

Lecture 4.1

Spin Hamiltonians and Exchange interactions

This version of Modern Models, Lec. 4.1, edited for P654, Spring 2008. Sections 4.1 D ff, about the microscopic origin of spin interactions, were cut.

This lecture develops the idea of spins as a degree of freedom, with which models are built. There is a tension in how we think of spins. On the one hand, definitions and calculations are easiest using the z -basis description, with operators S_z, S_{\pm} obeying an operator algebra (reminiscent of fermion or boson operators). On the other hand, a *semiclassical* picture in which the spin is approximately a fixed-length vector is more useful for intuitive thinking and as a starting point for calculations in *ordered* states (Sec. 4.1 B).

Besides the spin degrees of freedom, a spin model needs a Hamiltonian, and the typical terms are surveyed in Sec. 4.1 C. Most important is the dot-product spin-spin coupling called an exchange interaction: this is the second key physical idea of this lecture. The (omitted!) next two sections (and Sec. 4.1 X) develop the origin of exchange interactions – both ferromagnetic and antiferromagnetic – as a consequence of fermion statistics when we reduce the Hilbert space (by eliminating charge fluctuations as a degree of freedom). This story (the derivation of spin Hamiltonians from a more microscopic level) will be continued in Lec. 4.3, which [in its present form] focuses on “superexchange”.

4.1 A Spins as objects

A “spin” \mathbf{S} is a discrete degree of freedom that transforms like an angular momentum under rotations. It is a shorthand for a quantum-mechanical degree of freedom with a discrete set of basis states $|S_z\rangle$ labeled by the quantum number $S_z = -S, \dots, +S$ (the “ z basis”). Furthermore, the basis states $|S_z\rangle$ transform like angular momenta under spin-space rotations.

All components of a spin \mathbf{S} are axial vectors – i.e., they should change sign under time reversal. Thus “time reversal symmetry” in a spin Hamiltonian means “symmetry under reversal of all spins.”

We typically arrive at a spin Hamiltonian by eliminating portions of the Hilbert space as first described in Lec. 1.1 E : the subspace we project onto no longer allows variations of the number of electrons (or whatever the spin-bearing particle is), such that

the low-lying states form a representation of the rotation group. Thus, microscopically, \mathbf{S} might be (i) the spin of a single electron localized on an impurity in a semiconductor; (ii) the combined spin of several d electrons in a transition-metal ion (commonest case); (iii) a *nuclear* spin (of course this depends on the isotope) of an atom in a crystal; or (iv) the combined spin and orbital moment of a rare-earth ion. *But if the Hamiltonian has the same form, the system has the same behavior, no matter what the spins are built from.*

Now we imagine a lattice with a “spin” on each of the N sites. This system has $(2S + 1)^N$ basis states, which are the direct product of the basis states for each spin. They can be labeled

$$|S_{z1}, S_{z2}, \dots, S_{zN}\rangle \quad (4.1.1)$$

When we specialize for simplicity to the spin-1/2 case, it is convenient to rewrite the S_z labels $\pm 1/2$ as “ \uparrow ” and “ \downarrow ”.

Any Hamiltonian $\mathcal{H}_{\text{spin}}(\{\mathbf{S}_i\})$ in terms of spins (in a finite system) can always be written as a polynomial in the $3N$ spin components. The same spin Hamiltonian could come from diverse origins. Once we have it, it is irrelevant what the internal degrees of freedom were that led to it – they only describe high-lying excited states. I think of the spin as a quantum object with a finite state space.

Algebra of spin operators

Most readers should be familiar with the following algebraic relations, collected here for reference. But keep in mind that we now picture the spin as an abstract object in its own right, rather than an angular momentum.

The Hamiltonian for such a system is naturally built out of spin operators (S_{ix}, S_{iy}, S_{iz}) , which transform as a vector and are defined to act as follows on the basis states:¹

$$\hat{S}_{iz}|S_{iz}\rangle_i = S_{iz}|S_{iz}\rangle_i \quad (4.1.2)$$

$$\hat{S}_{i+}|S_{iz}\rangle_i = \sqrt{S(S+1) - S_{iz}(S_{iz}+1)} |S_{iz}+1\rangle_i \quad (4.1.3)$$

$$\hat{S}_{i-}|S_{iz}\rangle_i = \sqrt{S(S+1) - S_{iz}(S_{iz}-1)} |S_{iz}-1\rangle_i \quad (4.1.4)$$

Here $|\dots\rangle_i$ means the basis state for the spin on *lattice site* i . Also S is the total length quantum number of the spins, a constant, which depends on the ion species (including its ionization state); Lec. 4.2 [omitted] shows how you could figure it from the start. When different spin sites are inequivalent, their spins *might* have different S values.

We’re usually interested in a *lattice* with a macroscopic number of spins. So the i indices are written explicitly in (4.1.2), (4.1.3), (4.1.4), to make the point that each spin operator acts on just one site. When the basis states are written as in (4.1.1), the operator with index i affects only the label with index i , e.g. in a chain of five $S = 1/2$ spins:

$$S_{3+}|\uparrow\downarrow\uparrow\uparrow\rangle = |\uparrow\downarrow\uparrow\uparrow\rangle \quad (4.1.5)$$

From (4.1.2), (4.1.3), (4.1.4), the commutation relations follow²

$$[S_{iz}, S_{j\pm}] = \pm\delta_{ij}S_{i\pm} \quad (4.1.6)$$

¹I’ll usually omit the hats that indicate a quantum operator.

²Here’s how I remember the commutators. First, to know what operator I get, I notice e.g. that S_{i+} carries a net z spin of $+1$ so I know that either term in the first commutator, $S_{i+}S_{iz} - S_{iz}S_{i+}$ carries a net z spin of $+1$, their sum does too, thus it can only be $\propto S_{i+}$. To determine the coefficient (which is independent of the spin length S), I check the $S = 1/2$ case where $S_+|-\frac{1}{2}\rangle = |+\frac{1}{2}\rangle$ and $S_-|+\frac{1}{2}\rangle = |-\frac{1}{2}\rangle$.

$$[S_{i+}, S_{j-}] = \delta_{ij} 2S_{iz} \quad (4.1.7)$$

When we write $S_{i\pm} = S_{ix} \pm iS_{iy}$, we find commutation relations $[S_{ix}, S_{iy}] = iS_{iz}$ (also cyclic permutations of xyz) and indeed $\hat{\mathbf{S}}$ is a vector. The spin's length is $\mathbf{S}_i^2 = S(S+1)$.

Comparison to fermion and boson operators

In Table 4.1.1, the spinless fermions/bosons are in discrete orbitals, with just one orbital per lattice site. The full algebra of operators includes (i) what I called “label” operators – diagonal operators whose eigenvalues are used to label the basis states (ii) “ladder” operators – off-diagonal creation/annihilation or raising/lowering operators which connect between eigenstates with adjacent values of the label operators.

What	Labels	states/site	Ladder operators	Commutators
spinless fermions	$\hat{\rho}_i = 0, 1$	2	c_i, c_i^\dagger	$\{c_i, c_i^\dagger\} = 1$
bosons; harm. osc.	$\hat{\rho}_i = 0, 1, \dots$	discrete ∞	b_i, b_i^\dagger	$[b_i, b_i^\dagger] = 1$
spin	$S_{iz} = -S, \dots, +S$	$2S + 1$	S_{i+}, S_{i-}	$[S_{i+}, S_{i-}] = 2S_{iz}$

Table 4.1.1: Discrete quantum models on lattices: three kinds of operator

The mathematical structure is very similar to that of a boson or fermion operator (see Table 4.1.1). On the one hand, spins are like *fermions* in that their Hilbert space is finite-dimensional. On the other hand, they are like *bosons* in that operators from different spins commute ((4.1.7)). The similarity to bosons is exploited in various exact mappings to particle operators such as the *Schwinger bosons* or the *Holstein-Primakoff* representations, discussed in Lec. 5.5 .

Spin operators can also be written as bilinears in electron operators:

$$\begin{aligned}
 S_{iz} &= \frac{1}{2}(c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow}) \\
 S_{i+} &= c_{i\uparrow}^\dagger c_{i\downarrow} \\
 S_{i-} &= c_{i\downarrow}^\dagger c_{i\uparrow}
 \end{aligned} \quad (4.1.8)$$

The Wigner-Eckart relation says that, we project the Hilbert space of some electrons to a subspace labeled by a single spin operator, then any vector operator projects (within that space) to a multiple of the spin operator. Sorry, I'm not prepared with a a good explanation; it is an elementary consequence of group representation theory.

4.1 B Semiclassical viewpoint

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There is one big difference between spin and particle operators: in particles, the occupation number basis is natural to our semiclassical thinking since we think of a particle as being in a given place in a given time. Quantum perturbation terms can be visualized as “virtual” processes in which a particle hops to some other state temporarily, and this may be given a precise meaning within a path integral formalism.

In spins, on the other hand, it is natural to think of them as having a “direction”. But the uncertainty relations for spin say the direction on the unit sphere is uncertain to $O(1/\sqrt{S})$. This justifies approximately acting as though we could specify (S_x, S_y, S_z)

and represent the spin classically as a point on the unit sphere, a vector of fixed length. (This semiclassical viewpoint would be developed later in Part 4, or 5, for spin waves in particular.) The customary $|S_z\rangle$ basis is handier for doing calculations; in it the z component is perfectly definite and the others are completely uncertain.

There are systematic expansions in powers of $1/S$. Rather surprisingly, they often work – at least as a qualitative picture – even when $S = 1$ or $S = 1/2$.

Uncertainty principle for spins

Given a spin is in a state of definite and maximum $S_z = S$, the relative mean-squared deviation

$$\frac{\langle |\mathbf{S} - S_z \hat{z}|^2 \rangle}{\langle \mathbf{S}^2 \rangle} \approx \frac{\text{Const}}{S} \quad (4.1.9)$$

Thus, the angular uncertainty is of $O(S^{-1/2})$. This means that, in the limit $S \rightarrow \infty$, we may consider a spin as having a definite direction, just as in the limit of small \hbar we may consider an object as having both position and momentum well-defined.

Semiclassical spin dynamics

This result below can be thought of as the analog for spins of Newton's equations; the condition for static equilibrium is also there (that every spin be aligned with its "local field"). They are very convenient for visualization, since we are used to a classical world.

Quite generally, if $\mathcal{H}(\mathbf{S})$ is a single-spin Hamiltonian, we have

$$d\mathbf{S}/dt = \gamma \mathbf{S} \times \mathbf{h}(\mathbf{S}) \quad (4.1.10)$$

where

$$-g\mu_B \mathbf{h}(\mathbf{S}) \equiv \delta\mathcal{H}/\delta\mathbf{s}. \quad (4.1.11)$$

Here $\mathbf{h}(\mathbf{S})$ is called the "local field".

4.1 C Spin couplings

A spin Hamiltonian (almost always) consists of a sum of one-spin and two-spin terms. This is very analogous to the Hamiltonian of a particle system, where one has one-body terms (an external potential) plus two-body terms (particle-particle interactions). The terms are best visualized by pretending the spin length S is long and imagining \mathbf{S} to be a c -number vector.

Since we will be interested in extended arrays of spins, the (continuous or discrete) *symmetries* of the spin Hamiltonian with respect to rotations in spin space are all-important. There are two reasons for this.

(i) In an ordered state, symmetries of the Hamiltonian will be spontaneously broken. [See Lec. 1.3 and Lec. 1.4.] The possibilities of topological defects and of Goldstone modes depends on this.

(ii) Invariance of the Hamiltonian under continuous rotations about axis $\hat{\mathbf{a}}$ implies *conservation* of the $\hat{\mathbf{a}}$ spin component. Conservation laws affect the dynamics including the nature of the spin-wave dispersion as well as transport properties. *A more current interest: if you're doing spintronics, you care whether spin is conserved in your material!*

“Isotropic” terms of the Hamiltonian are invariant under rotations in spin space (unaccompanied by real space). Terms which violate rotation symmetry are called *anisotropies*. All of them are due to spin-orbit coupling except the dipolar. Frequently system is rotationally symmetric at zero order, but anisotropy terms are present as small perturbations. The form of anisotropic terms is directly dependent on the *local* symmetry rotation symmetry (of the site or sites being coupled plus their neighbors). When the crystal structure is not a Bravais lattice, the local symmetry may be lower than the crystal’s point group, or alternatively, an *approximate* but practically exact local symmetry may be *higher* than the point group.

A general spin Hamiltonian can be written in the following form,

$$\mathcal{H}_{\text{spin}} = (\mathcal{H}_H + \mathcal{H}_{\text{An}}) + (\mathcal{H}_{\text{ex}} + \mathcal{H}_{\text{DM}} + \mathcal{H}_{\text{an-ex}} + \mathcal{H}_{\text{dip}}) \quad (4.1.12)$$

I’ve grouped the single-spin and multiple-spin terms in (4.1.12); below, I’ll discuss each term, starting with the one-spin terms.

Magnetic field coupling

An external field \mathbf{H} couples as

$$\mathcal{H}_H = -\mathbf{H} \cdot \sum_i g_i \mu_B \mathbf{S}_i \quad (4.1.13)$$

This term looks anisotropic in that \mathbf{H} defines a special direction in space. ³ But the *material* is isotropic in spin space, in the sense that the strength of its field coupling is independent of the field’s direction.

It’s convenient to rewrite $\mathcal{H}_H = -\mathbf{H} \cdot \sum_i \mathbf{S}_i$, absorbing the $g\mu_B$ coefficient into the magnetic field \mathbf{H} , which thenceforth has the units of energy. This term is small compared to the others: recall $\mu_B = 0.0578\text{meV/T}$, that fields over $\sim 20\text{ T}$ require large and expensive magnets, and that a typical exchange constant is 10meV (often more). In particular, it is rarely possible to apply a field large enough to force a system into a nearly saturated state (all spins nearly parallel), if the spin-spin couplings favor some other state.

Most generally, when microscopic spin-orbit scattering is important and the local symmetry is less than cubic, we should replace (4.1.13) by $\mathcal{H}_H = -\mathbf{H} \cdot \sum_i \mathbf{g}_i \mu_B \mathbf{S}_i$ where \mathbf{g}_i (a 3×3 matrix) is the “g-tensor” of site i , which must have the same rotational symmetries as the site. ⁴

Single-ion anisotropy

This term has the form

$$\mathcal{H}_{\text{An}} = \sum_i \mathcal{E}_{\text{An}}^{(i)}(\mathbf{S}_i) \quad (4.1.14)$$

If a given point group operation around a site leaves all its neighbors in the same places, then the same point operation applied to (4.1.14) should leave it invariant.

A very common form is *uniaxial* anisotropy

$$\mathcal{E}_{\text{An}}(\mathbf{S}) = -\frac{1}{2}DS_z^2 \quad (4.1.15)$$

³Actually, if the only other terms are exchange, the only effect of (4.1.13) is to set the system into uniform precession around the \mathbf{H} axis at angular frequency $\omega = g\mu_B H$. (See Lec. 4.6 [Omitted] on spin resonance.)

⁴The anisotropic g tensor is to be explained in Lec. 4.2 [omitted] or Lec. 4.3 .

or $\mathcal{E}_{\text{An}}^{(i)}(\mathbf{S}) = -\frac{1}{2}D(S \cdot \hat{n}_i)^2$ where the unit vector \hat{n}_i is called the spin's “easy axis”.

The most general single-spin term, quadratic in spin components, can be written $\mathcal{H}_{\text{An}}(\mathbf{S}) = \frac{1}{2} \sum_{\alpha\beta} K_{\alpha\beta} S_\alpha S_\beta$ where $K_{\alpha\beta}$ must be symmetric. If we diagonalize the matrix $\{K_{\alpha\beta}\}$, then after a spin-space rotation that makes the principal axes into x', y', z' , the general form is

$$\mathcal{H}_{\text{An}} = -\frac{1}{2}DS_z'^2 + \frac{1}{2}D'(S_x'^2 - S_y'^2) \quad (4.1.16)$$

There were three independent eigenvalues of $\{K_{\alpha\beta}\}$, but one combination of them corresponds to the unit-matrix component of $\{K_{\alpha\beta}\}$ which gives a trivial constant $\mathbf{S}^2 = S(S+1)\dots$ A corollary of the symmetry lemma is that when the local environment has mirror planes (symmetric under reflection in those planes), the principal axis directions must lie in them or perpendicular to them.

Finally, if the environment has tetrahedral or cubic local symmetry, there is no nontrivial quadratic term; the first anisotropic term is

$$\mathcal{E}_{\text{An}}^{\text{cubic}}(\mathbf{S}) = K(S_x^4 + S_y^4 + S_z^4) \quad (4.1.17)$$

(there is only one such term). This *cubic* anisotropy favors spins along $\langle 111 \rangle$ axes when $K > 0$ or $\langle 100 \rangle$ axes when $K < 0$.

Exchange

The *exchange interaction* (sometimes called Heisenberg exchange) is bilinear in spins and isotropic under rotations:

$$\mathcal{H}_{\text{ex}} = - \sum_{i < j} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j \quad (4.1.18)$$

For us, the name “exchange” does not refer to any particular mechanism but merely to the dot-product form, which guarantees rotation symmetry. Notice The interactions in (4.1.18) may extend beyond first neighbors. Exchange couplings (the coefficients J_{ij}) are called “ferromagnetic” (resp. “antiferromagnetic”), when they favor favoring parallel (resp. antiparallel) alignment of interacting spins.

I now mention some algebraic tricks related to exchange couplings. Let \hat{P}_{12} be the operator that exchanges spin 1 and spin 2, i.e. $\hat{P}_{12}|\sigma_1\sigma_2\rangle \equiv |\sigma_2\sigma_1\rangle$. Then we can show

$$\hat{P}_{12} = \frac{1}{2} + 2\mathbf{S}_1 \cdot \mathbf{S}_2. \quad (4.1.19)$$

As you know from basic quantum mechanics, one may construct (using Clebsch-Gordan coefficients) combined states of two spins such that $\mathbf{S}_{\text{tot}} \equiv \mathbf{S}_1 + \mathbf{S}_2$ has a definite spin S_{tot} .

Then

$$\mathbf{S}_1 \cdot \mathbf{S}_2 = \frac{1}{2} [(\mathbf{S}_1 + \mathbf{S}_2)^2 - \mathbf{S}_1^2 \mathbf{S}_2^2] = \frac{1}{2} [S_{\text{tot}}(S_{\text{tot}} + 1) - 2S(S + 1)]. \quad (4.1.20)$$

It can be shown (see (Ex. 4.1.1)(b) that for spin 1/2 there are just two eigenvalues of $J\mathbf{S}_1 \cdot \mathbf{S}_2$, corresponding to a combined singlet or triplet; the splitting is J , and the average over the four eigenstates is zero.

Other two-spin terms

We could write a most general bilinear form, with terms $\sum_{\alpha\beta} M_{\alpha\beta} S_{i\alpha} S_{j\beta}$, where α, β label Cartesian components of the coupling matrix $\{M_{\alpha\beta}\}$. Any 3×3 matrix may be

decomposed into (i) a multiple of the identity matrix, (ii) an antisymmetric part (three different coefficients), and (iii) a traceless symmetric part (five different coefficients). [One could also say these correspond to the ways of combining two spherical harmonics of angular momentum 1 (as characterizes the vector operator \mathbf{S} , whatever the spin quantum number S), so as to make a net angular momentum 0, 1, or 2, respectively.] These three terms give respectively \mathcal{H}_{ex} , \mathcal{H}_{DM} , and $(\mathcal{H}_{\text{an-ex}} + \mathcal{H}_{\text{dip}})$ in (4.1.12). The bilinear terms, besides exchange, are anisotropic exchange ($\mathcal{H}_{\text{an-ex}}$ and antisymmetric or “Dzyaloshinskii-Moriya” term) and finally dipole-dipole.

The *Dzyaloshinskii-Moriya* interaction, or antisymmetric exchange, has the form

$$\mathcal{H}_{\text{DM}} = - \sum_{i < j} \mathbf{D}_{ij} \cdot \mathbf{S}_i \times \mathbf{S}_j \quad (4.1.21)$$

It is also possible to have anisotropic exchange, for example

$$\mathcal{H}_{\text{an-ex}} = - \sum_{i < j} J_{ij}^{xy} (S_{ix} S_{jx} + S_{iy} S_{jy}) + J_{ij}^z S_{iz} S_{jz} \quad (4.1.22)$$

As far as its symmetry in spin space, the *dipolar* interaction is a special case (extending beyond nearest neighbors) of the “traceless symmetric” case above, i.e., as part of $\mathcal{H}_{\text{an-ex}}$. However, in this case the interaction does not depend on the crystal axes, and its microscopic origin is not in exchange, so it makes sense to treat it separately:

$$\mathcal{H}_{\text{dip}} = \sum_{ij} \frac{(g\mu_B)^2}{r_{ij}^3} [3(\hat{\mathbf{r}}_{ij} \cdot S_i)(\hat{\mathbf{r}}_{ij} \cdot S_j) - S_i \cdot S_j] \quad (4.1.23)$$

This is long-range and responsible for the demagnetizing field, ferromagnetic domains, etc. Dipolar interactions are important when exchange is small, and also in nuclear magnets.

They can lead to different dynamics and to different critical exponents in phase transitions.

Multi-spin terms?

In modeling the stability of crystal structures (see Lec. 1.2E), three- and four-atom effective potentials can be important. By contrast, three- or four-spin potentials rarely appear in spin Hamiltonians. They arise (i) in solid ^3He (a nuclear spin $S=1/2$) arising from a ring tunneling of atoms *mentioned in Lec. 4.3*; (ii) the effective interaction when you have a magnetoelastic coupling and eliminate the elastic degrees of freedom. *In addition, ring-exchange interactions may appear in the cuprate antiferromagnets which become high- T_c superconductors upon doping.*

Exercises

Ex. 4.1.1 Spin 1/2 exchange interactions

(a) Here’s how a permutation can be converted into a dot product operation. Each operator in the table annihilates 3 of the 4 possible states, and turns the other one into its $(1 \leftrightarrow 2)$ permutation. The sum of the terms in the left column is thus the permutation exchange operator \hat{P}_{12} ; show that it adds up to (4.1.19).

(b). Use (4.1.20) to show that, if \mathbf{S}_1 and \mathbf{S}_2 are both $s=1/2$ spins, then $\mathbf{S}_1 \cdot \mathbf{S}_2 = +1/4$ or $-3/4$ are the only eigenvalues of this operator.

(c). Express $(\mathbf{S}_1 + \mathbf{S}_2)^2$ in terms of $\mathbf{S}_1 \cdot \mathbf{S}_2$ for the case of spin-1/2 spins.

Operator	$ \uparrow\downarrow\rangle$	$ \downarrow\uparrow\rangle$	$ \uparrow\uparrow\rangle$	$ \downarrow\downarrow\rangle$
$S_{1+}S_{2-}$	0	$ \uparrow\downarrow\rangle$	0	0
$S_{2+}S_{1-}$	$ \downarrow\uparrow\rangle$	0	0	0
$(\frac{1}{2} + S_{1z})(\frac{1}{2} + S_{2z})$	0	0	$ \uparrow\uparrow\rangle$	0
$(\frac{1}{2} - S_{1z})(\frac{1}{2} - S_{2z})$	0	0	0	$ \downarrow\downarrow\rangle$

Table 4.1.2: Pieces of two-spin-1/2 exchange operator

Ex. 4.1.2 Spin uncertainties

(a). Confirm (4.1.9). Also, what is the ratio

$$\frac{\langle |[s_{ix}, s_{iy}]|^2 \rangle}{\langle s_{ix}^2 \rangle \langle s_{iy}^2 \rangle} ? \quad (4.1.24)$$

What happens to (4.1.9) and (4.1.24) in the limit $S \rightarrow \infty$?**Ex. 4.1.3 Semiclassical spin dynamics**

(a). Consider

$$\mathcal{H}_0 = -g\mu_B \mathbf{H} \cdot \mathbf{s} \quad (4.1.25)$$

Use Heisenberg's equation of motion

$$\hbar i \frac{dX}{dt} = [X, \mathcal{H}_0] \quad (4.1.26)$$

to find

$$d\mathbf{s}/dt = \gamma \mathbf{s} \times \mathbf{H} \quad (4.1.27)$$

What is γ ?

(b). Now consider a generalization of (4.1.25)

$$\mathcal{H}_0(\mathbf{s}) = \sum_{klm} \lambda_{klm} s_x^k s_y^l s_z^m. \quad (4.1.28)$$

Construct a semiclassical equation of motion as follows: First expand the commutator from (4.1.26), so that each term in (4.1.28) produces many terms. Adopt the approximation that this result is made of c -numbers which commute freely: those many terms should collapse back to one term.

Within this approximation, does it matter in which order we write the factors in each term of (4.1.28)?

Show that the result can be expressed in the form (4.1.10) .

(c). Let $\bar{\mathbf{s}}_0$ be the direction for the *classical* ground state, minimizing $\mathcal{H}_0(\mathbf{s})$ (with the fixed-length constraint $|\mathbf{s}_0| = s$).

What relation must hold between the directions of \mathbf{s} and $\mathbf{h}(\mathbf{s})$ in a ground state? Does this make sense, in the light of (4.1.10)?

(d). (OPTIONAL) What is the frequency ω of small oscillations around the ground state direction \mathbf{s}_0 , in terms of \mathbf{h} evaluated at the ground state? (Hint: Eqs. (4.1.10) and (4.1.11) are rotationally invariant, as they ought to be, so you may choose your axes for *spin* space such that $\mathbf{h}(\mathbf{s}_0)$ is along z' .) Then linearize in the components transverse to \mathbf{s}_0 .

Ex. 4.1.4 Ferromagnetic exchange in a ring

assigned in 2003 only

Compare the exact-diagonalization exercise in Lec. 1.1 .

Consider a ring of three sites, at position 0, 1, 2, (so lattice constant =1). Each site has one orbital, with room for an up and a down spin. The Hamiltonian is a Hubbard model, with *positive* hopping matrix element $+t$ and a repulsive energy $\sum_{r=0}^2 U \hat{n}_{r\uparrow} \hat{n}_{r\downarrow}$ when two electrons (necessarily \uparrow and \downarrow) are on the same site. Two electrons are placed on the ring.

(a). The noninteracting (single-particle) dispersion is $\epsilon(k) = 2t \cos ka$, where $k_n = (2\pi/3)n$. Show that the single-particle ground state is doubly degenerate. (This is due to $t > 0$ and also to the ring having an odd number of sites.)

(b). Construct the noninteracting ground state for spins $|\uparrow\uparrow\rangle$. Imagine that U is small and evaluate its effect in first-order perturbation. Show $\langle \hat{n}_{r\uparrow} n_{r\downarrow} \rangle = 0$ for the $|\uparrow\uparrow\rangle$ case and $1/9$ for either of the two kinds of $|\uparrow\downarrow\rangle$ case. (You could place opposite spins both in the same orbital, or in two different ones.)

(c). Consider the case $|k_1\uparrow, k_2\downarrow\rangle$ (recall $k_2 \equiv -k_1$ modulo 2π , so the net “wavevector” is zero.) Expanding out its terms, and keep only those which have both electrons on the same site. Now do the same for $|k_2\uparrow, k_1\downarrow\rangle$. Verify that in either the sum or the difference (which!?) of these two wavefunctions, all the terms with double occupancy cancel, and therefore the noninteracting energy is obtained as for the $|\uparrow\uparrow\rangle$ wavefunction. What is the relation of this wavefunction to the $|\uparrow\uparrow\rangle$ state?

(d). OPTIONAL!! Consider instead the case $U = \infty$, meaning two particles are never allowed on the same site. Solve this exercise by writing a graph with all possible states of the spins in a ring. (There are three states in the $|\uparrow\uparrow\rangle$ case and six of the $|\uparrow\downarrow\rangle$ case). Find the ground state in either case, and verify that the ferromagnetic case is lower. In this case, the exchange energy scale is necessarily $O(t)$, and you can see the difference comes entirely through Fermi statistics.

Lecture 5.0

Overview of spin order

This version is edited for Physics 654. (Lec. 5.0A and 5.0B were an overview of the Hubbard model.)

5.0 A Semiclassical treatment of spin system

In this section, we consider a local-moment model. The degrees of freedom are N spins \mathbf{s}_i , each of length S . I'll explain how, in the limit $S \gg 1$, the spins behave as (nearly) classical objects. It's useful to have such a limit, as a means to visualizing spin behavior with our (classical) minds, or to approximate them using classical statistical mechanics. Furthermore, as with particle systems, any quantum result must pass the test of Bohr's correspondence principle – but the classical limit of a spin is not as obvious as Newtonian mechanics. In actuality, the spin of an ion is at most $S = 7/2$, but it turns out that $S \gtrsim 3/2$ seems to be sufficient that the large- S limit is qualitatively correct.

Spin coherent states

Consider, for now, just *one* spin \mathbf{S} . Let $|\psi_{\hat{\mathbf{z}}}\rangle$ be the state at the top of the ladder of S_z states : its wavefunction is entirely on the state $S_z = +S$; equivalently, it satisfies

$$\hat{S}^z |\psi_{\hat{\mathbf{z}}}\rangle = S |\psi_{\hat{\mathbf{z}}}\rangle. \quad (5.0.1)$$

Next, for any unit vector $\hat{\mathbf{n}}$, find a rotation matrix \mathbb{R} such that $\mathbb{R}\hat{\mathbf{z}} = \hat{\mathbf{n}}$, and let $\mathcal{R}_{\mathbb{R}}$ be a unitary operator that applies the same rotation to the spin. ¹ Obviously,

$$\hat{\mathbf{S}} |\psi_{\hat{\mathbf{n}}}\rangle = S \hat{\mathbf{n}} |\psi_{\hat{\mathbf{n}}}\rangle; \quad (5.0.2)$$

this state is pointing in the $\hat{\mathbf{n}}$ direction as strongly as it can. It turns out these states are the analog of minimum-uncertainty wavepackets.

Notice that coherent states in different directions aren't exactly orthogonal (only when in opposite directions). Namely

$$|\langle \psi_{\hat{\mathbf{n}}} | \psi_{\hat{\mathbf{n}}}' \rangle| = \left(\frac{1 + \hat{\mathbf{n}} \cdot \hat{\mathbf{n}}'}{2} \right)^S = \left| \cos \frac{1}{2} \theta(\hat{\mathbf{n}}, \hat{\mathbf{n}}') \right|^{2S} \approx \exp\left[-\frac{S}{4} \theta(\hat{\mathbf{n}}, \hat{\mathbf{n}}')^2\right] \quad (5.0.3)$$

¹There is more than one rotation matrix satisfying $\mathbb{R}\hat{\mathbf{z}} = \hat{\mathbf{n}}$; it turns out that you get the same state $\mathcal{R}_{\mathbb{R}}|\psi_{\hat{\mathbf{z}}}\rangle$, except there is a phase factor; this is exactly like the gauge freedom in defining the phase of the real-space state \mathbf{r} , in the case of a particle. Thus, for some calculations one must specify a gauge choice, or else work with manifestly gauge-invariant quantities; but none of that matters in this lecture.

where $\theta(\hat{\mathbf{n}}, \hat{\mathbf{n}}')$ is the angle between their directions, and this is obviously like the overlap between two offset Gaussian wavepackets.

Semiclassical limit notion

A spin vector has a well-defined direction in space in the limit $S \rightarrow \infty$ (this is the analog of $\hbar \rightarrow 0$ in a particle system.) For example, let's take a coherent state, and compute the spin's quantum fluctuations about its expectation. It turns out (see homework [?]) you get $\langle \delta \mathbf{S}^2 \rangle = S$, i.e. the relative angle fluctuation is

$$\frac{\langle \delta \mathbf{S}^2 \rangle^{1/2}}{S} \sim S^{-1/2} \rightarrow 0 \quad (5.0.4)$$

as $S \rightarrow \infty$.

This makes common sense: the Hilbert space of a spin has dimension $2S + 1$, with which it has to represent all possible directions. So, if we want basis states that are maximally localized in direction, each one must cover $4\pi/(2S + 1)$ of solid angle, which would be (for large S) a circle of radius $\sqrt{2/S}$ radians.

Conjugate variables

Take a coherent state along $\hat{\mathbf{z}}$. If $S \gg 1$, the quantum fluctuations are small and S_z can be approximated as a c -number. Consider the commutator $[\delta S_x, \delta S_y] = -iS_z \approx -iS$. So long as we can treat it as a c -number, this is the exact analog of $[\hat{X}, \hat{P}] = -i\hbar$ for a particle system, and hence the different components are the canonical conjugate variables. This is the basis (see below) for semiclassical spin wave and spin precession dynamics; also of spin tunneling.

But there's a difference. In a particle system, we think of position and momentum as different quantities, and they come in different units, so it's natural to write wavefunctions in terms of one of them, e.g. $\psi(x)$, or to define a Green's function (e.g. in Lec. 2.2) as the amplitude of a particle to get from position \mathbf{r} at time t to position \mathbf{r}' at time t' : we're not bothered that specifying the position exactly means that momentum is indefinite (hence our real-space basis function contains all possible wavevectors).

On the other hand, the different components of a spin are manifestly equivalent quantities, often related by symmetries; and our intuition leads us to think of a well-defined direction in spin space. (The analog of $\psi(x)$ would be a wavefunction in terms of say S_z , so the azimuthal angle would be totally indefinite.) However, the uncertainty relation (5.0.4) means a spin state with a truly definite direction is impossible: the coherent state basis is the best we can do (even though it's not an orthogonal basis)

Multi-spin states

In general, the wavefunction is $\Psi(S_1^z, S_2^z, S_3^z, \dots)$; it depends on the discrete $[(2S + 1)^N$ -dimensional] Hilbert space. We can write a product wavefunction

$$\Psi^{\text{coh}}(\{S_{iz}\}) = \prod_i \psi_{\hat{\mathbf{n}}_i}(S_{iz}) \quad (5.0.5)$$

thus

$$\langle \mathbf{S}_i \rangle_{\Psi^{\text{coh}}} = S \hat{\mathbf{n}}_i; \quad (5.0.6)$$

$$\langle \mathbf{S}_i \cdot \mathbf{S}_i \rangle_{\Psi^{\text{coh}}} = S^2 \hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_i. \quad (5.0.7)$$

(This follows since the wavefunction Ψ^{coh} incorporated no quantum correlations between sites; it's simply a direct product.)

Think of Ψ^{coh} as a variational wavefunction, specified by the set of classical directions $\{\hat{\mathbf{n}}_i\}$ as parameters. It plays the same role as the classical ground state of a many-particle system, the minimum of potential energy $U(\{\mathbf{x}_i\})$ as a function of positions. Minimizing $\langle \hat{\mathcal{H}}_{\text{hop}}^{\text{spin}} \rangle_{\Psi^{\text{coh}}}$ is equivalent to minimizing a *classical* function $\mathcal{H}^{\text{spin}}(\{\hat{\mathbf{n}}_i\})$. This is what we mean by a classical spin Hamiltonian.

A next step would be to incorporate the zero-point fluctuations about this minimum, as done for phonons in Lec. 1.5 .²

Alternatively, at $T > 0$, we could replace each coherent state by a thermal distribution: technically, a density matrix. The whole system's density matrix is the direct product of the density matrices for the respective spins. This yields a form of *mean field theory*, which somewhat takes into account the quantum nature of the spins, but also describes the high-temperature paramagnetic state and ordering transitions

Equations of motion

This subsection was missing in the previous notes I'm typing up... it may have been postponed to Lec. 5.5 in a previous version. So this is just a sketch, and in particular the signs and coefficients are not right.

The "local field" is

$$\mathbf{h}_i \equiv \frac{\delta \mathcal{H}}{\delta \mathbf{s}_i} \quad (5.0.8)$$

and thus is exactly the analog of a force (except, since \mathbf{S}_i has fixed length, we can't actually displace in that direction). In particular say the Hamiltonian is pure exchange,

$$\mathcal{H}_{\text{ex}} = -\frac{1}{2} \sum_{ij} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j; \quad (5.0.9)$$

then

$$\mathbf{h}_i = \sum_j J_{ij} \mathbf{s}_j. \quad (5.0.10)$$

This is called "local field" because $\mathbf{h}_i = \mathcal{H}$ if the Hamiltonian were just $-\mathcal{H} \cdot \sum_i \mathbf{s}_i$, an external field.

The condition for a local minimum is $\mathbf{s}_i = S \hat{\mathbf{n}}_i$, with

$$\hat{\mathbf{n}}_i = \mathbf{h}_i / |\mathbf{h}_i|. \quad (5.0.11)$$

The dynamics which follow (e.g.) from the commutators are simple: each spin precesses around its local field. It's like the motion of a gyroscope, or a particle in a strong magnetic field (see Part 9 on quantized Hall effect): it moves (along its unit sphere) perpendicular to the direction it's pushed:

$$\hbar \frac{d}{dt} \hat{\mathbf{n}}_i = \frac{1}{S} \hat{\mathbf{n}}_i \times \mathbf{h}_i. \quad (5.0.12)$$

²In a ferromagnet, Ψ^{coh} is actually the exact ground state so there are no fluctuations. The fluctuations are a consequence of the fact that the Hamiltonian doesn't commute with the order parameter.