Quantum Phase Transitions: T=0 vs. Finite T

In these lectures, much of the material concentrated on classical (thermal) phase transitions that we understand well. Much of the current research activity, on the other hand, focuses on quantum effects on phase transitions, that arise near $T = 0$ critical points. Many aspects of these fascinating phenomena we do not understand yet, and much work remains to be done before we have a complete theory. What we do understand, though, is that quantum effects are generally irrelevant when phase transitions take place at finite temperature. Here we discuss why this is generally true, and describe the structure of various crossover regimes around the quantum critical point.

Ising model in a transverse field

Instead of discussing the role of quantum fluctuations in abstract terms (which can often be confusing), we concentrate on a prototypical model system: an Ising model in a transverse magnetic field, given by the Hamiltonian

$$H = -\frac{1}{2}\sum_{ij} \boldsymbol{\sigma}_i^z J_{ij} \boldsymbol{\sigma}_j^z - \Gamma \sum_i \boldsymbol{\sigma}_i^x .$$

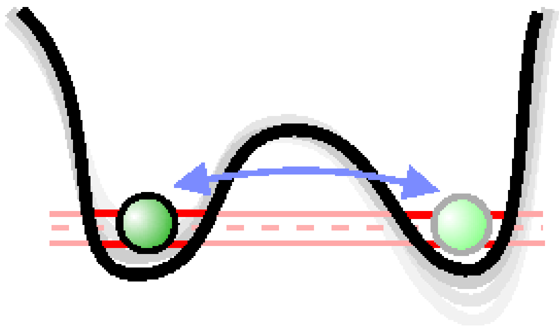
Here, the spin operators are represented by Pauli matrices

$$\boldsymbol{\sigma}_i^z = \begin{bmatrix} +1 & 0 \\ 0 & -1 \end{bmatrix}; \qquad \boldsymbol{\sigma}_i^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Physically, the spin operator $\boldsymbol{\sigma}_i^z$ represents any kind of two state system, e.g. a magnet with anisotropic spins , or even an atom in a double well potential. More precisely, the eigenstates $|\pm\rangle$ of $\boldsymbol{\sigma}_i^z$ represent the two corresponding states of the system. The interaction J favors the neighboring spins to align, just as in the classical Ising model.

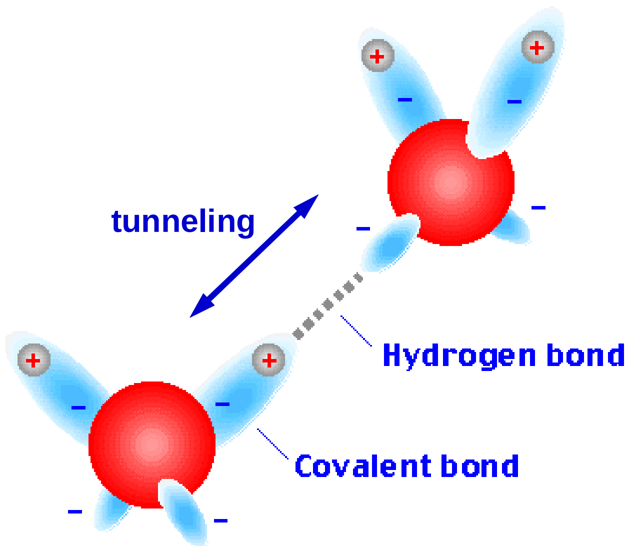
In many systems, though, there exist a finite probability for the local degrees of freedom to tunnel back-and-forth between the two states, as described by the off-diagonal Pauli matrix $\boldsymbol{\sigma}_i^x$, and of amplitude (tunneling rate) Γ. An isolated tunneling center is characterized by two (”bonding” and ”anti-bonding”) quantum states

$$|1/2\rangle = \frac{1}{\sqrt{2}}\left[|+\rangle \mp |-\rangle\right],$$



which have energy $E_{1/2} = \pm\Gamma$.

Because the tunneling process tends to oppose localizing the spin in one of two states, it introduces *quantum fluctuations* that generally reduce ordering. In many physical system one can experimentally tune the tunneling rate, by modifying the barrier between the two wells. This model can be used to represent the behavior of hydrogen-bonded ferroelectrics such as potassium di-hydrogen phosphate (KH_2PO_4), where the crystal lattice is formed of phosphate (PO_4) tetrahedra connected by "hydrogen bonds". In a hydrogen bond two



oxygens "share" one hydrogen ion, i.e. a proton. The proton can "sit" either close to one or the other oxygen; its energetics can be described by a double-well potential. If the proton happens to sit next to one of the two oxygens, this induces a dipole moment in the crystal lattice. It proves energetically favorable to line-up so formed electrical dipole moments, and the crystal assumes ferroelectric ordering.

However, since hydrogen is the lightest element, and the barriers separating the two wells are of moderate height, there proves to be appreciable tunneling between the two potential minima. This tunneling rate can be experimentally tuned by applying hydrostatic pressure which reduces the unit cell size, and thus the height of the barrier separating the wells. As the pressure increases, the critical temperature for ferroelectric ordering drops, and the ordered phase is completely destroyed at a critical pressure $P = P_c$. Such a $T = 0$ phase transition is called a quantum critical point, since in its vicinity quantum fluctuations cannot be ignored. In the following we outline a theoretical approach that can be used to describe the quantum critical behavior.

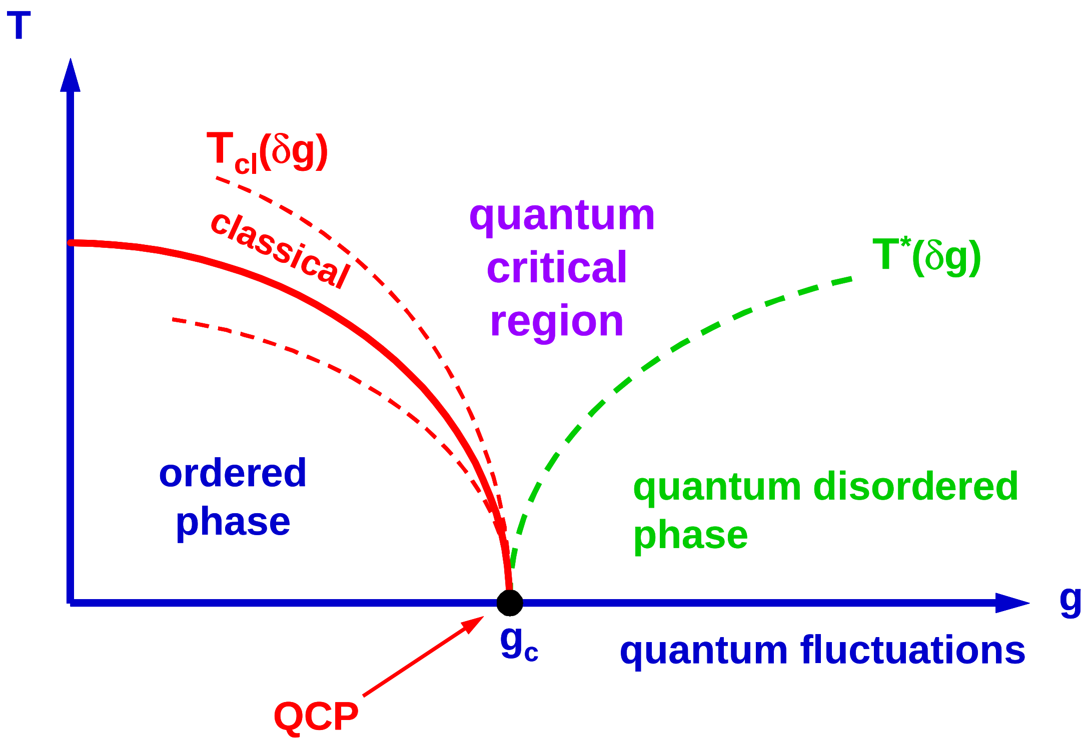


FIG. 1: Generic phase diagram around a quantum critical point (QCP). Classical critical behavior is expected in a narrow region around the finite-temperature critical line (red). Quanum effects modify the critical behavior if the transition is approached by tuning the quanum fluctuations at $T = 0$ (green), and even within the so-called "quantum critial" regime (purple). In the antiferroelectric potassium di-hydrogen posphate (KH_2PO_4), the tunneling rate within the hydrogen bonds can be tuned by applying pressure, driving the system through a quantum critical point.

Quantum statistical mechanics

For quantum systems the partition function can be written as the trace of the density matrix

$$Z = Tr\; T_\tau \exp\left\{ \frac{1}{2} \sum_{ij} \int_o^\beta d\tau \boldsymbol{\sigma}_i^z(\tau) J_{ij} \boldsymbol{\sigma}_j^z(\tau) + \Gamma \sum_i \int_o^\beta d\tau \boldsymbol{\sigma}_i^x(\tau) \right\}.$$

Here, T_τ represents the time (temperature) ordered product in the Heisenberg representation, where the operators become functions of the imaginary time τ. We assume that the reader is already familiar with this formalism, as discussed in many standard texts on quantum many-body problems.

To describe the critical behavior, we follow the same strategy as for classical models, where it proved useful to represent the partition function as a functional integral over the fluctuations of an appropriate order parameter field. To do this, we again perform a Hubbard-Stratonovich transformation to decouple the interaction term

$$-\frac{1}{2} \sum_{ij} \int_o^\beta d\tau\, \boldsymbol{\sigma}_i^z(\tau) J_{ij} \boldsymbol{\sigma}_j^z(\tau) \longrightarrow \frac{1}{2} \sum_{ij} \int_o^\beta d\tau\, \phi_i(\tau) J_{ij}^{-1} \phi_i(\tau) - \sum_i \int_o^\beta d\tau\, \boldsymbol{\sigma}_i^z(\tau) \phi_i(\tau).$$

The partition function takes the form

$$Z = \int D\varphi \exp\left\{ -\frac{1}{2} \sum_{ij} \int_o^\beta d\tau\, \phi_i(\tau) J_{ij}^{-1} \phi_i(\tau) \right\}$$
$$\times \prod_i Tr\; T_\tau \exp\left\{ \int_o^\beta d\tau\; [\phi_i(\tau) \boldsymbol{\sigma}_i^z(\tau) + \Gamma \boldsymbol{\sigma}_i^x(\tau)] \right\}.$$

In this expression, the last term looks precisely as the partition function of noninteracting quantum spins in presence of an (imaginary) time-dependent external (longitudinal) field $\varphi_i(\tau)$. To derive a quantum version of a Landau functional, we again formally expand the logarithm of this term in powers of the order-parameter field $\varphi_i(\tau)$. As usual, we only keep (see Appendix A) the lowest order contributions in (Matsubara) frequency and momentum, since we expect the rest to be irrelevant by power counting.

The resulting Landau functional takes the form

$$S = \frac{1}{2} \int d\mathbf{x} \int_o^\beta d\tau\, \phi(\mathbf{x},\tau) \left[r - \partial_\tau^2 - \nabla^2 \right] \phi(\mathbf{x},\tau) + \frac{u}{4} \int d\mathbf{x} \int_o^\beta d\tau \phi^4(\mathbf{x},\tau).$$

An explicit expression for the "mass" r in terms of the interaction J and the tunneling rate Γ takes the form

$$r = \frac{1}{Jz} - \frac{\tanh \beta\Gamma}{\Gamma}.$$

[Note here that in this quantum case, the definition of r and u differs by a factor β from the ones used in the classical model. Defined like this, r remains finite even in the $T = 0$ limit, were it indicates the stability of the paramagnetic phase for sufficiently large Γ.] The mean-field critical line is obtained by setting $r = 0$, or

$$\frac{1}{\beta J z} = \frac{\tanh \beta\Gamma}{\beta\Gamma}.$$

In the classical limit ($\beta\Gamma \ll 1$) we find $T_c/Jz = 1$, and in the opposite $T = 0$ limit ($\beta\Gamma \gg 1$) the quantum critical point is found at

$$\Gamma_c/Jz = 1.$$

In the above expression for the Landau functional, the fields $\varphi_j(\tau)$ representing Bosonic spin excitations are periodic functions of (imaginary) time $\varphi_j(\tau + \beta) = \varphi_j(\tau)$. The corresponding Matsubara frequencies are $\omega_n = 2\pi n$, with $n = 0, \pm 1, \pm 2, ...$ Note that in deriving this result we have chosen the units of both the length and the time (i.e. the temperature) so that the action assumes a "Lorentz-invariant" form (i.e. the coefficients of ∂_τ^2 and ∇^2 are the same).

We pause to fully appreciate this important result. At $T = 0$, $\beta \longrightarrow \infty$, and the partition function takes precisely the same form as in classical statistical mechanics for a system in $D = d + 1$ dimensions. The time effectively plays a role of an additional dimension, but no essentially new features are added. All the results that we have obtained so far still hold, and we can immediately read-off the critical behavior. At $T = 0$, the quantum fluctuations play the role of thermal fluctuations in the classical problem, and magnetic ordering is destroyed when they are sufficiently large.

Finite temperature crossovers

The situation is more complicated at finite temperature. Here, partition function still looks just like that of a classical system in $D = d - 1$ dimensions, but with an important difference. Namely, the system "size" is still infinite in d spatial dimensions, but now becomes finite in the "time" direction. This new feature has important consequences for the critical behavior. The same situation is found in a classical system where the sample has finite size in one of the d dimensions.

We should emphasize that this subtlety proves of relevance only if fluctuation corrections to mean-field theory are examined. This is true since the fluctuation corrections acquired singular contributions precisely from long-wavelengths, and these will be cut-off if we have a finite system size. Physically, as soon as the correlation length becomes longer then the "thickness" of our system, the "infrared" divergence in the appropriate dimensions will be cut-off, and the system effectively behaves as that of a reduces dimensionality.

In the quantum case we consider, the finite temperature introduces a cutoff in the time dimension. We conclude that the leading critical behavior will be exactly the same as that of the corresponding classical system. The quantum fluctuations are, therefore, irrelevant for the leading critical behavior at finite temperature. To be precise, at very low temperature the relevant temperature cutoff will be very small. We thus expect its effects to be important only in an infinitesimally narrow crossover regime between the critical temperature T_c and the quantum-classical crossover scale T_{cl}. We expect this "classical" crossover regime (shown by dashed red lines on the phase diagram) to shrink to a point precisely at the QCP, i.e. at $T = 0$.

Similarly, within the quantum disordered phase, the fluctuations are "massive", i.e. $r > 0$. Quantities like the order parameter susceptibility thus remain finite down to $T = 0$. However, finite temperature again introduces a new cutoff that should be compared to r. As soon as the temperature cutoff is large enough, it washes out the effects of the mass r, and the behavior is modified. We thus expect another crossover scale T^* to emerge, separating the quantum critical region and the low temperature quantum disordered regime. This scale is also expected to vanish in a powerlaw fashion as the QCP is approached. The genuine quantum effects dominate within the quantum critical regime, which is expected to broaden as temperature increases. This makes it possible to observe such quantum critical behavior even in finite temperature experiments, despite the fact that the QCP is located at $T = 0$.

Infrared divergences and finite temperature cutoffs

A precise description of the quantum critical behavior and the associated finite temperature crossovers requires careful analysis which is beyond the scope of our presentation. Within the quantum Landau landau formulation we discussed, this calculation is *in principle* straightforward, since it reduces to an appropriate finite size scaling analysis of an effective classical model. For our purposes it will be sufficient to illustrate these ideas by examining the leading fluctuation corrections to mean-field theory, and by determining how their form is modified at finite temperature.

To be specific, let us examine the one-loop "mass" renormalization. The expression derived in the classical model not generalizes to

$$\widetilde{r} = r + 3uT \sum_{\omega_n} \int \frac{d\mathbf{k}}{(2\pi)^d} \frac{1}{\widetilde{r} + \omega_n^2 + k^2} + O(u^2).$$

At $T = 0$, the Matsubara sum can be replaced by an integral

$$T \sum_{\omega_n} \longrightarrow \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi},$$

and we get

$$\begin{aligned}\widetilde{r} &= r + 3u \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \int \frac{d\mathbf{k}}{(2\pi)^d} \frac{1}{\widetilde{r} + \omega^2 + k^2} \\ &= r + 3u \int \frac{d^{d+1}\mathbf{q}}{(2\pi)^{d+1}} \frac{1}{\widetilde{r} + q^2},\end{aligned}$$

where $\mathbf{q} = (\omega, \mathbf{k})$ is a $(d+1)$-dimensional vector. The calculation clearly reduces to that of a classical $(d+1)$-dimensional system.

The situation is different at $T \neq 0$. Now we separate the $\omega_n = 0$ contribution, and write

$$\widetilde{r} = r + 3uT \int \frac{d\mathbf{k}}{(2\pi)^d} \frac{1}{\widetilde{r} + k^2} + 3uT \sum_{\omega_n \neq 0} \int \frac{d\mathbf{k}}{(2\pi)^d} \frac{1}{\widetilde{r} + \omega_n^2 + k^2}.$$

In the last term we can again replace the Matsubara sum by an integral, but this time with a lower cutoff $\omega_o = 2\pi T$, which provides a "mass"

$$\widetilde{r} = r + 3uT \int \frac{d\mathbf{k}'}{(2\pi)^d} \frac{1}{\widetilde{r} + k^2} + 3u \int \frac{d^{d+1}\mathbf{q}}{(2\pi)^{d+1}} \frac{1}{\widetilde{r} + \omega_o + q^2}.$$

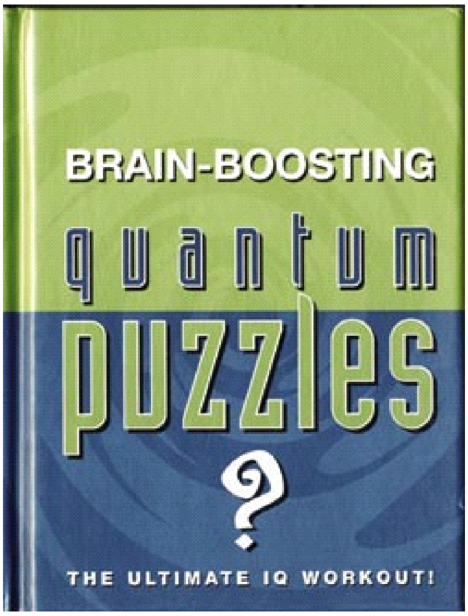
We can now explicitly evaluate these integrals and get

$$\widetilde{r} = r + \delta r_o + \frac{3uTK_d}{d-2} \widetilde{r}^{(d-2)/2} + \frac{3uK_{d+1}}{d-1} \left(\widetilde{r} + \omega_o\right)^{(d-1)/2}.$$

We have two fluctuation corrections. The first one $\sim \widetilde{r}^{(d-2)/2}$ is the same as in the classical case, corresponding to the static ($\omega_n = 0$) fluctuations. The second one is, on the other hand, cut-off close to the critical line ($\widetilde{r} \longrightarrow 0$), and can be ignored there. We conclude that the most singular correction to the critical behavior is precisely of the same form as in the classical theory, just as we anticipated. However, the last term dominates sufficiently far from the transition ($\widetilde{r}$ not too small), and the behavior is modified.

Epilogue

We will not explore further details of this rich crossover behavior. Still, what we have seen is sufficient to start appreciating why quantum fluctuations are irrelevant near finite temperature critical points. This phenomenon is, of course, much more general then the specific example we have discussed, and represents one of the lessons that we consider as well established.



In contrast, there are still many questions in the area of quantum critical phenomena that remain hard to understand, and which perhaps indicate some fundamental limitations of the paradigm that we have explored. In recent years, more and more examples of quantum critical phenomena seem to emerge that do not fit well in the Landau-based picture that we cherish. Most puzzling phenomena are found when quantum critical phenomena are examined in strongly correlated metals, such as heavy fermion compounds and oxides close to the Mott transition. In many of these systems, standard power counting approaches suggest that mean-field predictions should be sufficient in $d = 3$. Yet most experiments seem at odds to what simple theories predict. Many researchers believe that excitations other then long-wavelength spin wave modes may be crucial at the critical point, and that Kondo-like processes must be reexamined more carefully. Others search for even more exotic topological excitations, generalizing the ideas of Kosterlitz and Thouless. What will be the final answer? Time only will tell. One thing is certain: we have a long way to go...

Appendix A: cumulant expansion

We now carry out the cumulant expansion to obtain an appropriate Landau functional. We also add a small (longitudinal) field at each lattice site

$$\delta S_h(i) = -\int_o^\beta d\tau\, h_i(\tau)\boldsymbol{\sigma}_i^z(\tau),$$

in order to calculate correlation functions

$$\chi_{ij}(\tau-\tau') = \frac{\delta^2}{\delta h_i(\tau)\delta h_j(\tau')}\ln Z[h].$$

We can write the effective Action in the form

$$S[\phi,h] = \frac{1}{2}\sum_{ij}\int_o^\beta d\tau\,\phi_i(\tau)J_{ij}^{-1}\phi_j(\tau) + \sum_i V_{loc}[\phi+h],$$

where

$$V_{loc}[\phi] = -\ln TrT_\tau \exp\left\{\int_o^\beta d\tau\ \left[\phi_i(\tau)\boldsymbol{\sigma}_i^z(\tau) + \Gamma\boldsymbol{\sigma}_i^x(\tau)\right]\right\}$$

Let us first shift the ϕ-fields by the external field h

$$\phi_i(\tau) \longrightarrow \phi_i(\tau) - h_i(\tau),$$

in order to eliminate $h_i(\tau)$ from $V_{loc}[\phi+h]$. We get

$$\begin{aligned} S[\phi,h] &= \frac{1}{2}\sum_{ij}\int_o^\beta d\tau\ \left(\phi_i(\tau)-h_i(\tau)\right) J_{ij}^{-1}\left(\phi_j(\tau)-h_j(\tau)\right) + \sum_i V_{loc}[\phi_i] \\ &= \frac{1}{2}\sum_{ij}\int_o^\beta d\tau\, h_i(\tau)J_{ij}^{-1}h_j(\tau) - \sum_{ij}\int_o^\beta d\tau\,\phi_i(\tau)J_{ij}^{-1}h_j(\tau) + S[\phi], \end{aligned}$$

with

$$S[\phi] = \frac{1}{2}\sum_{ij}\int_o^\beta d\tau\,\phi_i(\tau)J_{ij}^{-1}\phi_j(\tau) + \sum_i V_{loc}[\phi_i].$$

From this expression, we find

$$\frac{\delta}{\delta h_i(\tau)}\ln Z[h] = \frac{1}{Z[h]}\left[\sum_j\int_o^\beta d\tau\ J_{ij}^{-1}\left\langle -h_j(\tau)+\phi_j(\tau)\right\rangle_{S[\phi,h]}\right],$$

and

$$\chi_{ij}(\tau-\tau') = \frac{\delta^2}{\delta h_i(\tau)\delta h_j(\tau')} \ln Z[h]$$
$$= \frac{\delta}{\delta h_j(\tau')} \frac{1}{Z[h]} \left[\sum_j J_{ij}^{-1} Tr \left[(-h_j(\tau) + \phi_j(\tau))\, e^{-S[\phi,h]} \right] \right]$$
$$= J_{ij}^{-1} \left[G_{ij}(\tau-\tau') - \delta(\tau-\tau') \right],$$

where $G_{ij}(\tau-\tau') = \langle \phi_i(\tau)\phi_j(\tau) \rangle_c$ denotes the connected Green's function corresponding to the Action $S[\phi]$.

Next, we perform the cumulant expansion of $V_{loc}[\phi]$, as follows

$$V_{loc}[\phi_i] = \frac{1}{2} \int_o^\beta d\tau \int_o^\beta d\tau' \, \phi_i(\tau) \Gamma^{(2)}(\tau-\tau') \phi_i(\tau') + O(\phi^4).$$

We explicitly calculate only the form of the two-point vertex $\Gamma_{ij}^{(2)}(\tau-\tau')$

$$\Gamma^{(2)}(\tau-\tau') = \frac{\delta^2}{\delta\phi_i(\tau)\delta\phi_i(\tau')} \left[- \ln Tr T_\tau \exp \left\{ \int_o^\beta d\tau \, \left[\phi_i(\tau) \boldsymbol{\sigma}_i^z(\tau) + \Gamma \boldsymbol{\sigma}_i^x(\tau) \right] \right\} \right]$$
$$= \langle \boldsymbol{\sigma}_i^z(\tau) \boldsymbol{\sigma}_i^z(\tau') \rangle_o = -\chi_o(\tau-\tau')$$

where $\langle \cdots \rangle_o$ indicates a isolated-spin correlation function, corresponding to the noninteracting quantum Hamiltonian

$$H_o = -\Gamma \sum_i \boldsymbol{\sigma}_i^x.$$

It is not difficult to explicitly calculate $\chi_o(\tau-\tau')$ [see, e.g. V. Dobrosavljevic and R. M. Stratt, Phys. Rev. B **36**, 8484 (1987)], and one finds

$$\chi_o(\tau) = \frac{\cosh\left[\beta\Gamma\,(1-2\tau)\right]}{\cosh\left[\beta\Gamma\right]}.$$

At low frequency, we can write

$$\chi_o(\omega_n) = \chi_o - a\omega_n^2 + \cdots,$$

where

$$\chi_o = \int_o^\beta d\tau \chi_o(\tau) = \frac{\tanh\beta\Gamma}{\beta\Gamma}.$$

Finally, we get an expression for the Landau Action of the form

$$S[\phi] = \frac{1}{2} \sum_{ij} \int_o^\beta d\tau \int_o^\beta d\tau \phi_i(\tau) \left[\delta(\tau-\tau') J_{ij}^{-1} + \chi_o(\tau-\tau') \right] \phi_j(\tau) + \frac{u}{4} \sum_i \int_o^\beta d\tau \phi_i(\tau).$$

From this result we can immediately read-off an expression for the "mass"

$$r = \frac{1}{Jz} - \frac{\tanh\beta\Gamma}{\Gamma}.$$