Quantum Magnetism Approaches to Strongly Correlated Electrons

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Abstract
Problems of strongly interacting electrons can be greatly simplified by reducing them to effective quantum spin models. The initial step is renormalization of the Hamiltonian into a lower energy subspace. The positive and negative U Hubbard models are explicitly transformed into the Heisenberg and -x-xz models respectively. Basic tools of quantum magnetism are introduced and used: spin coherent states path integral, spin wave theory, and continuum theory of rotators. The last lecture concerns pseudospin approaches to superconductivity and superfluidity. The SO(3) rotator theory for the -x-xz model describes the charge density wave to superconductor transition for e.g. doped bismuthates. Analogously, Zhang’s theory for collective modes of high $T_c$ cuprates describes the antiferromagnet to d-wave superconductor transition using SO(5) rotators. Finally, the Magnus force on two dimensional vortices and their momentum, are derived from the Berry phase of the spin path integral.
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Part I

Deriving the Effective Hamiltonian

Let us consider the Hubbard model for conduction electrons hopping on a lattice with short range interactions

\[ H = \mathcal{T} + \mathcal{U} \]
\[ \mathcal{T} = -t \sum_{\langle ij \rangle s=\uparrow,\downarrow} c_{i,s}^\dagger c_{j,s} \]
\[ \mathcal{U} = U \sum_i n_{i,\uparrow} n_{i,\downarrow}, \]  

(1)

It is always tempting to reduce the interaction term \( \mathcal{U} \) to fermion bilinears (single electron terms) using the Hartree Fock (HF) variational approximation. However this approach is known to be seriously flawed in several important cases. For example, while the HF spin density wave is energetically favorable for \( U > 0 \) at half filling, it breaks spin symmetry too readily in one and two dimensions, in violation of the Mermin Wagner theorem. This implies that Fock states might be too restrictive as a variational basis. We can illustrate this point using a simple toy model: the Hubbard model on two sites. It will also teach us something about onsite interactions and their effect on spin correlations.

1 Two-site Hubbard model

The two-site Hubbard model with two electrons, is

\[ H = -t \sum_{s=\uparrow,\downarrow} \left( c_{1,s}^\dagger c_{2,s} + c_{2,s}^\dagger c_{1,s} \right) + U \sum_{i=1,2} n_{i,\uparrow} n_{i,\downarrow}, \]  

(2)

where we take \( U > 0 \). The total spin \( S = S_1 + S_2 \), commutes with the Hamiltonian, we restrict ourselves to the \( S = 0 \) and \( S = 1 \) subspaces. The singlet subspace is spanned by three states

\[ \frac{c_{1,\uparrow}^\dagger c_{2,\downarrow}^\dagger - c_{1,\downarrow}^\dagger c_{2,\uparrow}^\dagger}{\sqrt{2}} |0\rangle, \quad c_{1,\uparrow}^\dagger c_{1,\downarrow}^\dagger |0\rangle, \quad c_{2,\uparrow}^\dagger c_{2,\downarrow}^\dagger |0\rangle. \]  

(3)

In this subspace, the Hamiltonian is

\[ H_{S=0} = \begin{pmatrix} 0 & \sqrt{2}t & \sqrt{2}t \\ \sqrt{2}t & U & 0 \\ \sqrt{2}t & 0 & U \end{pmatrix}. \]
Figure 1: Noninteracting ($U=0$) eigenstates of the two-site Hubbard model. The ground state is the “two electron Fermi sea”.

Diagonalizing the Hamiltonian in the singlet sector, one gets

$$H_{S=0} \rightarrow \begin{pmatrix} (U - \sqrt{U^2 + 16t^2})/2 & 0 & 0 \\ 0 & U & 0 \\ 0 & 0 & (U + \sqrt{U^2 + 16t^2})/2 \end{pmatrix},$$

which, in the strong coupling limit ($U \gg t$) is

$$H_{S=0} \underset{U\gg t}{\rightarrow} \begin{pmatrix} -4t^2/U & 0 & 0 \\ 0 & U & 0 \\ 0 & 0 & U + 4t^2/U \end{pmatrix}.$$

The triplet subspace is spanned by the states:

$$\frac{1}{\sqrt{2}} \left( \left| \uparrow\downarrow_1, \downarrow\uparrow_2 \right> - \left| \downarrow\uparrow_1, \uparrow\downarrow_2 \right> \right), \quad \frac{1}{\sqrt{2}} \left( \left| \uparrow\downarrow_1, \downarrow\uparrow_2 \right> + \left| \downarrow\uparrow_1, \uparrow\downarrow_2 \right> \right).$$

which all have zero energy.

The comparison of the spectrum and wave functions of the non-interacting case and the strong coupling limit is displayed in Figs. 1 and 2.

The non-interacting groundstate is the two-site version of the Hartree-Fock two electron “Fermi sea”. This state, and the lowest excited multiplet, contain sizeable contributions from the doubly occupied singlets

$$\frac{1}{\sqrt{2}} \left( \left| \uparrow\downarrow_1, 0 \right>, \quad \left| 0, \uparrow\downarrow_2 \right> \right).$$
The Hubbard interaction pushes these states to energies of order $U$. At strong coupling therefore, the ground state becomes a valence bond singlet, of singly occupied sites with no charge fluctuations. It also cannot be expressed, even approximately, as a Fock state.

The lessons to be learned from this toy model is that repulsive interactions can

- enhance magnetic correlations,
- reduce double occupancies in the ground state,
- separate spin and charge excitations.

## 2 Renormalization to Low Energy Subspace

Low temperature phases and their interesting DC transport properties, are determined by the ground state and low energy excitations. This chapter is slightly formal, as it shows what is precisely meant by the Renormalization Group (RG) transformation which replaces an orginal non diagonal Hamiltonian with an effective one for a lower energy subspace. Let us consider any Hamiltonian written as

$$H = H_0 + V,$$  \hspace{1cm} (6)
where $H_0$ is diagonal and $V$ is a non diagonal perturbation. We define the Hilbert space using the eigenstates of $H_0$, and $P_0(\Lambda)$ is projector onto the subspace with energies less than $\Lambda$.

The resolvent operator, $G = (E - H)^{-1}$, projected onto the latter subspace is given by a well known matrix inversion identity [1]

$$G_{00}(E) = P_0 G(E) P_0 =$$

$$= P_0 \left( \begin{array}{cc} E - P_0(H_0 + V)P_0 & \frac{P_0 V(1 - P_0)}{(1 - P_0)(E - (H_0 + V))(1 - P_0)} \\ (1 - P_0)V P_0 & \frac{P_0 V(1 - P_0)}{(1 - P_0)(E - (H_0 + V))(1 - P_0)} \end{array} \right)^{-1} P_0 =$$

$$= \left\{ \begin{array}{c} E - P_0(H_0 + V)P_0 - \\ \end{array} \right.$$  

$$- P_0 V(1 - P_0) [(1 - P_0)(E - (H_0 + V))(1 - P_0)]^{-1} (1 - P_0) V P_0 \right\}^{-1} \equiv \left( E - \mathcal{H}_{eff}(E) \right)^{-1} , \quad (7)$$

where the last equality defines the effective Hamiltonian $\mathcal{H}_{eff}(E)$. Then the spectrum of $H$, which corresponds to states with non-zero weights in the subspace considered, is given by the zeros of the characteristic polynomial of $\mathcal{H}_{eff}(E)$,

$$\det (E_n - \mathcal{H}_{eff}(E_n)) \quad (8)$$

that is by the poles of the function $\text{Tr} G(E)_{00}$. The effective Hamiltonian can be also written as

$$\mathcal{H}_{eff}(E) = P_0 \left\{ (H_0 + V) + V(1 - P_0) \times \right.$$  

$$\times \left[ (1 - P_0) \left(1 - (E - H_0)^{-1} V(1 - P_0) \right) \right]^{-1} (1 - P_0)(E - H_0)^{-1} V \right\} P_0 =$$

$$= P_0 \left\{ (H_0 + V) + V \sum_{n=1}^{\infty} \left[ \frac{1 - P_0}{E - H_0} V \right]^{n} \right\} P_0 . \quad (9)$$

If $P_0$ projects onto the ground state manifold of $H_0$, Eq. (9) defines the Brillouin-Wigner perturbation theory [1]. For two cut-off energies $\Lambda' < \Lambda$, Eq. (10) is a Renormalization Group transformation

$$\mathcal{H}(\Lambda) \rightarrow \mathcal{H}(\Lambda') = H_0(\Lambda') + V(\Lambda') \quad (10)$$

where

$$\mathcal{H}(\Lambda') = P(\Lambda') \left\{ \mathcal{H}(\Lambda) - V(\Lambda) \sum_{n=1}^{\infty} \left[ \frac{1 - P(\Lambda')}{E - H_0(\Lambda)} V(\Lambda) \right]^{n} \right\} P(\Lambda') . \quad (11)$$

\footnote{Note that the sum $\sum_{n=1}^{\infty}$ in Eq. (11) does not correspond to a perturbation series for the ground state energy, since the terms depend on $E$.}
After doing the best job we can to evaluate $\mathcal{H}(\Lambda')$ (it is clear one needs to truncate the infinite sum and do something about the energy dependence of the denominators), the terms separate naturally into a diagonal operator $H_0$ and residual interactions $V(\Lambda')$. Sometimes we are lucky, and complicated terms of $V(\Lambda')$ become relatively smaller as $\Lambda'$ is reduced. These are called *irrelevant interactions* which scale to zero. We end this section by remarking that the RG transformation should preserve all the symmetries of the Hamiltonian. If $\mathcal{H}$ has explicit symmetry-breaking terms, those terms may grow or shrink under the RG transformation rendering the low energy correlations less or more symmetrical, as the case may be.

3 From Hubbard to $t-J$ and Heisenberg Models

As an explicit derivation of an effective Hamiltonian outlined in Sec. 2, we consider the Hubbard model $\mathcal{H} = T + U$ of Eq. (1) in the strong coupling regime ($U/t \gg 1$). The diagonal part $H_0$ we choose as $U$, the onsite interactions. This term divides the Fock space into two subspaces, the singly occupied and empty sites configurations

$$S = \{ |n_{1,\uparrow}, n_{1,\downarrow}, n_{2,\uparrow}, n_{2,\downarrow}, \ldots \rangle / \forall i, n_{i,\uparrow} + n_{i,\downarrow} \leq 1 \},$$

and configurations with one or more doubly occupied sites

$$D = \{ |n_{1,\uparrow}, n_{1,\downarrow}, n_{2,\uparrow}, n_{2,\downarrow}, \ldots \rangle / \exists i, n_{i,\uparrow} + n_{i,\downarrow} = 2 \}.$$

The hopping term $T$ couples the $S$ and $D$ subspaces by moving an electron into, or out of, a doubly occupied state. We define $P_0$ to project onto the ground state manifold of subspace $S$, and thus

$$G_{00}(E) = P_0 G(E) P_0 = (E - \mathcal{H}_{eff}(E))^{-1},$$

where the effective Hamiltonian $\mathcal{H}_{eff}$, is given by Eq. (7)

$$\mathcal{H}_{eff}(E) = P_0 T P_0 + P_0 T \left[ (1 - P_0)(E - (U + T))(1 - P_0) \right]^{-1} T P_0.$$

In the strong coupling limit, expanding the effective Hamiltonian to zeroth order in $E/U$ and to second order in $t/U$ one gets

$$\mathcal{H}_{eff}(E) \xrightarrow{t/U \ll 1} \mathcal{H}^{t-J},$$

$$\mathcal{H}^{t-J} = P_0 \left( T - \frac{t^2}{U} \sum_{i,j,k,s,s'} c_{i,s}^\dagger c_{j,s} n_{j,\uparrow} n_{j,\downarrow} c_{j,s'}^\dagger c_{k,s'} \right) P_0,$$
i.e., the low energy excitations of the Hubbard model are described by the Hamiltonian of the so called \( t - J \) model.

The fermion operators appearing in Eq. (17), can be rearranged in the following way:

\[
\mathcal{H}_{t - J} = P_0 \left( T + T' + \mathcal{H}^H \right) P_0 ,
\]

\[
T' = -\frac{t^2}{2U} \sum_{i,j,k} \left[ \sum_s c_{i,s}^\dagger c_{k,s} n_j - c_{i,s}^\dagger \vec{\sigma} c_{k,s} \cdot c_{j,s} \right] ,
\]

\[
\mathcal{H}^H = \frac{J}{2} \sum_{\langle i,j \rangle} \left( \mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right) ,
\]

where \( J = 4t^2/U \) and the \( S = 1/2 \) spin operators \( \mathbf{S}_i \) are

\[
S_i^\alpha = \frac{1}{2} \sum_{s,s'} c_{i,s}^\dagger \sigma_{s,s'}^\alpha c_{i,s'} ,
\]

\( \sigma^\alpha \) being the Pauli matrices.

At half filling, i.e., when \( n_i = 1 \), \( P_0 \) annihilates \( T \) and \( T' \) since there can be no hopping processes within subspace \( S \) when there are no empty sites. The transport of charge is prevented by an energy gap of order \( U \). This is the Mott insulator, which describes the undoped (parent compounds) of the high \( T_c \) superconductors of the cuprate family.

In this limit, the \( t-J \) model simply reduces to the spin \( S = 1/2 \) Heisenberg model

\[
\mathcal{H}_{t - J} \to \frac{J}{2} \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \text{const.}
\]

As in the two site Hubbard model of two electrons (see Sec.3), the low energy excitations are purely magnetic.

4 The Negative-U Hubbard Model

The negative-U Hubbard model describes local attractive interactions between electrons which could be produced by several microscopic mechanisms e.g., phonons, plasmons or spin fluctuations. We choose, for convenience to write the model as follows

\[
\mathcal{H}^{-U} = -t \sum_{\langle i,j \rangle,s} c_{i,s}^\dagger c_{j,s} - \frac{U}{2} \sum_i (n_i - 1)^2 +
\]

\[
+ \frac{1}{2} \sum_{\langle i,j \rangle} V_{ij}(n_i - 1)(n_j - 1) - \mu \sum_i n_i ,
\]
where the negative-U term favors pairs of electrons on the same site in competition with the hopping term which delocalizes the electrons; $V_{ij}$ is intersite Coulomb interactions and $\mu$ the chemical potential. The following canonical transformation

$$c_{i,\uparrow} \rightarrow \tilde{c}_{i,\uparrow}, \quad (24)$$

$$c_{i,\downarrow} \rightarrow \tilde{c}_{i,\downarrow}^\dagger, \quad (25)$$

maps the negative-U to a positive-U Hamiltonian:

$$H^{-U} \rightarrow H^{+U} = -t \sum_{\langle i,j \rangle} (\tilde{c}_{i,\uparrow}^\dagger \tilde{c}_{j,\uparrow} - \tilde{c}_{i,\downarrow}^\dagger \tilde{c}_{j,\downarrow}) + \frac{U}{2} \sum_i (\tilde{n}_i - 1)^2 +$$

$$+ \frac{1}{2} \sum_{i,j} J^x_{ij} \tilde{S}_i^x \tilde{S}_j^x - h \sum_i \tilde{S}_i^z - N(\mu + \frac{U}{2}), \quad (26)$$

where

$$J^z_{ij} = 4V_{ij}, \quad (27)$$

$$h = 2\mu, \quad (28)$$

$$\tilde{S}_i^z = \frac{1}{2}(\tilde{n}_i - 1), \quad (29)$$

and $N$ is the total number of sites.

Following the derivations of Sec. 3 and using the fact that $H^{+U}$ is at half filling (for a proof see Sec. 3.3.1 in [3]), this model at large $|U|/t$ can be directly mapped onto an effective pseudospin model

$$H^{+U} \rightarrow H^{-x-xz} + O(t^2/U)$$

$$H^{-x-xz} = \frac{1}{2} \sum_{i,j} \left[ J^z_{ij} \tilde{S}_i^z \tilde{S}_j^z - J^x_{ij} (\tilde{S}_i^x \tilde{S}_j^x + \tilde{S}_i^y \tilde{S}_j^y) \right] - \sum_i h_i \tilde{S}_i^z \quad (30)$$

where the pseudospin operators are

$$\tilde{S}_i^z = \frac{1}{2}(\tilde{n}_i - 1)$$

$$\tilde{S}_i^x = \frac{1}{2}(\tilde{c}_{i,\uparrow}^\dagger \tilde{c}_{i,\downarrow}^\dagger + \tilde{c}_{i,\downarrow} \tilde{c}_{i,\uparrow})$$

$$\tilde{S}_i^y = \frac{1}{2i}(\tilde{c}_{i,\uparrow}^\dagger \tilde{c}_{i,\downarrow} - \tilde{c}_{i,\downarrow} \tilde{c}_{i,\uparrow}). \quad (31)$$

We see that the local charge operator and the pair operator have the same commutation relations as angular momenta along the $z$-axis and $xy$ plane respectively. The quantum properties of the pseudospins explains Josephson commutation relation between charge and superconducting phase, $[N, \phi] = 1$. 


At weak coupling $|U|/t < 1$, it can be also argued that the negative-$U$ model renormalizes onto a similar effective model as (30) albeit with different lattice constant and interaction parameters. The Fermi sea is unstable with respect to attractive interactions as seen diagrammatically by the divergence of the vertex function in the BCS or charge density wave channels. Since the attractive interaction scales to strong coupling, at the scale where the cut-off energy equals the BCS gap, the effective Hamiltonian can be transformed to the $-x$-$xz$ model to obtain the strong coupling fixed point Hamiltonian. This procedure however, has not yet been carried out, to the best of our knowledge.

In Lecture III, we shall use the classical $\mathcal{H}^{-x}$-$xz$ model to describe superconductivity, and charge density wave phases.
Part II
Quantum Magnetism

This lecture is technical in nature. It contains a brief review of the spin path integral and how to obtain the classical and semiclassical approximations to it. A fuller background for this subject, with compatible notations, can be found in Ref.\[2\]. Here, a new emphasis is placed on anisotropic models and their rotator representation.

5 Spin Coherent States

Path integrals provide formal expressions which can lead to useful approximation schemes. A path integral representation of spin models can be constructed using spin coherent states. Let us consider the eigenstates $|S, m\rangle$ of $S^2$ and $S^z$ with eigenvalues $S(S+1)$ and $m$, respectively. Spin coherent states are a family of spin states labelled by a unit vector $\hat{\Omega} = (\theta, \phi)$, where $\theta$ and $\phi$ are the latitude and longitude angles respectively. They are defined by applying the SU(2) rotation operator to the highest weight state in representation $S$:

$$|\tilde{\Omega}\rangle_S = e^{i\phi S^z} e^{i\theta S^y} e^{-i\phi S^z} |S, S\rangle$$

$$= e^{-iS\phi} \sqrt{(2S)!} \sum_{m=-S}^{+S} \frac{u(\theta, \phi)^{S+m} v(\theta, \phi)^{S-m}}{\sqrt{(S+m)!(S-m)!}} |S, m\rangle , \quad (32)$$

with

$$u(\theta, \phi) = \cos (\theta/2) e^{i\phi/2} \quad (33)$$

$$v(\theta, \phi) = \sin (\theta/2) e^{-i\phi/2} \quad (34)$$

Using Eq. (32), two useful identities can be readily proven:

- The resolution of identity

$$\frac{2S+1}{4\pi} \int_{-1}^{1} d\cos \theta \int_{0}^{2\pi} d\phi \ |\tilde{\Omega}\rangle \langle \tilde{\Omega}| = \sum_{m=-S}^{+S} |S, m\rangle \langle S, m| = I_S \quad (35)$$

- The overlap of two states with closeby unit vectors

$$\langle \tilde{\Omega}|\tilde{\Omega}'\rangle \simeq \left(1 + \hat{\Omega} \cdot \hat{\Omega}'\right)^{S} e^{(iS(1-\cos \bar{\theta})(\phi - \phi'))} \quad (36)$$

where $\bar{\theta}$ is the average latitude of the two vectors.

\[2\]The phase $e^{-iS\phi}$ represents a gauge choice with one singularity on the sphere: at the south pole.
6 Spin Path Integral

The partition function of a single spin with Hamiltonian $H$ is

$$Z = Tr[e^{-\beta H}] = Tr\left(e^{-\epsilon H}e^{-\epsilon H} \ldots e^{-\epsilon H}\right),$$

(37)

with $\beta = 1/T$, $T$ being the temperature. By inserting $N_\epsilon - 1$ resolutions of the identity (35), and in the limit $\epsilon \rightarrow 0$, by expanding each exponential to first order, one gets

$$Z \simeq \int d\tilde{\Omega}_1 \ldots d\tilde{\Omega}_N \prod_{n=0}^{N_\epsilon - 1} \langle \tilde{\Omega}(\tau_n) \left| 1 - \epsilon H | \tilde{\Omega}(\tau_{n+1}) \right\rangle,$$

(38)

with the boundary condition $\tilde{\Omega}_0 = \tilde{\Omega}_N$. In the limit $N_\epsilon \rightarrow \infty$ (and $\epsilon \rightarrow 0, \beta = N_\epsilon \epsilon = \text{const}$.) Eq. (38) defines a path integral

$$Z = \oint D\tilde{\Omega}(\tau) \exp \left[-\int_0^\beta d\tau \left(i S(1 - \cos \theta(\tau))\dot{\phi}(\tau) + H[\tilde{\Omega}(\tau)]\right)\right],$$

(39)

The time dependent term in Eq. (39)

$$i S \omega [\tilde{\Omega}] = i S \int_0^\beta d\tau (1 - \cos \theta) \dot{\phi}$$

(40)

derives from the overlap between coherent states (36). It is known as the Berry phase of the spin history and it is geometric, i.e., depends on the trajectory of $\tilde{\Omega}(\tau)$ on the unit sphere. In fact it measures the area enclosed by the path $\tilde{\Omega}(\tau)$ on the unit sphere (Fig. 3).

The classical Hamiltonian is defined as

$$H[\tilde{\Omega}(\tau)] = \langle \tilde{\Omega}(\tau) \left| H \right| \tilde{\Omega}(\tau) \rangle.$$

(41)

An implicit assumption in Eq. (39) is that the path integral is dominated by smooth (differentiable) paths. This turns out to be unjustified, since discontinuous paths matter for the correct ordering of quantum operators. For that reason, path integral results should be checked whenever possible against operator methods. Ordering ambiguities give rise to erroneous quantum corrections to energies and local spin correlations. They do not effect, however, long distance and long timescale correlation functions.

The partition function for a system of $N$ spins is

$$Z = \oint D\tilde{\Omega}_1(\tau) \exp \left[i S \sum_{i=1}^N \omega[\tilde{\Omega}_i] - \int_0^\beta d\tau H[\{\tilde{\Omega}_i(\tau)\}]\right].$$

(42)
Figure 3: The Berry phase $\omega[\hat{\Omega}]$ measures the area enclosed by the trajectory of $\Omega(\tau)$ on the unit sphere which does not include the south pole.

For example, the nearest neighbor Heisenberg model partition function is

$$Z_H = \oint D\hat{\Omega} \exp \left[ iS \sum_{i=1}^{N} \omega[\hat{\Omega}_i] - \frac{J}{2} \int_0^\beta \sum_{(i,j)} \hat{\Omega}_i \cdot \hat{\Omega}_j \right].$$  \hspace{1cm} (43)

The spin coherent states path integral (42) are convenient starting points for deriving semiclassical, i.e. large $S$, approximations. The integration variables are unit vectors, i.e. classical spins. The quantum effects enter through their time dependent fluctuations. Keeping $JS^2 \rightarrow J$ fixed and sending $S \rightarrow \infty$, suppresses the contributions of fluctuating paths with $\dot{\hat{\Omega}} \neq 0$. This leaves integration over frozen spin configurations precisely as in the classical partition function

$$Z \xrightarrow{S \rightarrow \infty} \int \prod_{i=1}^{N} d\hat{\Omega}_i e^{-\beta H\{\hat{\Omega}_i\}}.$$  \hspace{1cm} (44)

Now it is possible to use $S$ as the control parameter for a systematic expansion of the partition function. In particular, applying the saddle point approximation (analytically continued to real time $t = i\tau$) yields

$$S \frac{\delta \omega[\hat{\Omega}_i]}{\delta \hat{\Omega}_i} - \int_0^t dt \frac{\delta H}{\delta \hat{\Omega}_i} = 0,$$  \hspace{1cm} (45)

which are the *Euler-Lagrange* equations of motion for classical spins

$$S\dot{\hat{\Omega}}_i^c(t) \times \hat{\Omega}_i^c(t) = \frac{\partial}{\partial \hat{\Omega}_i} H \left\{ \{\hat{\Omega}_j^c\} \right\}.$$  \hspace{1cm} (46)
7 Spin Wave Theory

When spin symmetry is broken, either spontaneously or by explicit symmetry breaking terms, it is quite natural to use the semiclassical expansion of the path integral. We consider small fluctuations around a classical spin configuration, $\hat{\Omega}_i^{\text{cl}}$ which minimizes $H[\Omega]$.

$$\hat{\Omega}_i(\tau) = \hat{\Omega}_i^{\text{cl}} + \delta \hat{\Omega}_i(\tau).$$  

(47)

To leading gaussian order, the partition function is approximated by

$$Z \simeq e^{-\beta H[\hat{\Omega}^{\text{cl}}]} \int D\delta \hat{\Omega}(\tau) \exp \left[ i S \sum_{i=1}^{N} \delta^2 \omega[\hat{\Omega}_i] - \int_0^\beta d\tau \delta^2 H[\{\hat{\Omega}_i(\tau)\}] \right],$$

(48)

where

$$\delta^2 \omega[\hat{\Omega}_i] = \frac{1}{2} \sum_{i=1}^{N} \int_0^\beta d\tau \hat{\Omega}_i \cdot \delta \hat{\Omega}_i \times \delta \hat{\Omega}_i,$$

$$\delta^2 H[\hat{\Omega}_i] = \frac{1}{2} \sum_{(i,j)} \frac{\delta \hat{\Omega}_i}{\delta \hat{\Omega}_i} \frac{\delta^2 H[\{\hat{\Omega}_i\}]}{\delta \hat{\Omega}_j \delta \hat{\Omega}_j} \delta \hat{\Omega}_i \delta \hat{\Omega}_j.$$

(49)

$\delta \hat{\Omega}_i$, which are perpendicular to $\hat{\Omega}_i$ can be projected onto the two tangential unit vectors which defines the harmonic oscillator degrees of freedom

$$q_i = \delta \hat{\Omega}_i \cdot \hat{\phi}_i,$$

$$p_i = S \delta \hat{\Omega}_i \cdot \hat{\theta}_i.$$

(50)

(51)

These variables can be used to represent the gaussian fluctuations as

$$Z \simeq e^{-\beta H[\hat{\Omega}^{\text{cl}}]} \int Dp_i Dq_i \exp \left[ \int_0^\beta d\tau \left( \frac{\dot{p}_i \cdot \dot{q}_i - \dot{p}_i \cdot \dot{q}_i}{2} - \frac{1}{2} (q, p) H^{(2)} (q, p) \right) \right],$$

(52)

where $H^{(2)}$ is a dynamical matrix of coupled harmonic oscillators

$$H^{(2)} = \begin{pmatrix} K & P \\ P^t & M^{-1} \end{pmatrix},$$

(53)

where

$$K_{ij} = \frac{\partial^2 H}{\partial q_i \partial q_j} \bigg|_{q=p=0},$$

$$M_{ij}^{-1} = \frac{\partial^2 H}{\partial p_i \partial p_j} \bigg|_{q=p=0}. $$

(54)

(55)
are the force constant and reciprocal mass matrices respectively and

\[ P_{ij} = \left. \frac{\partial^2 H}{\partial p_i \partial q_j} \right|_{q=p=0}, \]  
(56)

couples coordinates and momenta. Eq. (52) is the harmonic spin wave partition function of any quantum spin Hamiltonian, whose classical ground state is known. By diagonalizing its action one readily obtains the spin wave excitation energies and wavefunctions, and spin correlations can be evaluated to the sub-leading order in \( S^{-1} \). The complexity of the calculation depends on the lattice symmetry of the classical ground state, i.e. such as the size of its magnetic unit cell. For example, for the Néel state, it is two lattice unit cells.

For completeness, we work out the spin wave dispersion of the antiferromagnetic Heisenberg model with a Néel state given by

\[ (\theta_i^c, \phi_i^c) = \begin{cases} (\frac{\pi}{2}, 0) & i \in A \\ (\frac{\pi}{2}, \pi) & i \in B \end{cases} \]  
(57)

where \( A \) and \( B \) are the two sublattices in which the lattice can be divided. The harmonic degrees of freedom are

\[ q_i(t) = \begin{cases} \phi_i(t) & i \in A \\ \pi + \phi_i(t) & i \in B \end{cases} \]  
(58)

and

\[ p_i(t) = S \cos \theta_i(t). \]  
(59)

The dynamical matrix of the model (43) is

\[ H^{(2)} = \frac{J}{2} \sum_{\langle i,j \rangle} \left[ \left( \frac{p_i - p_j}{S^2} \right)^2 - (q_i - q_j)^2 \right] = \right. \]

\[ = \frac{1}{2} \sum_k (p_k, q_k) \begin{pmatrix} zJ(1 + \gamma_k) & 0 \\ 0 & zJS^2(1 - \gamma_k) \end{pmatrix} \begin{pmatrix} p_k \\ q_k \end{pmatrix}, \]  
(60)

where

\[ \gamma_k = \frac{1}{z} \sum_d e^{i\mathbf{k} \cdot \mathbf{d}}, \]  
(61)

\( z \) and \( \mathbf{d} \) being respectively the coordination number and the vector connecting one site to its nearest-neighbours. The dispersion relation of the small fluctuations around the ground state configuration, i.e., of the spin waves, can be found solving the characteristic equation

\[ \det \begin{pmatrix} S^{-2}zJ(1 + \gamma_k) & i\omega_k \\ -i\omega_k & zJ(1 - \gamma_k) \end{pmatrix} = 0, \]  
(62)

and \( \omega_k = \frac{1}{S} z J \sqrt{1 - \gamma_k^2}, \) for two distinct spin wave modes.
8 Continuum Theory for Anisotropic Models

Spin wave theory is restricted to the ordered phases of the Heisenberg model. However, one can still use a semiclassical approach even in the absence of spontaneously broken symmetry. A short range classical Hamiltonian is mostly sensitive to short-range correlations. Thus the Heisenberg Hamiltonian, in the large $S$ limit, has at least short range antiferromagnetic order. In the path integral approach it is possible to utilize the short lengthscale correlations to define a continuum theory without assuming broken symmetry.

In this section we spend some time preparing the ground for Lecture II. To that end, we derive the continuum theory for the anisotropic $xxz$ model in a magnetic field. The resulting path integral will be later used in the context of quantum properties of superconductors. The continuum theory is shown to be equivalent to SO(3) quantum rotators. The rotator formulation is readily generalizable to SO(5) symmetry, which is the topic of section 14. Subsequently, for the isotropic case we review Haldane’s mapping of the quantum Heisenberg antiferromagnet in $d$ dimensions into the nonlinear sigma model (NLSM) in $d+1$ dimensions, and the main results which can be obtained by that mapping.

The first step is to parametrize the spins using two continuous vector fields $\hat{n}$ and $\vec{L}$,

$$\hat{\Omega}_i^\alpha = \eta_i \hat{n}^\alpha(\vec{x}_i) - \frac{1}{S} \frac{\vec{L}(\vec{x}_i)}{S},$$

where $\eta_i = e^{i\pi \cdot \vec{x}_i}$ has opposite signs on the two sublattices. Each pair of neighboring spins (4 degrees of freedom) is replaced by $\hat{n}$, $\vec{L}$. We can choose $\hat{n}$ to be a unimodular ($|\hat{n}|^2 = 1$) Néel field (2 degrees of freedom), and $\vec{L}$ is the perpendicular canting field, with the constraint $\vec{L} \cdot \hat{n} = 0$ (2 degrees of freedom). The spin measure of Eq. (42) becomes

$$D\hat{\Omega} \rightarrow D\hat{n}D\vec{L}\delta\left(\vec{L} \cdot \hat{n}\right)$$

where the $\delta$ functionals are local space-time constraints.

Let us consider a general anisotropic spin model in a magnetic field $\vec{h}$,

$$\mathcal{H} = \frac{1}{2} \sum_{ij,\alpha} J_{ij}^\alpha \hat{\Omega}_i^\alpha \hat{\Omega}_j^\alpha - \vec{h} \cdot S \sum_i \hat{\Omega}_i.$$  

Using (63) and expanding to lowest order in $L^\alpha$, $\partial_i n^\alpha$ and $\partial_i L^\alpha$ we obtain the energy density

$$\mathcal{H} \rightarrow \int d^d x \left[ L, \hat{n} \right]$$

$$H = E^{cl}[n] + \frac{1}{2} \sum_\alpha \left( \lambda_\alpha^{-1} (L^\alpha)^2 + \rho_\alpha^2 (\partial_i n^\alpha)^2 \right) - a^{-d} \vec{n} \cdot \vec{L},$$

(66)
where the energy, spin stiffness, and susceptibility parameters are respectively:

\[
E^{cl}[n] = - \frac{1}{2Na^d} \sum_{\alpha} (n^\alpha)^2 \left( \sum_{ij} J_{ij}^\alpha \eta_i \eta_j \right),
\]

\[
\rho^\alpha = \frac{1}{2dNa^d} \sum_{ij} J_{ij}^\alpha \eta_i \eta_j |\vec{x}_i - \vec{x}_j|^2,
\]

\[
\frac{1}{\chi^\alpha} = \frac{2S^{-2}}{Na^d} \left( \sum_{ij} J_{ij}^\alpha \right) - 2S^{-2}E^{cl}
\]

(67)

\(a\) and \(N\) are the lattice constant and size respectively. Expansion of the Berry phase term to the same order yields two terms

\[
iS \sum_i \omega \left[ \Omega_i \right] = -i\Upsilon + i \int_0^\beta d\tau \int d^d x \hat{n} \times \dot{\hat{n}} \cdot \vec{L},
\]

(68)

where

\[
\Upsilon(\hat{n}) = S \int d^d x e^{i\vec{\pi} \cdot \vec{x}} \omega(\hat{n}(\vec{x})).
\]

(69)

Collecting the terms together, we have the path integral

\[
Z_{x=0} = \int D\hat{n} D\vec{L} \delta(\vec{L} \cdot \hat{n}) e^{-i\Upsilon} \exp \left( \int d\tau d^d x i\hat{n} \times \dot{\hat{n}} \cdot \vec{L} - H[\vec{L}, \hat{n}] \right).
\]

(70)

9 Anisotropic Quantum Rotators

Eq. (70) can be physically understood as a path integral of rotators. Consider the phase space path integral over an \(N\)-dimensional field \(\hat{n}\), and canonical momenta \(\vec{p}\) with a “Mexican hat” potential

\[
Z_{K \to \infty} \propto \int D\hat{n} \exp \left( \int d\tau d^d x i\hat{n} \cdot \vec{p} - \tilde{H}[\vec{p}, \hat{n}] \right).
\]

(71)

If \(K\) is taken to be very large, fluctuations of \(\delta \hat{n} = |\vec{n}| - 1\), and its conjugate momentum \(\vec{p}_\parallel\) become high frequency harmonic oscillators, which can be integrated out in the adiabatic approximation. This leaves us with the slow degrees of freedom \(\hat{n} = \vec{n}/|\vec{n}|\), and \(\vec{p}_\perp\), and a renormalized Hamiltonian

\[
Z_{K \to \infty} \propto \int D\hat{n} \exp \left( \int d\tau d^d x i\hat{n} \cdot \vec{p}_\perp - \tilde{H}[\vec{p}_\perp, \hat{n}] \right).
\]

(72)
A Faddeev-Jackiw quantization of a particle on an N-sphere leads to the same constraints, as shown in Ref. [3].

For the N=3 model, the angular momenta and the transverse momenta are both vectors, related by

\[ \vec{L} = \hat{n} \times \vec{p}_\perp, \quad \vec{p}_\perp = \vec{L} \times \hat{n}. \] (73)

A change of variables \( \vec{p}_\perp \rightarrow \vec{L} \) has a unit Jacobian

\[ D\vec{p}\delta(\vec{p} \cdot \hat{n}) = D\vec{L}\delta(\vec{L} \cdot \hat{n}). \] (74)

Substituting (73) and (74) into (72) yields a path integral of the form (70), without the Berry phase \( e^{-i\Upsilon} \).

For general \( N \), the \( N(N-1)/2 \) angular momenta are defined as

\[ L_{ab} \equiv n_a p_b - n_b p_a, \quad a, b = 1, \ldots, N. \] (75)

Note, that it is not useful for \( N > 3 \) to write the path integral measure in terms of \( L_{ab} \), because they are not independent degrees of freedom, and more constraints are required. On the other hand, the transverse momenta, which obey \( \sum_a n_a(p_\perp)_a = 0 \), can be expressed as

\[ (p_\perp)_a = \sum_b L_{ab} n_b. \] (76)

Therefore it is always possible to express the rotator Hamiltonian \( \tilde{H}^{rot} \) of (72) in terms of \( L_{ab} \) and \( \hat{n} \).

The opposite direction, might be even more useful. For example, as in Eq. (66), the starting point could be a Hamiltonian whose kinetic energy is expressed using symmetry generators

\[ H^{rot}[\vec{L}, \hat{n}] = E^{cl}[\hat{n}] + \frac{1}{2} \sum_{a < b} \chi^{-1}_{ab} L_{ab}^2 + \frac{1}{2} \sum_a \rho^a_s (\partial_i n_a)^2 \]

\[ - a^{-d} \sum_{a < b} h_{ab} L_{ab}, \] (77)

where \( h_{ab} \) and \( \chi_{ab} \) are SO(N) fields and susceptibilities respectively. (For SO(3) their vector notation is given by \( X^a \equiv \sum_{bc} \epsilon^{abc} X_{bc} \)). Substituting (77) into \( H^{rot} \) yields

\[ H^{rot}[\vec{p}, \hat{n}] = E^{cl}[\hat{n}] + \frac{1}{2} \sum_{ab} M^{-1}_{ab} p_a p_b \]

\[ + \sum_a \rho^a_s (\partial_i n_a)^2 - a^{-d} \sum_{a < b} h_{ab} (n_a p_b - n_b p_a), \]

\[ M^{-1}_{ab} \equiv \delta_{ab} \left( \sum_c \chi^{-1}_{ac} n_c^2 \right) - \chi^{-1}_{ab} n_a n_b \] (78)
where $M[\hat{n}]$ is an anisotropic “mass” matrix in the Cartesian basis.

We note that by (78), the path integral (72) is Gaussian in momenta $p_a$. One must be careful and integrate only over the transverse components to $\hat{n}$. For a given direction $\hat{n}$, we choose the transverse basis $\hat{e}_i$, $i = 1, N - 1$ which obeys the following conditions

$$\hat{e}_i \cdot \hat{n} = 0, \quad i = 1, N - 1$$

$$\sum_{a,b}^{N} \hat{e}_i^a M^{-1}_{ab} \hat{e}_j^b = \delta_{ij} \tilde{M}_{\hat{n}}^{-1}[\hat{n}] .$$

(79)

This is always possible since the first condition leaves the freedom to perform an SO(N-1) rotation on the transverse basis. For an arbitrary transverse basis $\{\hat{f}_i\}$, we find the rotation which diagonalizes $\hat{f}_i M^{-1} \hat{f}_j$, and the resulting eigenbasis is chosen as $\{\hat{e}_i\}$.

Thus, we parametrize

$$\vec{p} = \sum_i p_i \hat{e}_i$$

and integrate unrestrictedly over $\int D\hat{n}$ to obtain

$$Z = \int D\hat{n} \exp \left( - \int_0^\beta d\tau \int d^d x \left( E_{\text{cl}}[\hat{n}] + \sum_{l,a}^{1} \frac{1}{2} \rho^a (\partial_l \hat{n}^a)^2 \right. \right.

$$

$$\left. \left. + \frac{1}{2} \sum_j M_j \left( \hat{n} \cdot \hat{e}_j - i h_j \right)^2 \right) \right)$$

$$h_j \equiv a^{-d} \sum_{a<b} a_{ab} (n_b \hat{e}_j^a - n_a \hat{e}_j^b) .$$

(81)

This expression is ready for the evaluation of the classical (time independent) ground state $\hat{n}^{\text{cl}}$ as a function of applied field $h_{ab}$, and a spinwave expansion about it. In the next section however, we shall only deal with the isotropic case.

### 10 Haldane’s Mapping

We now return to (81) but specialize to the isotropic Heisenberg model without a field, where life simplifies considerably.

The inverse mass matrix is simply

$$M^{-1} = \chi^{-1} \delta_{ab} - n_a n_b .$$

(82)

Any choice of transverse basis $\hat{e}_i$ yields a diagonal $M_i = \chi$ in Eq. (79). Omitting the constant $E_{\text{cl}}$, and inserting the Berry phase $e^{-i\tau[\hat{n}]}$ the partition function
(81) reduces to Haldane’s result

\[ Z = \int D\hat{n} e^{-i\Upsilon(\hat{n})} \exp \left( -\frac{1}{2} \int_0^\beta d\tau \int d^d x (\chi |\hat{n}|^2 + \rho_S \sum_{l=1}^d |\partial_l \hat{n}|^2) \right) = \int D\hat{n} e^{-i\Upsilon(\hat{n})} \exp \left( -\frac{a^{1-d}}{2f} \int d\tau d^d x (\partial_\mu \hat{n})^2 \right), \]  

(83)

where \( x_0 = c\tau \), and \( c = \sqrt{\rho_S/\chi} \) is the spin wave velocity. For the nearest neighbor model with interaction \( J \), one obtains from (67):

\[ \chi = \frac{S^2}{(4dJa^d)}, \]  

(84)

\[ \rho_S = Ja^{2-d}, \]  

(85)

\[ f = \frac{ca^{1-d}}{\rho_S} = 2\sqrt{d}/S. \]  

(86)

Eq. (83) is the partition function for a NLSM with an additional Berry phase term.

In 1 + 1 dimensions the NLSM is disordered for all \( f \), as required by the classical Mermin Wagner theorem. Its correlations are known to fall off exponentially at large distances with a correlation length which goes as \( \xi \propto e^{2\pi/f} \). By the (Lorentz) symmetry of the action between spatial and temporal dimensions, this implies a gap (Haldane’s gap) for all excitations above the ground state. However one should also consider the effects of the phases brought about by the term \( \Upsilon(\hat{n}) \).

For \( d = 1 \), \( \Upsilon(\hat{n}) \) is a topological winding number of the two dimensional NLSM. For all continuous fields, it yields \( e^{-\Upsilon(\hat{n})} = e^{-i2\pi Sk} \) with \( k \) an integer number. Thus, the Berry phase factor is 1 for all integer \( S \), while it can be \( \pm 1 \) for half integer spins. As a result, it produces interference effects for half odd integer spins, and drastically changes the ground state properties and the elementary excitations spectrum of the Heisenberg chain.

In \( d = 2 \) the topological phase is zero for all continuous fields. For the nearest neighbours Heisenberg model, Neves and Perez \[4\] proved that the ground state is ordered for all \( S \geq 1 \). Also, series expansions and numerical simulations provide evidence of the presence of an ordered ground state even for \( S = 1/2 \).

11 Spin Liquid States

For most antiferromagnetic Heisenberg models the ground state is not explicitly known. While for finite bipartite lattices, ground state theorems require the ground state to be a total singlet, and have positivity conditions (Marshall’s signs). The discussion of the previous section expects them to exhibit long range order in two dimensions. Considering these conditions, particularly useful
variational states for the $S = \frac{1}{2}$ antiferromagnetic Heisenberg model are Fazekas and Anderson’s *Resonating Valence Bond* (RVB) states

$$|\{d_\alpha\}\rangle = \sum_\alpha d_\alpha |\alpha\rangle ,$$  \hspace{1cm} (87)

where

$$|\alpha\rangle = \prod_{(i,j) \in \Lambda_\alpha} \frac{1}{\sqrt{2}} \left( |\uparrow_i\rangle |\downarrow_j\rangle - |\downarrow_i\rangle |\uparrow_j\rangle \right) ,$$  \hspace{1cm} (88)

and $d_\alpha$ can be chosen to have the form

$$d_\alpha = \left( \prod_{(i,j) \in \Lambda_\alpha} u_{ij} \right) .$$  \hspace{1cm} (89)

Since the states $|\alpha\rangle$ are not orthogonal to each other, it is not possible to evaluate correlations of RVB states analytically. Monte Carlo simulations of Liang, Doucot and Anderson\cite{6}, and Havilio\cite{7}, have found that the RVB states have long range Néel order for $u_{ij}$ that decay slower than

$$u_{ij} \simeq |x_i - x_j|^{-p}, \ p \leq 3 .$$  \hspace{1cm} (90)

The RVB states Eq.(87) can thus be used as variational ground states for both ordered and disordered phases. This makes them appealing candidates for studying the transitions from the Néel phase to possible quantum disordered phases, particularly in the presence of hole doping\cite{7}. 

Part III
Pseudospins and Superconductivity

The -x-xz model, encountered in Lecture I, will be considered as an effective Hamiltonian for the low temperature, long wavelength properties of s-wave superconductors and charge density waves. Such transitions are observed in e.g. doped bismuthates $\text{Ba}_{1-x}\text{K}_x\text{BiBO}_3$. Recall Eq. (30):

$$
\mathcal{H}_{-x-xz} = \frac{1}{2} \sum_{ij} \left[ J^z_{ij} \hat{S}^z_i \hat{S}^z_j - J^x_{ij} \left( \hat{S}^y_i \hat{S}^y_j + \hat{S}^y_i \hat{S}^y_j \right) \right] - \sum_i h_i \hat{S}^z_i. \quad (91)
$$

\(\hat{S}\) are spin 1/2 operators, and \(h = 2\mu\), where \(\mu\) is the electron chemical potential. As shown later, it can also be used to describe superfluids. In this lecture we use the continuum rotator model, and its classical limit to obtain the phase diagram. The generalization to Zhang’s SO(5) rotators, which describe the collective modes of high $T_c$ cuprates, and the transition from antiferromagnetism to $d$-wave superconductivity, is straightforward. The last section uses the -x-xz model to describe dynamics of vortices in superfluids.

12 Charge Density Wave to Superconductivity

In bipartite lattice with sublattices $A$ and $B$ (e.g. square, simple cubic, etc.), the negative $J^x$ terms of the -x-xz model can be rotated to positive terms by a global $e^{iS^z\pi}$ rotation on sublattice $B$. Obviously, for frustrated (non bipartite) lattices the xxz and the -x-xz models are not equivalent. For example, the triangular, Kagomé, and face centered cubic lattices[8], the -x-xz model prefers to order in the $xy$ plane even when $J^z > |J^x|$ at zero doping[1].

Here we specialize to the classical model on a bipartite (square or cubic) lattice

$$
H = \frac{1}{z} \sum_{\langle i,j \rangle} \left[ J^z_{ij} \tilde{\Omega}^z_i \tilde{\Omega}^z_j - J^x_{ij} \left( \tilde{\Omega}^y_i \tilde{\Omega}^y_j + \tilde{\Omega}^y_i \tilde{\Omega}^y_j \right) \right] - \hbar S \sum_i \tilde{\Omega}^z_i + H_{nnn}
$$

$$
H_{nnn} = \frac{1}{z} \sum_{i,j} K \tilde{\Omega}^z_i \tilde{\Omega}^z_j \quad (92)
$$

---

3This helps to explain superconductivity in $K_3\text{C}_{60}$ which is an FCC compound with a half filled conduction band.
where \( z \) and \( z' \) are nearest neighbor (nn) and next nearest neighbor (nnn) coordination numbers respectively.

By (31) we note that the electron charge expectation value and the superconducting order parameters are

\[
\langle n_i \rangle - 1 = \hat{\Omega}_z^i \\
\langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle = \hat{\Omega}_x^i + i\hat{\Omega}_y^i \\
x = -N^{-1} \sum_i \hat{\Omega}_z^i
\]

(93)

\( x \) is the hole doping concentration away from half filling.

At finite temperatures, molecular mean field theory for \( S = 1/2 \) gives the critical temperatures as a function of doping \( x \) to be

\[
T_c^{CDW}(x) = \frac{1}{4}(J^z - K)(1 - x^2) \\
T_c^{SC}(x) = \frac{J^x x}{4 \text{arctanh}(x)}
\]

(94)

The two curves meet at \( T^* \) (See Fig. 4). This point is tetracritical or bicritical, depending on whether the transition (as a function of field \( h \)) is second or first order respectively. In Fig. 4 this is reflected by the nature of the intermediate region which would be either a mixed (“supersolid”) phase, or phase separation between pure CDW and SC domains respectively. The next section is devoted to determining the criteria for the order of the transition.

Near \( T^* \), the lowest order expansion of the Ginzburg Landau free energy functional has SO(3) symmetry. Thus even though the model might have high...
anisotropy $J^z >> J^x$, near the bicritical point the Heisenberg symmetry is approximately restored. This “symmetry restoring” is also argued to happen near the multicritical point of the anisotropic SO(5) model\(^\text{[10]}\).

13 Order of Transition from Rotator Theory

Finding out the order of the CDW-SC transition at zero $T$, requires the energy of the putative mixed state (M), which interpolates between the pure CDW and pure SC. The rotator partition function (81) comes in handy for that purpose. We write (92) as (65) by letting $-J^x \rightarrow +J^x$, and take the continuum limit with unit lattice constant $a = 1$ following the prescriptions of section 8. The M ground state is parametrized by one Néel angle $\hat{n} = (\sin \theta, \cos \theta)$, where $0 < \theta < \pi/2$. $\theta = 0$, $\theta = \pi/2$ are the pure CDW, SC respectively.

First we evaluate the inverse mass matrix of (78)

$$M^{-1}_{ab} = \begin{pmatrix} \chi^{-1}_y \cos^2 \theta & 0 & 0 \\ -\chi^{-1}_y \cos \theta \sin \theta & \chi^{-1}_y \cos^2 \theta + \chi^{-1}_z \sin^2 \theta & -\chi^{-1}_y \cos \theta \sin \theta \\ 0 & 0 & \chi^{-1}_z \sin^2 \theta \end{pmatrix}.$$  \hspace{1cm} (95)

The transverse vectors which diagonalize the projected inverse mass matrix are $\hat{e}_1 = \hat{y} \times \hat{n}$ and $\hat{e}_2 = \hat{y}$. The mass eigenvalues are

$$\tilde{M} = \begin{pmatrix} \chi_y & 0 & 0 \\ 0 & (\chi^{-1}_y \cos^2 \theta + \chi^{-1}_z \sin^2 \theta)^{-1} & 0 \\ 0 & 0 & \chi_z^{-1} \sin^2 \theta \end{pmatrix}.$$  \hspace{1cm} (96)

Set the lattice constant to unity $a = 1$, using (67) and (92) we obtain

$$h_j = -h \sin \theta \delta_{j,2}$$

$$\chi^{-1}_z(\theta) = \frac{2}{S^2} ((J^z + K) + (J^z - K) \cos^2 \theta + |J^x| \sin^2 \theta)$$

$$\chi^{-1}_y(\theta) = \frac{2}{S^2} (|J^x| + (J^z - K) \cos^2 \theta + |J^x| \sin^2 \theta).$$  \hspace{1cm} (97)

Here we have set the lattice constant to unity $a = 1$. Thus, the classical ground state $\theta^{cl}$ minimizes the energy

$$E^{rot}[\theta, h] = -(J^z - K) \cos^2 \theta - J^x \sin^2 \theta - \frac{1}{2} \sum_{j=1,2} M_j h_j^2$$

$$= -(J^z - K) + (J^z - K - J^x) \sin^2 \theta - \frac{1}{2} \frac{S^2 h^2 \sin^2 \theta}{J^z - K + J^x + 2K \sin^2 \theta}.$$  \hspace{1cm} (98)

A simple analysis of (98) reveals that the order of the transition depends on the sign of $K$.\[\text{\textcopyright} 2023\]
For $K < 0$,

$$\left. \frac{\partial^2 E}{\partial (\sin^2 \theta)^2} \right|_{K < 0} < 0, \quad 0 < \theta < \pi/2 \quad (99)$$

i.e., there is a first order transition between $\theta_{cl} = 0$ to $\theta_{cl} = \pi/2$ called a "spin flop". This happens at a magnetic field $h_{sc}$ given by

$$E_{\text{rot}}[0, h_{sc}] = E_{\text{rot}}[\pi/2, h_{sc}] \rightarrow h_{sc} = 2S^{-1} \sqrt{(J^z - K - J^x)(J^z + K + J^x)} . \quad (100)$$

For any $h$, the doping concentration is given by

$$x(h) = 2S^{-1} \left( \min_{\theta} E \right) \frac{\partial h}{\partial h} \quad (101)$$

In the case of a first order transition, there is phase separation between the doping concentrations of pure CDW and pure SC at densities

$$x_{\text{cdw}} = 0, \quad x_{\text{sc}} = \frac{\sqrt{J^z - K - J^x}}{J^z + K + J^x} . \quad (102)$$

On the other hand, for $K > 0$, $E(\theta)$ is minimized at

$$\sin^2 \theta_{cl} = \left( \frac{1}{2} hS \sqrt{\frac{J^z - K + J^x}{J^z - K - J^x} - (J^z - K + J^x)} \right) / 2K \quad (103)$$

which indicates the existence of a mixed phase for fields in the range $h_{\text{cdw}} < h < h_{sc}$, where

$$h_{\text{cdw}} = 2S \sqrt{(J^z - K + J^x)(J^z - K - J^x)}, \quad x_{\text{cdw}} = 0 .$$

$$h_{sc} = 2S \sqrt{\frac{J^z - K - J^x}{J^z - K + J^x} (J^z + K + J^x)}, \quad x_{\text{sc}} = \sqrt{\frac{J^z - K - J^x}{J^z - K + J^x}} . \quad (104)$$

For the pure nearest neighbor model ($K = 0$), it is easy to see by (28), that at $h_{sc} = h_{\text{cdw}}$ the mixed state is degenerate with a Maxwell construction of phase separation into SC and CDW. This degeneracy is lifted in the quantum version of the same model, which favors phase separation [11].

14 SO(5) Rotator Theory and High-$T_c$ Superconductors

Recently an SO(5) theory of high $T_c$ cuprate superconductors has been proposed by Shou-Cheng Zhang [10]. The order parameters of antiferromagnetism (AFM)
and $d$-wave superconductivity (dSC) are written as the cartesian components of a 5 dimensional vector

$$\hat{n} = (n_1, n_2, n_3, n_4, n_5), \quad |\hat{n}| = 1$$

$$\langle n_2, n_3, n_4 \rangle = \langle \sum_i e^{i\hat{x}_i \cdot \hat{S}_i} \rangle$$

$$n_1 + in_5 = \langle \sum_{\vec{p}} g(\vec{p}) c_{\vec{p}1}^\dagger c_{\vec{p}2}^\dagger \rangle$$

$g(\vec{p})$ is the Fourier transform of the pair wavefunction which for $d$-wave pairing transforms as $\cos(p_x) - \cos(p_y)$ under lattice rotations. Zhang has found explicit, second quantized constructions for the 10 SO(5) generators $\{L_{a,b}\}_{ab}, a, b = 1, \ldots, 5$ which rotate $\hat{n}$ in 5 dimensions. Particularly interesting are the $\Pi$ operators, i.e. generators $L_{1,a}, a = 2, 3, 4$, which rotate between the AFM and dSC hyperplanes. These are expected to create new low lying pseudo-Goldstone modes near the transition.

Zhang has proposed that the long wave fluctuations are described by an effective rotator Hamiltonian of the form (78),

$$H[L, n] = \frac{1}{2} \sum_{a<b} \chi_{ab} L_{ab}^2 + \frac{1}{2} \rho \sum_a |\nabla n_a|^2$$

$$+ g(n_1^2 + n_5^2) - 2\mu L_{15}$$

where $L_{ab}$ are the generators of SO(5) algebra, and $L_{15}$ is the charge operator whose expectation value yields half the doping concentration $\langle L_{15} \rangle = x/2$. Using the substitution (75), the momenta can be integrated out of the partition function, leaving us with

$$Z = \int D\hat{n} \exp \left( - \int_{0}^{\beta} d\tau \int d^d x \left( \frac{1}{2} \sum_{j=1}^{4} M_j \left( \hat{n} \cdot \hat{e}_j - i h_j \right) \right)^2$$

$$+ \frac{1}{2} \rho \sum_{a=1}^{5} |\nabla n_a|^2 + g(n_1^2 + n_5^2) \right)$$

$$h_j = 2\mu(n_5 \hat{e}_j^1 - n_1 \hat{e}_j^5) .$$

We set $\dot{\hat{n}} = 0$, and search for the classical ground state.

Let us first consider the SO(5) symmetric model, where all $\chi_{ab} = \chi$, and $g = 0$. For any finite $\mu \neq 0$, the ground state flops into $(n_1, n_5)$ plane, i.e. is superconducting.

Experimentally, a transition from AFM to dSC is observed at low hole concentrations $x$ in many of the high $T_c$ systems. Appealing to the analogy with the $-x-xz$ model, this suggests that the symmetry breaking terms of $SO(5) \rightarrow SO(3) \times SO(2)$ should not be forbiddingly large. Symmetry breaking
terms can be included by $g > 0$, and letting the charge susceptibility $\chi_c = \chi_{1,5}$ be different than all other susceptibilities $\chi_{ab} = \chi; a, b \neq 1, 5$. Without loss of generality, we can choose the order parameter to tilt between the AFM and dSC hyperplanes $\hat{n} = (\sin \theta, \cos \theta, 0, 0, 0)$. Following the same derivation as for xxz rotators\(^\text{[8]}\), the classical energy is

$$E[\theta, \mu] = g \sin \theta^2 - \frac{2 \sin^2 \theta \mu^2}{\chi^{-1} \cos^2 \theta + \chi_c^{-1} \sin^2 \theta}. \quad (108)$$

It is now straightforward to verify that the ground state is in the $(n_2, n_3, n_4)$ sphere at $\mu = 0$, and will “flop” into the SC state $\theta = \pi/2$ at large enough $\mu$. It also follows, using the same path as in Section 13, that the order of the transition depends on the relative magnitudes of susceptibilities\(^\text{4}\):

- $\chi_c > \chi \implies$ First order transition at $\mu_{dsc} = \sqrt{g/(2\chi_c)}$
- Phase separation at $0 < x < 4\sqrt{g\chi_c}/2$
- $\chi_c < \chi \implies$ Mixed phase for $\sqrt{g/(2\chi)} < \mu < \sqrt{g\chi}/2 (\chi_c^{-1} + \chi^{-1})$
- At densities $0 < x < 4\sqrt{g\chi}/2$

\(^{109}\)

In the mixed phase, the relation between the SC order parameter and the doping concentration is linear

$$\langle n_1^2 + n_2^2 \rangle = \sin^2 \theta^{el} = \frac{x}{4\sqrt{g\chi}/2} \quad (110)$$

Before attempting to compare these results to experiments, we must remember that this is merely the classical approximation.

### 15 Vortex Dynamics in Superfluids

We henceforth restrict ourselves to two dimensions. The quantum -$x$-xz Hamiltonian\(^\text{[30]}\) for spin $1/2$ can be written in terms of Holstein-Primakoff bosons defined as

$$S^x = a^\dagger a - \frac{1}{2}, \quad (111)$$
$$S^- = \sqrt{1 - a^\dagger a} a, \quad (112)$$
$$S^+ = a^\dagger \sqrt{1 - a^\dagger a} \quad (113)$$
yielding

\[ \mathcal{H}^{-x-xz} = \frac{1}{2} \sum_{ij} J_{ij} \left( \frac{1}{2} - a_i^\dagger a_i \right) \left( \frac{1}{2} - a_j^\dagger a_j \right) - J_{ij}^z \left[ a_i^\dagger a_j \sqrt{(1 - a_i^\dagger a_i)(1 - a_j^\dagger a_j)} + \text{h.c.} \right] - \hbar \sum_i \left( \frac{1}{2} - a_i^\dagger a_i \right). \]  

(114)

The partition function can be written as a Bose coherent state path integral

\[ Z = \int D^2 z \exp \left[ -i \int \partial_{\tau} z_i(z_{i+1} - z_{i-1}) - H^{-x-xz}[z_i(\tau), z_{i+1}(\tau)] \right], \]  

(115)

where \( Dz \) is an integration over the complex plane. Taking the continuum limit, \( z_i \rightarrow \phi(x_i) \), we can write

\[ Z = \int D^2 \phi e^{-S[\phi]} \]  

(116)

where

\[ S = \int d\tau d^d x \left[ \phi^* \partial_{\tau} \phi + \frac{1}{2} \nabla^2 \phi^2 + V(|\phi|) \right], \]  

(117)

is the time dependent Ginzburg-Landau action with

\[ V(\phi, \phi^*) = z J^x a^2 \left( \frac{1}{2} - |\phi|^2 \right)^2 - z J^x a^2 |\phi|^2 \left( 1 - |\phi|^2 \right) + \mu |\phi|^2. \]  

(118)

The classical equation of motion is given by analytically continuing \( \tau \rightarrow it \) and finding the saddle point

\[ \delta S \delta \phi^*(\phi) = 0 \rightarrow i \partial_{\tau} \phi = a \nabla^2 \phi + \frac{\delta V}{\delta \phi^*}(\phi, \phi^*), \]  

(119)

which is known as the Gross-Pitaeveski or Non Linear Schrodinger equation, whose solutions \( \phi(x, t) \) describe collective modes (phase fluctuations), and dynamics of vortex configurations.

A different approach to dynamics of superfluids, is to use the quantum spin model \((114)\) on a lattice with a lattice spacing \( a \) which is smaller than the interparticle spacing. as represented by the spin coherent states path integral \((12)\).

\[ Z = \int \mathcal{D} \cos \theta_i \mathcal{D} \phi_i \exp \left[ \int_0^\beta d\tau \left( i \sum_i (1 - \cos \theta_i(\tau)) \dot{\phi}_i(\tau) - H[\hat{\Omega}_i] \right) \right]. \]  

(120)
A superfluid state is characterized by an ordered state in the xy plane, with a constant two dimensional boson number density $a^2 \rho_s = |\phi|^2$. Using (113), the average spin direction is related to $\rho_s$ by

$$\frac{1}{2} (1 - \langle \cos \theta \rangle) = \rho_s a^2. \quad (121)$$

A vortex configuration can be parametrized by the azimuthal angles at lattice points $i$ by

$$\phi_i(t) = \text{arg} (x_i - x_V(t)) \quad (122)$$

where $x_V(t)$ is the vortex core trajectory. As one can see in Fig. 5, the Berry phase of a vortex path $x_V(t)$ can be written

$$\omega = \rho_s a^2 \sum_{i \in S_c} \oint d\phi_i = 2\pi \rho_s a^2 N_c \quad (123)$$

where the sum is extended to the $N_c$ lattice sites included by the vortex path since the contribution of the others is zero. This Berry phase generates a Magnus force on the moving vortex. This is evident when we write it as an integral over a gauge potential

$$\frac{\omega}{2\pi} = \int_c dx \vec{A} \cdot \vec{x} = \int_c \vec{A} \cdot d\vec{l} = BS_c \quad (124)$$
where \( S_c \) is the area included by the path \( c \), and \( B \) is an effective magnetic field (in dimensions of unit flux quantum). Thus, comparing Eq. (123) and Eq. (124), one can define \( B \) to be simply
\[
B \equiv \rho_s
\tag{125}
\]
and the Magnus force acting on the vortex can be written
\[
\vec{F}_{\text{Magnus}} = B \hat{z} \times \vec{x}_V = 2\pi \rho_s \hat{z} \times \vec{x}_V .
\tag{126}
\]
In the absence of any other time derivative terms, the vortex moves like a massless particle in a strong magnetic field restricted to the lowest Landau level. The semiclassical momentum \( \vec{p} \) of a vortex configuration can be evaluated by computing the expectation value of the translation operator \( T_\vec{a} \)
\[
e^{i\vec{a}.\vec{P}} \equiv \langle \hat{\Omega}|T_\vec{a}|\hat{\Omega} \rangle = \langle \hat{\Omega}(\vec{x})|\hat{\Omega}(\vec{x} + \vec{a}) \rangle
\approx \exp \left[ iS \sum_i (1 - \cos \theta_i) (\phi(\vec{x}_i) - \phi(\vec{x}_i + \vec{a})) \right]
\approx \exp \left( i \int d^2x \rho_s \vec{\nabla} \phi \cdot \vec{a} \right) = e^{2\pi \rho_s \hat{z} \times \vec{x}_V} .
\tag{127}
\]
Similarly, the momentum of a vortex-antivortex pair at positions \( \vec{x}_V, \vec{x}_{-V} \) can be computed
\[
\vec{P} = 2\pi \rho_s \hat{z} \times (\vec{x}_V - \vec{x}_{-V}) .
\tag{128}
\]
Since on a lattice the only distinguishable momenta are within the first Brillouin zone, Eq. (128) implies that vortex-antivortex pair configurations can tunnel between different separations which belong to the discrete family
\[
\vec{x}_V' - \vec{x}_{-V}' = -(2\pi \rho_s)^{-1} \left( \vec{P} + \vec{G} \right) \times \hat{z},
\tag{129}
\]
where \( \vec{G} \) is any reciprocal lattice vector. This is precisely an Umklapp scattering of the superfluid current by the lattice. This amounts to quantum dissipation of the supercurrent due to continuous translation symmetry breaking of a lattice potential [11].

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