Chapter 3

The XY model

In this chapter we will show that the system of Josephson junction arrays can be mapped from the XY model. A mean field analysis will be performed by treating the phases as classical variables.

3.1 The Quantum XY Model

In a two-dimensional square lattice of granular superconductors which are linked by weak couplings, each grain size has its phase ϕ_i. We treat the set of $\{\phi_i\}$ as the relevant variables. As we have shown in Chapter 2 that, each Josephson junction has its coupling energy $-E_J \cos(\phi_i - \phi_j)$. Thus for the 2D Josephson junction arrays, the Hamiltonian is

$$H = -E_J \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j) \qquad (3.1)$$

where $\sum_{\langle ij \rangle}$ denotes summation over pairs of nearest neighbors $\langle ij \rangle$. It is easy to show that eq.(3.1) comes from the mapping of the classical 2-dimensional XY model. Consider the XY model in 2D,

$$H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \qquad (3.2)$$

where $\mathbf{S}_i$ is a planar spin with $|\mathbf{S}_i| = 1$.

By treating spins as classical vectors $\mathbf{S}_i = (\cos \phi_i, \sin \phi_i)$ is the angle of the spin vector at site i. We can recast the Hamiltonian in eq.(3.2) as

$$H_{xy} = -J \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j). \qquad (3.3)$$

The angle ϕ_i can be treated as the phase variable of each grain in 2D Josephson junction arrays. In disordered systems, J is not uniform. We will investigate the disorder case later in Chapter 4 to see how disorder may cause the phase transition.

3.2   Mean Field Theory

It is instructive to consider to the mean field calculation to get some feeling about the problem.

To perform a mean-field analysis of ordered arrays of Josephson junctions, we follow the mean-field analysis of Shih and Stroud (Shih and Stroud, 1983) from which the thermodynamic properties of conventional arrays were obtained by treating the phases of the individual array islands, ϕ_i, as classical thermodynamic

variables in the canonical ensemble. In their paper, the authors begin with the model of an array of N interacting weakly coupled superconducting grains:

$$H = -\sum_{\langle ij \rangle} J_{ij} \cos(\phi_i - \phi_j - A_{ij}). \qquad (3.4)$$

Here J_{ij} is the coupling energy between the ith and jth grains, given in terms of the critical current by $J_{ij} = \left(\frac{h}{2e}\right) I_{ij}$; ϕ_i is the phase of the order parameter on the ith grain, and A_{ij} is given in terms of the vector potential $\mathbf{A}(\mathbf{x})$ by

$$A_{ij} = \frac{2e}{\hbar c} \int_{\mathbf{x}_i}^{\mathbf{x}_j} \mathbf{A} \cdot d\mathbf{l} \qquad (3.5)$$

where $\mathbf{x}_i$ is the position of the center of the ith grain, dl is the differential vector from grain site i to grain site j. The sum in eq.(3.4) runs over all pairs of Josephson coupled grains. In writing eq.(3.4) we have neglected charging effects (that is, we assume infinite grain capacitance). It is assumed that the phase is constant across each grain ("point grains") so that the integral in eq.(3.5) is well defined. The final approximation made is to ignore the temperature dependence of J_{ij}, i.e., of the critical current I_{ij}.

In principle, of course, A_{ij} should refer to the *local* magnetic field, including that produced by Josephson screening currents, and not just the applied field. But these induced fields are difficult to incorporate in practice, as they depend very much on simple geometry and boundary effects. Here, we neglect these screening fields. The neglect is probably justified in the "weak-coupling limit" in which the J_{ij}'s are small and the Josephson penetration depth is large compared with intergrain spacing.

The thermodynamic properties of eq.(3.4) are obtained by treating the phases ϕ_i's as classical thermodynamic variables within the canonical ensemble. Thus the expectation value of an operator O is

$$\langle O \rangle = \frac{1}{Z} \int \left(\prod_{i=1}^{N} d\phi_i \right) O(\phi_1, \ldots, \phi_N) e^{-\beta H}, \tag{3.6}$$

where the partition function Z is

$$Z = \int \left(\prod_{i=1}^{N} d\phi_i \right) e^{-\beta H}, \tag{3.7}$$

with $\beta = (k_B T)^{-1}$ being the inverse temperature and N being the number of grains. The mean-field approximation is then expressed by the condition

$$\eta_i \equiv \langle e^{i\phi_i} \rangle \sim Z_i^{-1} \int_0^{2\pi} d\phi_i e^{i\phi_i} e^{-\beta H_{eff}^{(i)}}, \tag{3.8}$$

$$Z_i = \int_0^{2\pi} d\phi_i e^{-\beta H_{eff}^{(i)}} \tag{3.9}$$

$$H_{eff}^{(i)} = -\sum_{j \neq i} J_{ij} \left[\cos\phi_i \langle \cos(\phi_j + A_{ij}) \rangle + \sin\phi_i \langle \sin(\phi_j + A_{ij}) \rangle \right] \tag{3.10}$$

where the expectation values in eq.(3.10) are to be calculated self-consistently from equations of the form eq.(3.8).

To derive eq.(3.10), we use the definition of the expectation value according to eq.(3.6), i.e.

$$\begin{aligned}
\langle n_{i'} \rangle &= \frac{1}{Z} \int \left(\prod_{i=1}^{N} d\phi_i \right) e^{i\phi_{i'}} e^{-\beta[-\sum_{\langle ij \rangle} J_{ij} \cos(\phi_i - \phi_j - A_{ij})]} \\
&= \frac{1}{Z} \int d\phi_{i'} e^{i\phi_{i'}} \\
&\quad \left\{ \int d\phi_1 \ldots d\phi_{i'-1} d\phi_{i'+1} \ldots d\phi_N e^{\beta \sum_{j \neq i'} J_{i'j} \cos(\phi_{i'} - \phi_j - A_{i'j})} \times e^{\beta \sum_{i \neq i'} \sum_j J_{ij} \cos(\phi_i - \phi_j - A_{ij})} \right. \\
&= \frac{1}{Z} \int d\phi_{i'} e^{i\phi_{i'}} \left\{ \int d\phi_1 \ldots d\phi_{i'-1} d\phi_{i'+1} \ldots d\phi_N e^{\beta H_{eff}^{(i')}} \langle e^{\beta \sum_{j \neq i'} J_{i'j} \cos(\phi_{i'} - \phi_j - A_{i'j})} \rangle \right\} \\
&= \frac{1}{Z} \int d\phi_{i'} e^{i\phi_{i'}} C \langle e^{\beta \sum_{j \neq i'} J_{i'j} \cos(\phi_{i'} - \phi_j - A_{i'j})} \rangle
\end{aligned}$$

where

$$\left\langle e^{\beta \sum_{j\neq i'} J_{i'j} \cos(\phi_{i'}-\phi_j-A_{i'j})}\right\rangle$$

$$\equiv \quad e^{\beta \sum_{j\neq i'} J_{i'j}[\cos\phi_{i'}\langle\cos(\phi_j+A_{i'j})\rangle+\sin\phi_{i'}\langle\cos(\phi_j+A_{i'j})\rangle]}$$

$$= \quad e^{-\beta H_{eff}^{(i')}},$$

$$H_{eff}^{(i)} \quad = \quad -\sum_{j\neq i} J_{ij}[\cos\phi_i\langle\cos(\phi_j+A_{ij})\rangle + \sin\phi_i\langle\cos(\phi_j+A_{ij})\rangle],$$

$$C \quad = \quad \int d\phi_1 \ldots d\phi_{i'-1}d\phi_{i'+1}\ldots d\phi_N e^{iH_{eff}^{(i')}}.$$

In the similar way,

$$Z \quad = \quad C\int d\phi_{i'}e^{-\beta H_{eff}^{i'}}$$

$$= \quad CZ_{i'}.$$

Therefore,

$$\eta_i \sim \frac{1}{Z_i}\int_0^{2\pi} d\phi_i e^{i\phi_i}e^{-\beta H_{eff}^{(i)}}. \tag{3.11}$$

Eqs.(3.8)-(3.10) constitute a set of N-coupled nonlinear complex equations in the unknown "phase-order parameters", η_i, and, in general, must be solved numerically. Note that as written the equations are applicable to both ordered and disordered arrays and to three-dimensional systems as well as two-dimensional ones.

28

3.3 Effect of Charging Energy

Let us consider the Josephson junction array in the presence of charging energy. The Hamiltonian in this case is described by

$$H = \frac{2e^2}{C_0} \sum_i n_i^2 - \frac{J}{2} \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j) \tag{3.12}$$

where C_0 is the capacitance of the grain size, n_i is the occupation number of Cooper pairs. Since n_i and ϕ_j are conjugate variables obeying the commutation relation

$$[n_i, \phi_j] = i\delta_{ij}. \tag{3.13}$$

We can represent n_i by

$$n_i = i\frac{\partial}{\partial \phi_i} \tag{3.14}$$

Then one can rewrite eq.(3.12) as

$$H = -2U \sum_i \frac{\partial^2}{\partial \phi_i^2} - \frac{J}{2} \sum_{\langle i,j \rangle} \cos(\phi_i - \phi_j). \tag{3.15}$$

In the self-consistent mean field approximation, assuming that the phase ordering is such that $\langle \cos \phi_i \rangle \neq 0$, and $\langle \sin \phi_i \rangle = 0$,

$$\cos(\phi_i - \phi_j) = [\langle \cos \phi_i \rangle + \delta(\cos \phi_i)][\langle \cos \phi_j \rangle + \delta(\cos \phi_j)] \tag{3.16}$$

$$\simeq \langle \cos \phi_i \rangle \cos \phi_j + \langle \cos \phi_j \rangle \cos \phi_i - \langle \cos \phi_i \rangle \langle \cos \phi_j \rangle. \tag{3.17}$$

Therefore, we arrive at the Hamiltonian within MFA,

$$H_{MFA} = -\sum_i \left(2U \frac{\partial^2}{\partial \phi_i^2} + ZJ\langle \cos \phi \rangle \cos \phi_i \right) \tag{3.18}$$

29

where Z is the coordination number.

We can see that within this approximation, the sites are decoupled, and the Hamiltonian, at each site, describes a quantum mechanical particle in a periodic, $\cos \phi_i$, potential. The corresponding Schrödinger equation now take the form,

$$[2U\frac{d^2}{d\phi^2} + ZJ\langle\cos\phi\rangle\cos\phi]|\psi_m^{(\phi)}\rangle = -E_m|\psi_m^{(\phi)}\rangle. \tag{3.19}$$

The order parameter $\langle\cos\phi\rangle$ can be calculated from the equation,

$$\langle\cos\phi\rangle = \frac{\sum_m e^{-E_m/kT}\langle\psi_m|\cos\phi|\psi_m\rangle}{\sum_m e^{-E_m/kT}}. \tag{3.20}$$

Eq.(3.19) is simply a Mathieu equation. Near the transition temperature T_c, the order parameter $\langle\cos\phi\rangle$ is small and so is the coefficient of the $\cos\phi$-term in eq.(3.19). There E_m and $|\psi_m\rangle$ can be expanded in term of a small dimensionless parameter, q, defined as

$$q = -\frac{ZJ}{U}\langle\cos\phi\rangle \tag{3.21}$$

To order q, the wave functions $|\psi_m\rangle$, are (Abramowitz and Stegun, 1972)

$$
\begin{aligned}
|\psi_0\rangle &= \frac{1}{\sqrt{2\pi}}\left(1 - \frac{1}{2}\cos\phi\right) \\
|\psi_1\rangle^{(e)} &= \frac{1}{\sqrt{2\pi}}\left(\cos\frac{\phi}{2} - \frac{q}{8}\cos\frac{3\phi}{2}\right) \\
|\psi_1\rangle^{(o)} &= \frac{1}{\sqrt{2\pi}}\left(\sin\frac{\phi}{2} - \frac{q}{8}\sin\frac{3\phi}{2}\right) \\
|\psi_2\rangle^{(e)} &= \frac{1}{\sqrt{2\pi}}\left[\cos\phi - q\left(\frac{\cos 2\phi}{12} - \frac{1}{4}\right)\right] \\
|\psi_2\rangle^{(o)} &= \frac{1}{\sqrt{2\pi}}\left(\sin\phi - q\frac{\sin 2\phi}{12}\right)
\end{aligned}
\tag{3.22}
$$

where for superscripts e and o stand for even and odd respectively. The corre-

sponding energy eigenvalues are, to order q,

$$E_0 = 0, \; E_1^e = \frac{U}{2}(1+q), \; E_1^o = \frac{U}{2}(1-q)$$

$$E_2^e = E_2^0 = 2U.$$

(3.23)

The wave functions $|\psi_m\rangle^{(e)}$ and $|\psi_m\rangle^{(o)}$ are the even and odd combinations resulting from the splitting of the degenerate doublets $|\psi_m^{(\pm)}\rangle$ that are eigenfunctions of eq.(3.19) in the absence of the periodic potential,

$$|\psi_m^{(\pm)}\rangle = \frac{1}{\sqrt{2\pi}} e^{\pm \frac{im\phi}{2}}.$$

(3.24)

These wave functions are also eigenstates of the number operator n_i with the eigenvalues

$$n = \langle \psi_m^{(\pm)} | \hat{n} | \psi_m^{(\pm)} \rangle = \pm \frac{m}{2}.$$

(3.25)

The $m = 2$ states are 2π periodic and correspond, according to eq.(3.25), to $n = \pm 1$. On the other hand, the $m = 1$ states are 2π antiperiodic (or 4π periodic) and correspond to $n = \pm\frac{1}{2}$ which can be interpreted as single-electron excitations on a grain.