

TAMU Winterschool: Spin in cold atom systems

Ian's outline

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I. Meaning of "spin" in atomic systems

$$(L, S) \rightarrow J, (J + I) \rightarrow F \text{ coupling}$$

~~II. Important levels of Alkali atoms $nS \rightarrow nP$ transition~~

III. Structure in ground state (hyperfine)

IV. Couplings to spin states

- Zeeman $\rightarrow$ Breit-Rabi equation, RF coupling
- ~~Electric Dipole (Raman)~~

V. Example (A): creating spin-orbit coupling

- Select two levels (pseudospins), then Raman Couple $\rightarrow$ SOC
- Introduce RWA, compare RF v.s. Raman (No SOC $\rightarrow$ SOC)

VI. Interactions: Spinor condensate physics

~~VII. Example (B): Phase separation in a two component gas.~~

This lecture doesn't derive the underlying physics, and instead seeks to reveal the effective Hamiltonians which matter for cold atom physics.

Spin in atomic systems, Basics

Today I will consider alkali atoms in their ground "s" orbital.

In this situation we will need to consider only the nuclear and electronic angular momenta

$S = 1/2$ and $I = \dots$ (we will see specifics later).

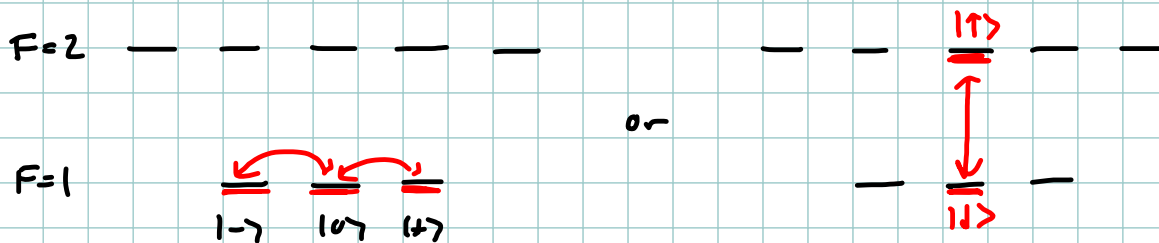
Lets think about I : it is a combination of nuclear spin and orbital angular momentum.

So already we know what I call "spin" isn't.

The name of the game is to construct a total angular momentum

$F = I + S$ (or $\overbrace{I+S}^J$), which takes on values

$f = i \pm 1/2$, e.g., $F=1$ and $F=2$ for ^{87}Rb . Given this we select some set of interesting pseudospins.



In this lecture I will explore some of the single particle and interaction physics that might go into such a selection.

Hyperfine structure + Zeeman Effect

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Here I will consider the properties of atoms in their ground electronic state in a uniform magnetic field.

I just introduced the components of $L=0$ atoms which make the spin

$$\vec{F} = \vec{S} + \vec{I}$$

In atoms these are coupled by the Hyperfine interaction (Magnetic dipole)

$$H_{HF} = A(\vec{I} \cdot \vec{S}), \text{ using the standard trick } F^2 = (S+I)^2 = S^2 + 2S \cdot I + I^2$$

$$\text{or } \frac{1}{2}(F^2 - S^2 - I^2) = \vec{S} \cdot \vec{I}$$

$$\text{So } \bar{H}_{HF} = \frac{A}{2}(\hat{F}^2 - \hat{S}^2 - \hat{I}^2) \rightarrow \frac{A}{2}[F(F+1) - S(S+1) - I(I+1)]$$

now in the Alkali atoms $S=1/2$, so $F = I \pm \frac{1}{2}$, for $I > 0$
 $= \frac{1}{2}$ for $I=0$

$$E_{HF} = \frac{A}{2}\left[\pm\left(i+\frac{1}{2}\right) - \frac{1}{2}\right], \Delta_{HFS} = A\left[i + \frac{1}{2}\right]$$

Now some examples:

	${}^6\text{Li}$	${}^7\text{Li}$	${}^{23}\text{Na}$	${}^{39}\text{K}$	${}^{40}\text{K}$	${}^{41}\text{K}$	${}^{85}\text{Rb}$	${}^{87}\text{Rb}$	${}^{133}\text{Cs}$
I	1	$3/2$	$3/2$	$3/2$	4	$3/2$	$5/2$	$3/2$	$7/2$
Δ_{HFS}	220 MHz	804 MHz	1.77 GHz	462 MHz	129 GHz	234 MHz	3.03 GHz	6.83 GHz	9.19 GHz
A	152 MHz	402 MHz	885 MHz	231 MHz	-286 MHz	127 MHz	1.01 GHz	3.42 GHz	2.30 GHz

So there are a wide range of possible hyperfine splittings which - as we shall see - has important effects.

Hyperfine structure + Zeeman Effect II

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Now with the hyperfine effect in the bag we move on to the Zeeman effect.

$$H_z = \mu_B (g_S \vec{S} + g_I \vec{I}) \cdot \vec{B}$$

↑ sometimes $\mu_B/\hbar$ depending on units (atomic physicists like $\hbar/2m_e$, or s^{-1})

So all together we consider $H = A(\vec{I} \cdot \vec{S}) + \mu_B (g_S \vec{S} + g_I \vec{I}) \cdot \vec{B}$

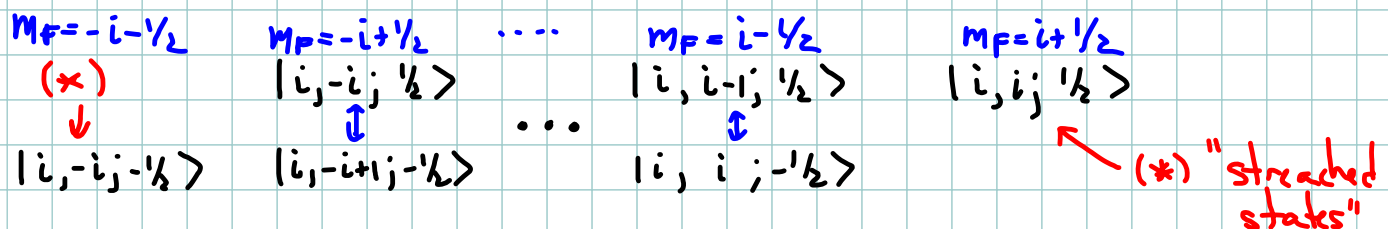
the solution to this equation is the Breit-Rabi equation

For $s=1/2$, and $B=B_z \hat{e}_z$

Recall that $J_{\pm} = J_x \pm iJ_y$ and $J_{\pm} |j, m_j\rangle = \hbar [(j \mp m_j)(j \pm 1 \pm m_j)]^{1/2} |j, m_j \pm 1\rangle$

So $J_x = \frac{1}{2}(J_+ + J_-)$, $J_y = \frac{1}{2i}(J_+ - J_-)$ giving $\vec{I} \cdot \vec{S} = I_z S_z + \frac{1}{2} I_+ S_- + \frac{1}{2} I_- S_+$

Thus in the uncoupled basis H_0 couples $|i, m_i; m_s=1/2\rangle$ to $|i, m_i \pm 1; -1/2\rangle$ which may be graphically depicted like:



So H_0 decomposes into 2×2 blocks labeled by m_F as above

$$\frac{\tilde{H}(m_F)}{\hbar} = \begin{pmatrix} \mu_B B \left[\frac{g_S - g_I}{2} \right] + g_I m_F + \frac{\hbar A}{2} (m_F - 1/2) & \frac{\hbar A}{2} (i + \frac{1}{2} + m_F)^{1/2} (i + \frac{1}{2} - m_F)^{1/2} \\ \text{---} & \text{---} \\ \text{C.C.} & -\mu_B B \left[\frac{g_S - g_I}{2} \right] - g_I m_F - \frac{\hbar A}{2} (m_F + 1/2) \end{pmatrix}$$

I will compute the eigenvalues of this matrix on the next page.

$$\# \text{ of } m_F \text{ doublets} \rightarrow \begin{pmatrix} |i, m_F - 1/2; 1/2\rangle \\ |i, m_F + 1/2; -1/2\rangle \end{pmatrix}$$

Hyperfine structure + Zeeman Effect III

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To recap, I started with

$$H_J = A(\mathbf{I} \cdot \mathbf{S}) + \mu_B(g_S \mathbf{S} + g_I \mathbf{I}) \cdot \mathbf{B} \quad \text{and transformed to}$$

$$\frac{\tilde{H}(m_F)}{\hbar} = \begin{pmatrix} \mu_B B \left[\frac{g_S - g_I}{2} + g_I m_F \right] + \frac{\hbar A}{2} (m_F - 1/2) & \frac{\hbar A}{2} (i + \frac{1}{2} + m_F)^{1/2} (i + \frac{1}{2} - m_F)^{1/2} \\ \text{---} & \text{---} \\ \text{C.C.} & -\mu_B B \left[\frac{g_S - g_I}{2} - g_I m_F \right] - \frac{\hbar A}{2} (m_F + 1/2) \end{pmatrix}$$

For today eigenvalues are enough:

$$\frac{E_{B-S}}{\hbar} = g_I \mu_B B m_F + \frac{\hbar A}{4} \left\{ -1 \pm \left[(2i+1)^2 + 4 m_F \left(\frac{2(g_S - g_I) \mu_B B}{A} \right) + \left(\frac{2(g_S - g_I) \mu_B B}{A} \right)^2 \right]^{1/2} \right\}$$

This is the Breit-Rabi equation, the eigenstates of which are the "spin states" usually used in cold atom systems

⊗ Now let's look at some examples See Slides

Keep in mind that $\sim 2 \text{ kG} = 0.2 \text{ T}$ is near the upper field limit for cold atom experiments

Clock States

depending on one's aims it can be useful to select a pair of states whose energy difference is 1st order insensitive to external magnetic fields.

In ^{87}Rb near $B=0$ there are two such pairs

$$\{ |F=1, m_F=0\rangle, |F=2, m_F=0\rangle \} \quad \text{and} \quad \{ |F=1, m_F=-1\rangle, |F=2, m_F=1\rangle \}$$

See Slides

RF coupling

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Lets focus on just one manifold at small field, then

$\swarrow$ Landé g factor

$$H = g_F \mu_B \vec{F} \cdot \vec{B}, \quad g_F = g_i \pm \frac{(g_s - g_i)}{2i+1}$$

make $B = B_0 \hat{e}_z + \delta \vec{B} \cos(\omega t)$

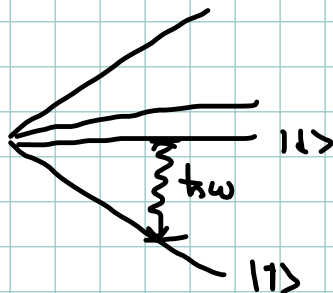
$$H = g_F \mu_B B_0 \hat{F}_z + g_F \mu_B \cos(\omega t) \vec{F} \cdot \delta \vec{B}$$

now I make a transformation into a frame rotating with angular frequency ω and make the RWA

to get: $H = \Omega \cdot F$, where

$$\Omega = \underbrace{(+g_F \mu_B \delta B_y, -g_F \mu_B \delta B_x)}_{\text{coupling terms}}, \overbrace{g_F \mu_B B_0 - \omega}^{\approx \delta}$$

- * only terms $\perp$ to bias matter
- * phase of drive affects Ω_x, Ω_y
- * frequency selects states



Dressed states: RF/Raman

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Now we have selected a pair of spin states and we want to couple them.

$$I. \hat{H} = \begin{pmatrix} \hbar^2 k^2 / 2m & 0 \\ 0 & \hbar^2 k^2 / 2m \end{pmatrix} + \begin{pmatrix} \delta/2 & \Omega/2 \\ \Omega/2 & -\delta/2 \end{pmatrix}$$

$$\hat{H} = \frac{\hbar^2 k^2}{2m} \hat{1} + \frac{\delta}{2} \hat{\sigma}_z + \frac{\Omega}{2} \hat{\sigma}_x, \text{ now some } U \text{ solves this hamiltonian}$$

Since U is position independent, it commutes with $k^2 \hat{1}$

$$\text{so } U H U^\dagger = \frac{\hbar^2 k^2}{2m} \hat{1} + \frac{(\delta^2 + \Omega^2)^{1/2}}{2} \hat{\sigma}_z \quad \left\{ \begin{array}{l} \text{standard} \\ \text{RF dressed state} \end{array} \right.$$

* RF evaporation

* RF dressed traps

* Quantum Control

I. Raman dressed ← "vector light shift" momentum displacement operator $|k-2k_r\rangle \langle k|$

$$\hat{H} = \frac{\hbar^2 k^2}{2m} \hat{1} + \frac{\delta}{2} \hat{\sigma}_z + \frac{\Omega}{2} \begin{pmatrix} 0 & e^{-2ik_r x} \\ e^{2ik_r x} & 0 \end{pmatrix}$$

It's most simple to write this out:

$$= \int \frac{dk}{2\pi} \frac{\hbar^2}{2m} \left(k^2 |k, \uparrow\rangle \langle k, \uparrow| + k^2 |k, \downarrow\rangle \langle k, \downarrow| \right) + \frac{\Omega}{2} \left(|k-2k_r, \uparrow\rangle \langle k, \downarrow| + H.c. \right) + \frac{\delta}{2} \hat{\sigma}_z$$

now I change my labeling so $|k, \uparrow\rangle \rightarrow |k+k_r, \uparrow\rangle$
 $|k, \downarrow\rangle \rightarrow |k-k_r, \downarrow\rangle$

$$= \int \frac{dk}{2\pi} \frac{\hbar^2}{2m} \left(k^2 |k+k_r, \uparrow\rangle \langle k+k_r, \uparrow| + k^2 |k-k_r, \downarrow\rangle \langle k-k_r, \downarrow| \right) + \frac{\Omega}{2} \left(|k-k_r, \uparrow\rangle \langle k-k_r, \downarrow| + H.c. \right) + \frac{\delta}{2} \hat{\sigma}_z, \text{ change integration}$$

Dressed states: RF/Raman

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Now we have selected a pair of spin states and we want to couple them.

$$= \int \frac{dk}{2\pi} \frac{\hbar^2}{2m} \left(k^2 |k+k_F, \uparrow\rangle \langle k+k_F, \uparrow| + k^2 |k-k_F, \downarrow\rangle \langle k-k_F, \downarrow| \right) + H.c. + \frac{\delta}{2} \check{\sigma}_z, \text{ change integration}$$

$$= \int \frac{dq}{2\pi} (|q, \uparrow\rangle, |q, \downarrow\rangle) \underbrace{\begin{pmatrix} \frac{\hbar^2}{2m} (q-k_F)^2 + \frac{\delta}{2} & \frac{\hbar^2}{2m} (q-k_F)^2 - \frac{\delta}{2} \\ \frac{\hbar^2}{2m} (q+k_F)^2 - \frac{\delta}{2} & \frac{\hbar^2}{2m} (q+k_F)^2 + \frac{\delta}{2} \end{pmatrix}}_{= \check{H}(q)} \begin{pmatrix} |q, \uparrow\rangle \\ |q, \downarrow\rangle \end{pmatrix}$$

$$\check{H}(q) = \frac{\hbar^2 q^2}{2m} \check{1} + \left(\frac{\hbar^2 k_F}{m} \right) \check{\sigma}_z + \frac{\delta}{2} \check{\sigma}_z + \frac{\hbar^2}{2m} \check{\sigma}_x$$

Rotation by $\pi/2$ about e_y (spins only)

$$H(q) = \frac{\hbar^2 q^2}{2m} \check{1} + \frac{\hbar^2 k_F}{2m} \check{\sigma}_x - \frac{\delta}{2} \check{\sigma}_x + \frac{\hbar^2}{2m} \check{\sigma}_z$$

To Experiment

Interactions

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So far my discussion has focused on single particle physics, but the "good stuff" has to do with interacting systems.

For the interatomic $V(r) \sim -C_6/r^6$ potential, it is possible to make a pseudo-potential approximation when

$$k \ll \frac{2\pi}{a_{vdw}}, a_{vdw} \sim 5\text{nm} \text{ (generally ok)}$$

Then $V(r) = g \delta(r_1 - r_2)$ for a single spin.

Lets consider two atoms with angular momentum F colliding with $B=0$. This implies that angular momentum is conserved

$$\text{so } \bar{V} = \delta(r_1 - r_2) \sum_{G=0}^{2F} g_G \hat{P}_G, \text{ where } g_G = \frac{4\pi\hbar^2 a_G}{m} \text{ and } \hat{P}_G = \sum_{M_G=-G}^G |G, M_G\rangle \langle G, M_G|$$

for Bosons only even G are allowed and odd for Fermions.
This is the first time spin statistics has come up!

So we have the closure relations for Bosons and Fermions

$$\underbrace{\mathbb{1} = \sum_{\substack{G=0 \\ \text{even}}}^{2F} \hat{P}_G}_{\text{Bosons}}, \quad \underbrace{\mathbb{1} = \sum_{\substack{G=0 \\ \text{odd}}}^{2F} \hat{P}_G}_{\text{Fermions}}$$

$$\text{Lastly recall } \hat{F}_1 \cdot \hat{F}_2 = \frac{\hat{G}^2 - \hat{F}_1^2 - \hat{F}_2^2}{2} = \frac{\hbar^2}{2} [g(g+1) - 2f(f+1)].$$

$$\text{multiplying this by our projector: } \hat{F}_1 \cdot \hat{F}_2 = \sum_{G=0}^{2F} \hat{F}_1 \cdot \hat{F}_2 \hat{P}_G = \sum_{G=0}^{2F} \lambda_G \hat{P}_G$$

At this point it's difficult to go farther w/o picking F

Interactions : Examples

$$\lambda_q = \frac{1}{2} [g(q+1) - 2f(f+1)]$$

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$$\bar{V} = \delta(r_1 - r_2) \sum_{q=0}^{2F} g_q \hat{P}_q$$

$$\hat{F}_1 \cdot \hat{F}_2 = \sum_{q=0}^{2F} \hat{F}_1 \cdot \hat{F}_2 \hat{P}_q = \sum_{q=0}^{2F} \lambda_q \hat{P}_q$$

$F=0$ (Bosons, trivial) : $V = \delta(r_1 - r_2) g_0 \hat{P}_0$, but $\mathbb{1} = \hat{P}_0$

$$\hat{V} = g_0 \delta(r_1 - r_2)$$

$F=1$ (Bosons) : $V = \delta(r_1 - r_2) (g_0 \hat{P}_0 + g_2 \hat{P}_2)$

This can be rewritten using $\hat{F}_1 \cdot \hat{F}_2 = -2\hat{P}_0 + \hat{P}_2$

$$V = \delta(r_1 - r_2) [C_0 (\hat{P}_0 + \hat{P}_2) + C_2 \hat{F}_1 \cdot \hat{F}_2]$$

$$\text{with } C_0 = \frac{g_0 + 2g_2}{3}, C_2 = \frac{g_2 - g_0}{3}$$

This is pretty stunning:

The most general potential is $V = \frac{1}{2} \int d^3x g_{ijkl} \psi_i^\dagger(x) \psi_j^\dagger(x) \psi_k(x) \psi_l(x)$

which has 81 coefficients

exchange symmetry $g_{ijkl} = g_{jilk}$ and time reversal $g_{ijkl} = g_{klij}$

reduces this to a still large 21!

whereas the above gives just 2!

If I look at just the C_0 term: $V_0 = \frac{C_0}{2} \int d^3x \psi_i^\dagger(x) \psi_j^\dagger(x) \psi_j(x) \psi_i(x)$

$$= \frac{C_0}{2} \int d^3x \left(\sum_i \hat{n}_i \right)^2 : \text{density-density}$$

Fermions

$F = 1/2$ fermions

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This is most simple in second quantized notation

$$V = \frac{1}{2} \int d^3x g_{ijkl} \psi_i^\dagger \psi_j^\dagger \psi_k \psi_l, \text{ with } \{ \psi_i^\dagger, \psi_j \} = \delta_{ij}$$
$$\{ \psi_i, \psi_j \} = 0$$

So $k \neq l$ and $i \neq j$

$$V = \frac{1}{2} \int d^3x (\psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\uparrow \psi_\downarrow g_{\uparrow\downarrow\uparrow\downarrow} + \psi_\downarrow^\dagger \psi_\uparrow^\dagger \psi_\uparrow \psi_\downarrow g_{\uparrow\uparrow\downarrow\downarrow} + \psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow g_{\downarrow\uparrow\uparrow\downarrow} + \psi_\downarrow^\dagger \psi_\uparrow^\dagger \psi_\downarrow \psi_\uparrow g_{\downarrow\downarrow\uparrow\uparrow})$$
$$= \frac{(g_{\uparrow\downarrow\uparrow\downarrow} + g_{\uparrow\uparrow\downarrow\downarrow} - g_{\downarrow\uparrow\uparrow\downarrow} - g_{\downarrow\downarrow\uparrow\uparrow})}{2} \int d^3x \psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow$$

$$V = \frac{\bar{g}}{2} \int d^3x \psi_i^\dagger \psi_j^\dagger \psi_j \psi_i = \frac{\bar{g}}{2} \int d^3x : (n_\uparrow + n_\downarrow)^2 :$$

so this is just a density-density interaction.

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