose-Hubbard Model.

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[37]This is quite complicated and has to do with the contact interaction.

8.3.2 Fermionic Systems

In bosons the strength of the effect in some sense is given as

$$\epsilon_{dd} = \frac{V_{dd}}{V_c}, \tag{8.69}$$

whereas in Fermison, there is a strength $\lambda = V_{dd}/\epsilon_F$. it was predicted that the BCS temperature in such a system would be given as

$$T_{BCS} \sim \epsilon_F \exp\left(\frac{-\pi \epsilon_F}{12nd^2}\right) = \epsilon_F e^{-\pi/(12\lambda)}, \tag{8.70}$$

which is about zero for magnetic atoms, but is closer to 100nk for heteronuclear molecules. The problem is that molecules tend to unstable. Often this is solved by loading molecules into a lattice to decrease the probability that two come into contact.

8.3.3 Challenges in Field

Here we address some of the challenges in dipolar physics.

Magnetic atoms have small dipoles, resulting in a weak interaction. Many of the the effects which occur through an interaction of the form of the dipole-dipole interaction cannot be seen except at experimentally difficult conditions like extremely low temperatures.

In contrast, ultracold molecules have a much strong dipole moment, however they are often unstable. This makes doing experiments difficult and often one needs a lattice to maintain stability. This limits the types of physics can can pursue.
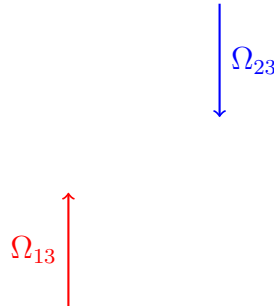
Figure 8: two counter propagating beams that are displaced from each other perpendicular to the axis of propagation

9 Gauge fields in optical lattices (Trey Porto)

9.1 Lecture 1

The motivation for artificial gauge fields mostly boils down to simulating condensed matter system. Most cold atoms are neutral and so there is no charge. In an optical lattice which freezes motion, this doesn't matter. However, when allowing the atoms to move, one needs coupling between a charge and a motion. This is basically a fictitious charge and a fictitious magnetic field.

9.1.1 Intuitive Picture

Classically, the force on a charged particle is given as

$$\vec{F} = e\vec{V} \times \vec{B}, \tag{9.1}$$

This has some nice properties:

- conservative

- velocity dependant

- transverse force

Optical lattices and dipole forces are conservative and laser cooling and trapping can create velocity dependant forces. However, these forces are all in the direction of motion. In order to get the transverse force, we consider two counter propagating beams that are displaced from each other perpendicular to the axis of propagation as shown in 8 and a three level system $|1\rangle, |2\rangle, |3\rangle$ where $|1\rangle, |2\rangle$ are both coupled only to $|3\rangle$. This can give rise to transverse force.

We will start with a review of gauge fields and quantum mechanics. We will work with a semiclassical model meaning light is classical and atoms are quantum mechanical.

9.1.2   Gauge Fields

in classical electrodynamics, we work with two potentials $\phi, \vec{A}$ which give rise to $\vec{E}, \vec{B}$ through the relations

$$\vec{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}$$
$$\vec{B} = \nabla \times \vec{A}, \tag{9.2}$$

and we can offset $\phi \to \phi + C$ without changing the physics and A can be chosen such that $A \to A + \nabla f(r)$ where f is any analytic function. Maxwell's equations are invariant to such changes. We can then write the Hamiltonian as

$$H = \frac{(\vec{p} - \frac{e}{c}\vec{A})^2}{2m} + e\phi, \tag{9.3}$$

which is governed by the time dependent Schrodinger equation

$$i\hbar\frac{\partial \psi}{\partial t} = H\psi. \tag{9.4}$$

When we change from $H \to H'$, where we have performed gauge transformations on $\phi, \vec{A}$ as stated before, then

$$\psi \to \psi e^{ief(r)/\hbar}, \tag{9.5}$$

which has no effect on observables as must be true.[38]

If one assumes that the physics is invariant under a local gauge transformation, $\psi \to \psi e^{if(r)}$, then this implies that gauge fields must exist. Gauge fields occur locally, and while it doesn't affect the physics of the system, we must keep track of the gauge to compensate for it in the wavefunction.

We cannot observe the vector potential $\vec{A}$ which implies that $\vec{p}$ is not observable. However, the mechanical momentum $\vec{\pi} = \vec{p} - \frac{e}{c}\vec{A}$ is observable.

One way in which to simulate this is to use rotation and move into the non-inertial frame, which gives rise to the coriolis force, which is given as

$$F_{cor} = 2m\vec{v} \times \vec{\Omega}, \tag{9.6}$$

which corresponds to the force we want with $2m \to E, \vec{\Omega} \to \vec{B}$. So we can write a Hamiltonian for this as

$$H = \frac{p^2}{2m} + V(r) - \Omega\hat{L}_z, \tag{9.7}$$

where $L_z = xp_y - yp_x = \vec{p}\cdot(x\hat{y} - y\hat{x})$. If we now complete the square, we get a Hamiltonian of

$$H = \frac{(p - M\Omega(x\hat{y} - y\hat{x}))^2}{2m} + V(r) - \frac{1}{2}M\Omega^2(x^2 + y^2), \tag{9.8}$$

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[38]If one calculates the local probability current $\vec{j} = -\frac{i\hbar}{2m}(\psi^*\psi - \psi\nabla\psi)$, then one finds that the phase is the important characteristic and not the amplitude.

which is the Hamiltonian we want with $\frac{e}{c}A \to M\Omega(x\hat{y} - y\hat{x})$ This has been done in the Cornell group, and it is difficult because one must overcome the centipetal force with the Harmonic trap. Additionally, the "equilibrium" state with $\vec{B} \neq 0$, is metastable. This makes using actual rotation difficult, and while it has been done, it is inaccessible to certain physics.

9.1.3　Adiabatic Dressed States

We will now review dressed states in a method applicable to gauge fields. Consider a Hamiltonian comprised of two parts

$$H = \underbrace{\frac{p^2}{2m}}_{H_{ext}} + \underbrace{\sum_i^N \delta_i(\vec{r}) \, |\phi_i\rangle \, \langle\phi_i| + \sum_{ij}^N \Omega_{ij}(\vec{r}) \, |\phi_i\rangle \, \langle\phi_j| + h.c.,}_{H_{int}} \tag{9.9}$$

and moving into the rotating frame, we can produce a time-independent Hamiltonian. So the Hamiltonian looks something like

$$\begin{pmatrix} 0 & \Omega_{12}^* & 0 & 0 & \dots & 0 \\ \Omega_{12} & \delta_1 & \Omega_{23}^* & 0 & \dots & 0 \\ 0 & \Omega_{23} & \delta_2 & \Omega_{34}^* & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \Omega_{N-1,N} & \delta_N \end{pmatrix} \tag{9.10}$$

note there must be one less coupling fields than number of states. The idea is to diagonalize in the internal basis

$$H_{int} \, |\psi_j(\vec{r})\rangle = E_j(r) \, |\psi_j(r)\rangle \,, \tag{9.11}$$

and thus a given full eigenfunction is

$$|\Psi(\vec{r}, t)\rangle = \sum_j c_j(\vec{r}, t) \, |\psi_j(\vec{r})\rangle \,. \tag{9.12}$$

If we assume that the function is initially

$$|\Psi_1\rangle = c_1(\vec{r}, t) \, |\psi_1(\vec{r})\rangle \,, \tag{9.13}$$

then we can write down the Schrodinger equation

$$(H_{ext} + H_{int})\Psi_1 = H_{ext} c_1(\vec{r}, t) \, |\psi_1(\vec{r})\rangle + E_1(r) c_1(\vec{r}, t) \, |\psi_1(\vec{r})\rangle \,, \tag{9.14}$$

where the second term is an effective potential energy sort of like a light shift. [39] So we have created a potential, but we still need to add in a gauge field.

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[39]The difference between this and the normal light shift is that it works for all cases, not just far detuning.
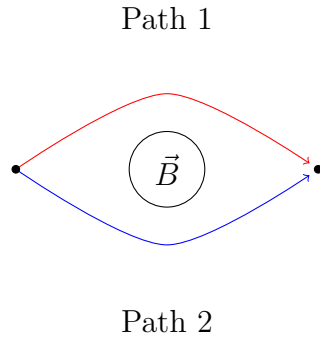
Path 1

Path 2

Figure 9: Aharamov-Bohm effect

9.1.4 Aharamov-Bohm effect

Consider a region with a magnetic field, and there is no magnetic field outside the region and two paths as shown in Figure 9 Now note that $\vec{A} = \nabla f(r)$, which means we can choose a vector potential which satisfied this zero magnetic field condition. So we can write the action of the momentum operator as

$$\vec{p}|\Psi\rangle = i\hbar \left[\nabla c_1(\vec{r}, t)\right] |\psi_1(\vec{r})\rangle + i\hbar c_1(\vec{r}, t)\nabla |\psi_1(\vec{r})\rangle$$
$$= \left[\vec{p} c_1(\vec{r}, t) - i\hbar \langle\psi_1|\nabla|\psi_1\rangle c_1(\vec{r}, t)\right] |\psi_1\rangle, \tag{9.15}$$

where we have used a completeness relation and then assumed adiabaticity. This gives us a Gauge field. Note this is only the lowest order terms, a more careful treatment is required for full information. To get some intuition, we can look at this in 1D and notice

$$\left\langle \psi(x) \left| \frac{\partial}{\partial x} \right| \psi(x) \right\rangle = \langle\psi| \left(\frac{|\psi(x + \delta x)\rangle - |\psi(x)\rangle}{\delta x} \right) = i\delta\theta, \tag{9.16}$$

which is imaginary thus when we multiply i, the term in the action of the momentum operator is real.

If one performs a careful analysis to higher order, there is an a adiabatic potential which is second order in the adiabaticity given as

$$w(\vec{r}) = \frac{\hbar^2}{2m} \sum_j^n |\langle\psi_j|\nabla|\psi_1\rangle|^2, \tag{9.17}$$

which couples the state to all other states in the problem. This naturally arises when working the adiabatic basis.

The final Hamiltonian is approximately

$$H \approx \frac{(p - \nabla A)^2}{2m} + U(r) + w(r), \tag{9.18}$$

where $\tilde{A} = i\hbar \langle\psi_1|\nabla|\psi_1\rangle$, $U(r) = E_1(r)$, and $w(r)$ is as previously defined. $\tilde{A}$ depends on $\Omega(r), \delta(r)$ and if we can engineer it to be curl free, we have an effective magnetic field which will give rise to transverse forces.

If we treat the center of mass motion as classical, then

$$i\hbar c_1 = (E_1(\vec{r}, t) - i\hbar\nabla \cdot \langle\psi_1|\nabla|\psi_1\rangle)c_1, \tag{9.19}$$

and ignoring the spatial variation of the wavefunction, one recovers

$$c_1(t) = \exp(i\phi_{dyn} + i\phi_{geo}), \tag{9.20}$$

where the dynamic phase is given as

$$\phi_{dyn} = \frac{1}{\hbar}\int_0^t E_1(\vec{r}, t)\, dt, \tag{9.21}$$

which depends on $\vec{r}(t)$, and the geometric phase

$$\phi_{geo} = \frac{1}{\hbar}\int_0^t \vec{v} \cdot \langle\psi|\nabla|\psi\rangle\, dt = \oint d\vec{r} \cdot \langle\psi|\nabla|\psi\rangle, \tag{9.22}$$

where we have assumed we are moving back in a complete path from starting point to starting point.[40]

In order for this to all work $\hbar\Omega \gg p^2/2m$, which defines a local basis and so geometrical phase develops along a curved path through Hilbert space. This resembles a magnetic field.

Now if we look at a two level problem with ground state $|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and an excited state $|2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ coupled by $\Omega(r)$, which has some detuning $\delta(r)$ and $\Omega(r) = \Omega(r)e^{i\phi(r)}$. So the ful Hamiltonian is

$$H_{int} = \frac{\hbar}{2}\begin{pmatrix} -\delta & \Omega e^{i\phi} \\ \Omega e^{-i\phi} & \delta \end{pmatrix}, \tag{9.23}$$

which can be diagonalized to get

$$H_{int} = \frac{\hbar}{2}\begin{pmatrix} \sqrt{\Omega^2 + \delta^2} & 0 \\ 0 & -\sqrt{\Omega^2 + \delta^2} \end{pmatrix}, \tag{9.24}$$

with eigenvectors given by

$$|\psi_1\rangle = \begin{pmatrix} \cos(\theta/2) \\ e^{i\theta}\sin(\theta/2) \end{pmatrix}; \ |\psi_2\rangle = \begin{pmatrix} -e^{-i\phi}\sin(\theta/2) \\ \cos(\theta/2) \end{pmatrix}, \tag{9.25}$$

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[40]The term $\langle\psi_1|\nabla|\psi_1\rangle$ is called Berry's connection and $\nabla \cdot \langle\psi_1|\nabla|\psi_1\rangle$ is called Berry's curvature

where we define
$$\cos\theta = \frac{\delta}{\sqrt{\Omega^2 + \delta^2}} \;;\; \sin\theta = \frac{|\Omega|}{\sqrt{\Omega^2 + \delta^2}}, \tag{9.26}$$

then if we assume we start in state $|\psi_1\rangle$, we have that

$$\begin{aligned}
\vec{A} &= i\hbar \langle\psi_1|\nabla|\psi_1\rangle \\
&= i\hbar(\cos(\theta/2), -e^{-i\theta}) \cdot \begin{pmatrix} -\sin(\theta/2)\nabla(\theta/2) \\ i\nabla\phi e^{i\phi}\sin(\theta/2) + e^{i\theta}\cos(\theta/2)\nabla(\theta/2) \end{pmatrix} \\
&= \frac{\hbar}{2}(\cos\theta - 1)\nabla\phi,
\end{aligned} \tag{9.27}$$

which tells us that
$$\vec{B} = \nabla \times \vec{A} = \frac{\hbar}{2}\nabla\cos\theta \times \nabla\phi, \tag{9.28}$$

which implies we need a coupling with a non-zero phase gradient perpendicular to a population gradient. The original two beam problem would give rise to such a vector gauge field.

9.2   Lecture 2

9.2.1   Review of previous results

If we consider a three level system with states at $\omega_1, \omega_2, \omega_3$, and picking $\omega_1 = 0$, and detuned by Δ_1, Δ_2. There is no coupling between state $|1\rangle, |2\rangle$. So we can write the Hamiltonian as

$$H = \begin{pmatrix} 0 & 0 & \Omega_{13}^* \\ 0 & -(\Delta_2 - \Delta_1) & \Omega_{23}^* \\ \Omega_{13} & \Omega_{23} & -\Delta_1 \end{pmatrix}, \tag{9.29}$$

and we can easily diagonalize to get dressed states and energy. From last time, we have the Hamiltonian

$$H = \frac{(\vec{p} - i\hbar\langle\psi_1|\nabla|\psi_1\rangle)^2}{2m} + E_1(r) + w(r), \tag{9.30}$$

where
$$w(r) = \frac{\hbar^2}{2m}\sum_j |\langle\psi_j|\nabla|\psi_1\rangle|^2. \tag{9.31}$$

We can use (9.25) independent of the two level Hamiltonian we are using, however the representation of $\cos\theta, \sin\theta$ is dependant on the specific Hamiltonian. [41] If we

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[41]We can write $w(r)$ for the two level system as

$$w(r) = \frac{\hbar^2}{2m}|\langle\psi_1|\nabla|\psi_1\rangle|^2 = \frac{\hbar^2}{8m}((\nabla\theta)^2 + \sin^2\theta(\nabla\phi)^2), \tag{9.32}$$

which is second order in the gradient.

consider a Gaussian beam propagating in the x direction, the phase gradient must be along the x direction and the gradient along the y direction. The magnetic field will be in the z direction which will be pointing up and pointing down on both sides of the zero in the center.

9.2.2   Examples

Consider the case with a homogeneous beam e^{ikx} and there will be a detuning gradient along the transverse direction y. The population will vary across the beam and so the magnetic field will be maximal in the middle. This is because for large y all the population would be in state $|1\rangle$ and for very negative y, all the population would be in state $|2\rangle$.

   This would be difficult because the the upper state has a lifetime and it would scatter light.

   For a three level system where $|1\rangle , |2\rangle , |3\rangle$, where $|3\rangle$ is the excited state and state $|1\rangle$ and state $|2\rangle$ are coupled to $|3\rangle$, but not to each other with equal detunings, where Ω_{23} has positive detuning and the other negative. Ordering the state $|1\rangle , |3\rangle , |2\rangle$ and setting $|3\rangle$ to zero, we have the Hamiltonian

$$H = \begin{pmatrix} 2\delta & \Omega_1^* & 0 \\ \Omega_1 & 0 & \Omega_2^* \\ 0 & \Omega_2 & 2\delta \end{pmatrix}, \tag{9.33}$$

which can be diagonalized to get that

$$|\psi_1\rangle = \frac{\Omega_2 |1\rangle - \Omega_1 |2\rangle}{\sqrt{\Omega_1^2 + \Omega_2^2}}$$

$$|\psi_{2/3}\rangle = \frac{\Omega_2 |1\rangle + \Omega_1 |2\rangle}{\sqrt{2}\sqrt{\Omega_1^2 + \Omega_2^2}} \pm \frac{|3\rangle}{\sqrt{2}}, \tag{9.34}$$

and we can write

$$|\psi_1\rangle = \begin{pmatrix} \frac{\Omega_2}{\sqrt{\Omega_1^2 + \Omega_2^2}} \\ \frac{\Omega_1}{\sqrt{\Omega_1^2 + \Omega_2^2}} \end{pmatrix}, \tag{9.35}$$

we can parametrize

$$\cos(\theta/2) = \frac{\Omega_2}{\sqrt{\Omega_1^2 + \Omega_2^2}} \implies \cos\theta = 2\cos^2(\theta/2) - 1, \tag{9.36}$$

and thus we get a magnetic field

$$\vec{B} = \frac{\hbar}{2} \nabla \frac{\Omega_2^2}{\Omega_1^2 + \Omega_2^2} \times \nabla\phi. \tag{9.37}$$

Now we can apply this to a particular case of a three level system with two laser beams offset in position perpendicular to the direction of propagation.

An intuitive (and hand-wavy) argument for this is as follows, if one is moving, then the atom is lagging behind the dressed state by something like

$$|\psi_1\rangle + \frac{kv_y}{\sqrt{2}\sqrt{\Omega_1^2 + \Omega_2^2}}\,|3\rangle\,, \tag{9.38}$$

and so this mixing of the excited state causes a force from differing light shifts from the two beams. This gives rise to a force in the transverse direction.

For a third example, we will consider a system which is four levels, with three ground states all coupled to an excited state, and if we set $\hbar$ to 1 and adiabatically eliminated the exited state, and ordered the states $|3\rangle, |2\rangle, |1\rangle$, we can write the Hamiltonian as

$$H = \begin{pmatrix} -\delta & \Omega/2 & 0 \\ \Omega/2 & 0 & \Omega/2 \\ 0 & \Omega/2 & \delta \end{pmatrix} \tag{9.39}$$

where $\Omega = \Omega_1\Omega_2/(2\Delta)$. So now we can also work in a plane wave basis. For a two level system where we have adiabatically eliminated the third level, we can only couple states whose momentum differ by $2\hbar k$. So we will index by the quasimomentum q, where $q = 0$ means k is coupled to $2\hbar k$. For each q_x and y, we will have an internal coupling Hamiltonian which will look like in the basis $|q - k_r, 1\rangle, |q + k_r, 2\rangle$

$$H_x + H_{int} = \begin{pmatrix} (q - k_r)^2 + \delta/2 & \Omega/2 \\ \Omega/2 & (q + k_r)^2 - \delta/2 \end{pmatrix}, \tag{9.40}$$

which can be diagonalized exactly as

$$E_\pm = q^2 + 1 \pm \sqrt{(4q - \delta)^2 + \Omega^2/2}, \tag{9.41}$$

which depends only on $q, y(\Omega, \delta)$. The nice thing about the plane wave basis is that the adiabaticity requirement can be relaxed

Now we can Taylor expand the energy expression about the minimum, giving

$$E_\pm \approx \underbrace{\left(\frac{\Omega \pm 4}{\Omega}\right)}_{\text{effective mass}} \underbrace{\left(q - \frac{\delta}{4 \pm \Omega}\right)^2}_{(p-A)^2} + \underbrace{1 \pm \frac{\Omega}{2}}_{\text{eigenenergy}} + \underbrace{\frac{\delta^2(4 \pm \Omega)}{4(4 + \Omega)^2}}_{w(r)}. \tag{9.42}$$

9.2.3   Lecture 3

9.2.4   Limitations of 3 level system

There are limitations of the the 3 level system. The first is that that the vector potential in this picture is limited such that $A \leq 2k_r$. The sets no limitation on the magnitude of $\vec{B}$, however, $B \propto A/\Delta y$, which means large B will only exist in a very narrow region of space. By defining

$$\Phi_0 = \frac{h}{e} = Bl_{mag}^2, \tag{9.43}$$

then on can define a magnetic length of $l_{mag} = \sqrt{\hbar/eB}$.[42] So in this system

$$eB - \frac{A_{max}}{\Delta y}, \tag{9.44}$$

and

$$l_{mag} = (k_r/\Delta y)^{-1/2} = \left(\frac{\lambda \Delta y}{2\pi}\right)^{1/2}, \tag{9.45}$$

so in order to get into a correlation regime, one wants the interparticle spacing to be on the order of the magnetic length. Here the system will stop acting like a classical field and start having real "quantum" effects.

If one takes $\Delta y = 5\mu$m and $k_r = 2\pi/800$nm, then $l_{mag} \approx 0.8\mu$m. $\Delta_y \gg l_{mag}$ and densities are needed on order $10^{12}/\text{cm}^3$. This is difficult, although not impossible and there are ways to do this in lattices.

Another problem, which is more serious, is that in the alkali atoms, there is a ground state $nS_{1/2}$ and two excited state $nP_{1/2}, nP_{3/2}$ and in order to use three states in the lowest manifold coupled to a single higher manifold, one needs $\Delta m = 1$. The light shift scales as Ω^2/Δ and the scattering scales as Ω^2/Δ^2, yet the Raman coupling scales as Ω^2/Δ and so you want to detune far and raise the laser power to send scattering to zero.

The issue is that at far detuning the electron spin and hyperfine spin don't really matter, so the transition is basically from an $S \to P$ which means $\Delta m = 0$ as there is no angular momentum in the S state. One can work this out properly and in the far detuned limit the Raman coupling also goes as Ω^2/Δ^2 which means it is impossible to overcome the spontaneous emission. So what is needed is a ground state with electronic angular momentum.[43]

9.2.5 Non-Abelian gauge Fields

One can extend this to non-Abelian gauge fields in a system with with $n \geq 2$ quaside-generate states. So take the case of three quasi-degenerate ground states all coupled to a higher state. One gets a similar argument to before, however $\vec{A}$ is now an $n \times n$ matrix where the definition of the matrix elements are

$$A_{ij} = i\hbar \langle \psi_j | \nabla | \psi_i \rangle, \tag{9.46}$$

which means that $[A_x, A_y] \neq 0$ which makes this non-abelian. One can see interesting transfer amongst the populations.

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[42] This can be thought of as like the cyclotron limit

[43] In order to perform a $\Delta m = 1$ transition $\Delta \leq \Delta_{fs}$ and in order to perform a $\Delta M = 2$ transition $\Delta \leq \Delta_{HFs}$.

9.2.6   Realization of gauge fields on a lattice

In order to have orbital effects, one needs to have a lattice in at last two dimensions. The Hamiltonian of the lattice goes as

$$H = -J \sum_i a_i^\dagger a_{i+1} + h.c., \tag{9.47}$$

and we can define a phase

$$\phi_{ij} = \int_{r_{ij}}^{r_{i+1,j}} \vec{A} \cdot d\vec{r} = 2\pi \frac{e}{h} B d^2 j = 2\pi \underbrace{\frac{\Phi_j}{\Phi_0}}_{\alpha} \tag{9.48}$$

where the Gauge is given as $A = (-By, 0, 0)$ and we can write the Hamiltonian as

$$H = -J \sum (e^{i\phi_{ij}} a_{i+1,j}^\dagger a_{i,j} + h.c.) + J \sum_{i,j} a_{i,j+1}^\dagger a_{i,j}. \tag{9.49}$$

Now if one looks at the phase around a square, then this will be given by $2\pi\alpha$ which will be gauge independent.