Introduction to Cold Atom Physics
Notes and Assignments

Chen-Chao Zhao

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1 Atomic Physics

Exercise 1. Calculate the Zeeman splittings as functions of applied field **B** of atomic Rb^{87} and Li^6.

Solution.
The Hamiltonian reads

$$H = A\mathbf{J}\cdot\mathbf{I} + B(\mu_J J_z + \mu_I I_z)$$

and notice that

- $B \downarrow 0$, the atom is in the eigenstates of $\mathbf{F} \equiv \mathbf{J}+\mathbf{I}$, $\{|JIF, M_F\rangle\}$, all vector quantities are projected along **F** direction according to Wigner-Eckart theorem, the effective Hamiltonian reads

$$\begin{aligned} H &= g_F \mu_B B M_F \\ g_F &= \frac{F(F+1)+J(J+1)-I(I+1)}{2F(F+1)} g_J \\ g_J &= \frac{3}{2} + \frac{S(S+1)-L(L+1)}{2J(J+1)} \end{aligned}$$

- $B \uparrow \infty$, the atom is dominated by Zeeman effect of electron angular momentum ($\mu_J \gg \mu_I$), and hence in basis $\{|J, M_J; I, M_I\rangle\}$ and the effective Hamiltonian reads

$$H = g_J \mu_B B M_J + A M_I M_J$$

- $0 < B < \infty$, competition is expected.

Quantum numbers of atomic Rb^{87} and Li^6 are summarized in Table 1.1.

Table 1.1: Quantum numbers of Rb^{87} and Li^6

Atom	Statistics		S	L	J	I	F
Rb^{87}	boson	$5s^1$	$\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{3}{2}$	$1, 2$
Li^6	fermion	$2s^1$	$\frac{1}{2}$	0	$\frac{1}{2}$	1	$\frac{1}{2}, \frac{3}{2}$

In order to obtain the full spectra with arbitrary B, I will numerically diagonalize the Hamiltonian in basis $\{|JM_JIM_I\rangle\}$. And the full Hamiltonian can be explicitly written as

$$\mathcal{H} = A\left[I_zJ_z + \frac{1}{2}(I_+J_- + I_-J_+)\right] + \mu_B B g_J J_z$$

and notice that the magnetic coupling of nuclear spin is completely negligible.

For our two atoms, there is only one J and I component, then we only need to scan over M_J and M_I to fill up the matrix.

The total "spinor" takes the form, $\psi = (-J : J)^T \otimes (-I : I)^T$, and the matrix will be $H = \psi^T \mathcal{H} \psi$. The results are shown in Figure 1.1. In the weak B limit, it is effectively the linear Zeeman effect of hyperfine levels ($|F, M_F\rangle$) and at $B = 0$, diagonalization gives the hyperfine splittings which are small comparing to Zeeman splittings at large B. In the limit $\mu_B B \gg A$, it is effectively the linear Zeeman effects of total electron angular momentum J which in both cases $J = \frac{1}{2}$, hence the splittings are two-fold. The further splittings at the ends result from hyperfine structure which in (a) three-fold ($I = 1$) and (b) four-fold ($I = \frac{3}{2}$). Note that the splittings at the end is the result of $A\mathbf{J} \cdot \mathbf{I}$ rather than $\mu_I B I_z$.

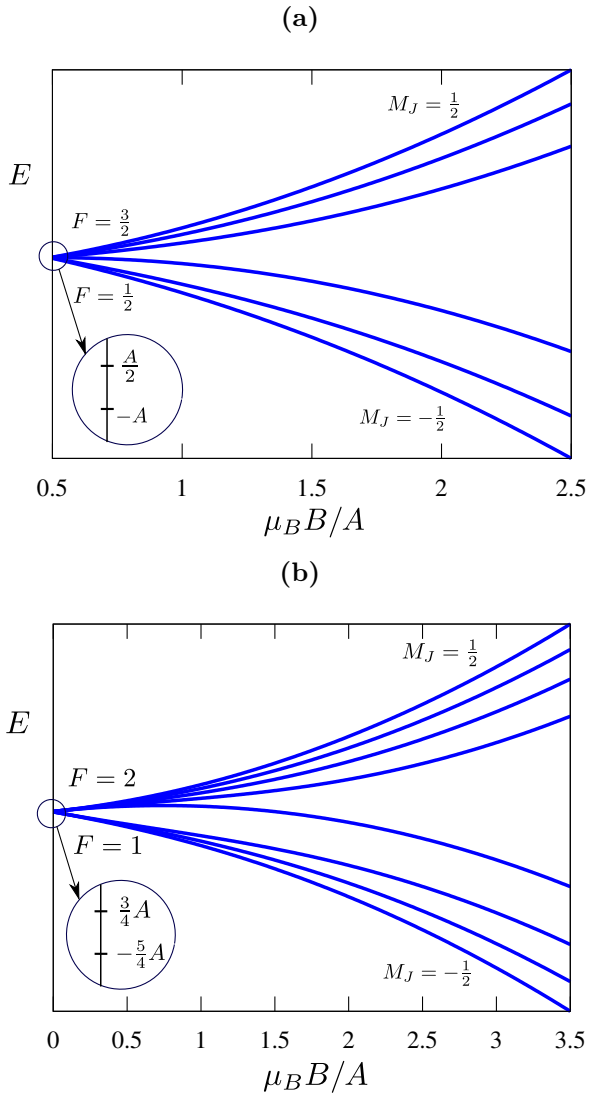

Figure 1.1: Zeeman effects of (a) Li^6 and (b) Rb^{87} including hyperfine interaction. In the weak limit $\mu_B B \ll A$, it is effectively the linear Zeeman effect of hyperfine levels ($|F, M_F\rangle$) and at $B = 0$, diagonalization gives the hyperfine splittings as indicated schematically. In the limit $\mu_B B \gg A$, it is effectively the linear Zeeman effects of total electron angular momentum J which in both cases $J = \frac{1}{2}$, hence the splittings are two-fold. The further splittings at the ends result from hyperfine structure which in (a) three-fold ($I = 1$) and (b) four-fold ($I = \frac{3}{2}$).

2 Two-Body Scattering

- For the neutral cold atomic gas considered here, the following assumptions are made

  1. Interaction is short-ranged[1] (force range r_0);
  2. The gas is dilute ($n^{-\frac{1}{3}} \gg r_0$);
  3. The gas is cold (low kinetic energy $kr_0 \ll 1$).

- The spherical potential $V(r)$ is
  - non-universal if $r < r_0$,
  - identically zero if $r > r_0$[2].

- We consider two-body scattering.
  - The two-body Hamiltonian can be recombined into center of mass part and relative part[3]

$$\hat{H}_{12} = \hat{H}_1 + \hat{H}_2 = \hat{H}_{\rm CM} + \hat{H}_{\rm relative}$$

    - ⇨ Mass in the center of mass part $M = m_1 + m_2$, and $M = 2m$ if $m_1 = m_2$.
    - ⇨ Mass in the relative part $m_r = m_1 m_2/(m_1+m_2)$, and $m_r = m/2$ if $m_1 = m_2$.
  - We are only concerned with the relative part, abbreviated as $\hat{H}$,

$$\begin{aligned} \hat{H} &= -\frac{\hbar^2}{m}\nabla^2 + V(r) \\ \hat{H}\Psi(\mathbf{r}) &= E\Psi(\mathbf{r}) \end{aligned}$$

    where $\mathbf{r}$ is the relative distance and m the reduced mass.
  - The Laplacian can be generically written as

$$\nabla^2 = -\frac{m}{\hbar^2}\frac{1}{r^2}\hat{\mathbf{L}}^2 + \frac{1}{r^2}(\mathbf{r}\cdot\nabla)(\mathbf{r}\cdot\nabla) + \frac{1}{r^2}\mathbf{r}\cdot\nabla$$

    while in spherical coordinates $\mathbf{r}\cdot\nabla = r\partial_r$ with $\mathbf{r} = r\hat{\mathbf{e}}_r$, it becomes

$$\begin{aligned} \nabla^2 &= \frac{1}{r}\partial_r(r\partial_r) + \frac{1}{r}\partial_r - \frac{m}{\hbar^2}\frac{1}{r^2}\hat{\mathbf{L}}^2 \\ \frac{1}{r}\partial_r r &= \frac{1}{r}\partial_r(r\partial_r) + \frac{1}{r}\partial_r \end{aligned}$$

[1] Van de Waals type of interaction. We also assume that the potential is of spherical symmetry.

[2] Later we will show that in the low energy limit, various atomic gases can be characterized by a universal parameter, s-wave scattering length a_s.

[3] This is not straight forward.

- Since the Hamiltonian is rotation invariant, the angular part decouples and the radial part is labeled by quantum numbers of $\hat{\mathbf{L}}^2$ subspaces. Therefore we write $\Psi_l(\mathbf{r}) = R_l(r)Y_{lm}(\theta,\phi)$.
- The Schrödinger equation reads

$$\begin{aligned}\left[\nabla^2 + \frac{m}{\hbar^2}(E - V(r))\right]\Psi(\mathbf{r}) &= 0\\ Y\frac{1}{r}\partial_r^2(rR) - \frac{R}{r^2}\hat{\mathbf{L}}^2 Y &= -\frac{m}{\hbar^2}(E-V(r))RY\\ \frac{1}{rR}\partial_r^2(rR) - \frac{l(l+1)}{r^2} &= -\frac{m}{\hbar^2}(E-V(r))\end{aligned}$$

  define $u(r) = rR(r)$

$$\partial_r^2 u + \frac{m}{\hbar^2}\left(E - V(r)\right)u - \frac{l(l+1)}{r^2}u = 0 \tag{2.1}$$

- Scattering length and phase shift
  - There are two ways of writing the scattered state
    - ⇨ Solve Eq 2.1
    - ⇨ In terms of scattering amplitude $f(\mathbf{k}', \mathbf{k})$
  - For a dilute degenerate quantum gas, the thermal wavelength Λ is large compared to inter-atomic distance $n^{-\frac{1}{3}}$, or $n^{-\frac{1}{3}}\Lambda^{-1} \ll 1$. It is equivalent to angular momentum $L \ll \hbar$. Therefore, we set $l = 0$ in Eq 2.1.
  - Solve Eq 2.1 out side the force range where $V(r > r_0) = 0$ and write $E = \hbar^2k^2/m$, then we have $\left(\partial_r^2 + k^2\right)u(r) = 0$, whose solutions can be read out directly,

$$\begin{aligned}u(r) &= A\sin(kr + \delta_0)\\ &\propto \sin kr + \tan\delta_0 \cos kr\\ &\propto \mathrm{e}^{2i\delta_0}\mathrm{e}^{ikr} - \mathrm{e}^{-ikr}\end{aligned}$$

    where $\delta_{l=0}$ is the scattering phase shift.
  - At the boundary $r = r_0$, the radial part should be $\mathcal{C}^1$, namely $u_>(r_0) = u_<(r_0)$ and $u'_>(r_0) = u'_<(r_0)$. Assume $u'_<(r_0)/u_<(r_0) = \text{const.} = -1/a_s$ in the limit $kr_0 \ll 1$. Clearly,

$$\frac{k\cos(kr_0 + \delta_0)}{\sin(kr + \delta_0)} \approx \frac{k}{\tan\delta_0} \equiv -\frac{1}{a_s}$$

  - For a general l, we define scattering length a_l related to phase shift δ_l as

$$a_l(k) = -\lim_{k\downarrow 0}\frac{\delta_l(k)}{k}$$

Exercise 2. Explicitly show that scattering is dominated by s-wave channel in the low energy limit. Using a spherical square well potential

$$V(r) = \begin{cases} V_0 & r < r_0 \\ 0 & r > r_0 \end{cases},$$

the low energy limit can be written as $kr_0 \ll 1$. The scattering phase shift a_s should also be independent of k.

Solution.

I will solve Schrödinger equation both inside and outside the square well, rewrite Eq 2.1

$$\partial_r^2 u + k'^2 u - \frac{l(l+1)}{r^2} u = 0$$

where $k'^2 = \frac{m}{\hbar^2}(E - V(r)) = k^2 - \frac{m}{\hbar^2}V(r)$ and $k' = k$ if $r > r_0$.

The solutions are $u_l(k'r) = rk'(Aj_l(k'r) + By_l(k'r)) = rk'(Ch_l^{(1)}(rk') + Dh_l^{(2)}(rk'))$ where j_l, y_l are spherical Bessel and Neumann functions and $h_l^{(1,2)}$ are Hankel functions.

Take $V_0 \uparrow \infty$, the solution is $\mathcal{C}^0$, since $u_< = 0$, $u_>(kr_0) = 0$. Set $l = 0$, $j_l(kr) = \sin kr/kr$, $y_l(kr) = \cos kr/kr$.

Clearly, $B/A = \tan \delta_l$.

Therefore, we have $Aj_l = -By_l$

$$\delta_l(k) \quad = \quad -\frac{j_l(kr_0)}{y_l(kr_0)} \propto \frac{(kr_0)^l}{(kr_0)^{-(l+1)}} \propto (kr_0)^{2l+1}$$

in the low energy limit $kr_0 \ll 1$, scattering is dominated by $l = 0$ channel, in which a_s is independent of k.

The above, we took a hard shell potential. For a general V_0, the calculations are subtle for $l \neq 0$ but feasible for $l = 0$ case.

3 BEC

Exercise 3. Calculate the T_c of free boson gases in 1 and 2 dimensions.

Solution.

The critical temperature is defined as the temperature where $\mu = 0$ but still $N_{\mathbf{0}} \ll N$.

Therefore, we have

$$N = \sum_{\mathbf{k} \neq \mathbf{0}} n_{\mathbf{k}}^{\mathrm{BE}} = V \int \frac{d^D k}{(2\pi)^D} \frac{1}{\mathrm{e}^{\epsilon_{\mathbf{k}}/k_B T_c} - 1}$$

where $\epsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m}$ and the measure $\frac{d^D k}{(2\pi)^D}$ and $n = N/V$ take the following forms in dimension $D = 1, 2, 3$

❒ $D = 1$

$$\begin{aligned}\int_{-\infty}^{\infty} \frac{dk}{2\pi} &= \frac{m^{\frac{1}{2}}}{2^{\frac{1}{2}}\pi\hbar} \int_0^{\infty} \epsilon^{-\frac{1}{2}} d\epsilon \\ C_1 &= \frac{m^{\frac{1}{2}}}{2^{\frac{1}{2}}\pi\hbar}\end{aligned}$$

$$\begin{aligned}n &= C_1 \int_0^{\infty} \frac{\epsilon^{-\frac{1}{2}}}{\mathrm{e}^{\epsilon/k_B T_c} - 1} d\epsilon \\ &= C_1 \sqrt{k_B T_c} I_1\end{aligned}$$

where

$$\begin{aligned}I_1 &= \int_0^{\infty} \frac{x^{-\frac{1}{2}}}{\mathrm{e}^x - 1} dx \\ &= \int_0^{\infty} \frac{\mathrm{e}^{-x} x^{-\frac{1}{2}}}{1 - \mathrm{e}^x} dx \quad (x > 0) \\ &= \int \mathrm{e}^{-x} x^{-\frac{1}{2}} \sum_{p=0}^{\infty} \mathrm{e}^{-px}\, dx \\ &= \int x^{-\frac{1}{2}} \sum_{p=1}^{\infty} \mathrm{e}^{-px}\, dx \\ &= \Gamma\left(\frac{1}{2}\right) \sum_{p=1}^{\infty} p^{-\frac{1}{2}} \\ &= \Gamma\left(\frac{1}{2}\right) \zeta\left(\frac{1}{2}\right)\end{aligned}$$

Then $T_c = (n/C_1 I_1)^2 / k_B$

❒ $D = 2$

$$\int \frac{kdk}{(2\pi)^2} d\Omega_2 = \frac{1}{2\pi} \int_0^{\infty} kdk = \frac{m}{2\pi\hbar^2} \int_0^{\infty} d\epsilon$$

Similarly we have

$$\begin{aligned}n &= C_2 \int_0^{\infty} \frac{1}{\mathrm{e}^{\epsilon/k_B T_c} - 1} d\epsilon \\ &= C_2 k_B T_c I_2\end{aligned}$$

with

$$\begin{aligned}I_2 &= \int_0^{\infty} \frac{1}{\mathrm{e}^x - 1} dx \\ &= \Gamma\left(\frac{1}{2}\right) \zeta(1)\end{aligned}$$

But $\zeta(z)$ is not well-defined at $z = 1$, hence there is no BEC in 2D.

❒ $D = 3$

$$\int \frac{k^2 dk}{(2\pi)^3} d\Omega_3 = \frac{1}{2\pi^2} \int_0^\infty k^2 dk = \frac{m^{\frac{3}{2}}}{2^{\frac{1}{2}} \pi^2 \hbar^3} \int \epsilon^{\frac{1}{2}} d\epsilon$$

We have

$$\begin{aligned} n &= C_3 \int_0^\infty \frac{\epsilon^{\frac{1}{2}}}{\mathrm{e}^{\epsilon/k_B T_c} - 1} d\epsilon \\ &= C_3 (k_B T_c)^{\frac{3}{2}} I_3 \\ I_3 &= \int_0^\infty \frac{x^{\frac{1}{2}}}{\mathrm{e}^x - 1} dx \\ &= \Gamma\left(\frac{1}{2}\right) \zeta\left(\frac{3}{2}\right) \\ T_c &= (n/C_3 I_3)^{\frac{2}{3}} / k_B \end{aligned}$$

Exercise 4. Tabulate the degeneracy temperatures of electron gases, ^{4}He and ultracold atomic gases.

Table 3.1: Degeneracy temperatures

	density	distance	mass	$T_{\text{degeneracy}}$
electron gases	10^{28}-10^{29}m^{-3}	10^{-9}-10^{-10}m	9.1×10^{-31}kg	10^4-10^5K
superfluid ^{4}He	10^{24}m^{-3}	10^{-10}m	4u $\sim 10^{-26}$kg	1K
ultracold atoms	10^{18}-10^{21}m^{-3}	10^{-7}-10^{-6}m	10u $\sim 10^{-26}$kg	0.1-10 nK

The degenerate temperature is defined as $k_B T \sim \hbar^2 k^2/2m = \hbar^2/2md^2$ while the distance d is related to density n as $d = n^{-\frac{1}{3}}$. In the case of fermions, the average distance is $\sim 1/k_F$ and for electrons in metal, $\epsilon_F \approx 1 \sim 10$ eV hence $k_F = \sqrt{2m\epsilon_F}/\hbar \sim 10^{-10}$m and the degeneracy temperature is also known as the Fermi temperature $T_F = \epsilon_F/k_B \approx 10^4 \sim 10^5$K. The unified atomic unit is $1\text{u} = 1.66 \times 10^{-27}$kg.

Exercise 5. Rewrite the ODLRO criterion for for free bosons.

The density matrix for a many-boson system is given by

$$\hat{w} = \sum_\alpha w_\alpha |\Psi_\alpha\rangle\langle\Psi_\alpha|$$

where $|\Psi_\alpha\rangle$ is a many-body wave function for all particles. The 1-particle density

matrix is evaluated by tracing out all other particles

$$\begin{aligned}\rho_1(\mathbf{r},\mathbf{r}') &= \langle \mathbf{r}|\mathrm{tr}'(\hat{w})|\mathbf{r}'\rangle \\ &= \sum_\alpha w_\alpha \int \prod_{j\neq 1}^{N} d\mathbf{r}_j \Psi_\alpha^*(\mathbf{r},\cdots,\mathbf{r}_j,\cdots\mathbf{r}_N)\Psi_\alpha(\mathbf{r}',\cdots,\mathbf{r}_j,\cdots\mathbf{r}_N) \\ &= \left\langle \psi^\dagger(\mathbf{r})\psi(\mathbf{r}')\right\rangle\end{aligned}$$

Since the 1-particle density matrix is hermitian, it can be written in eigenvectors χ_i with real eigenvalues n_i.

- ❒ A system without ODLRO $\Longleftrightarrow \forall i$, $\lim_{N\uparrow\infty}\frac{n_i}{N}=0$;
- ❒ Simple BEC $\Longleftrightarrow \exists n_0$ such that $\lim_{N\uparrow\infty}\frac{n_0}{N}>0$ and $\forall i\neq 0$, $\lim_{N\uparrow\infty}\frac{n_i}{N}=0$;
- ❒ Fragmented BEC $\Longleftrightarrow$ there are more than one eigenvalues that satisfy the condition above.

For free bosons, the many-body state is the product state of each free boson state, namely a plane wave. And the 1-particle density matrix is simply

$$\begin{aligned}\rho_1(\mathbf{r},\mathbf{r}') &= \sum_{\mathbf{k}} n_{\mathbf{k}}\chi_{\mathbf{k}}^*(\mathbf{r})\chi_{\mathbf{k}}(\mathbf{r}') \\ &= \frac{1}{V}\sum_{\mathbf{k}} n_{\mathbf{k}} \mathrm{e}^{-i\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})}\end{aligned}$$

This goes back to our previous analyses, above T_c, $n_{\mathbf{0}} \ll N$ and below T_c, $n_{\mathbf{0}}/N \sim 1$.