What is wrong with paramagnons?*

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Systems with itinerant fermions close to a zero temperature quantum phase transition like the high temperature superconductors exhibit unusual non-Fermi liquid properties. The interaction of the long-range and low-energy fluctuations of the incipient order with the fermions modify the dynamical properties of the fermions strongly by inducing effective long-range interactions. Close to the transition the interaction of the order parameter fluctuations becomes important. In this paper we discuss the physics of the non-Gaussian order parameter fluctuations on the electronic spectrum and illustrate their effect by considering the charge-density-wave transition. We show how to generalize the one-dimensional problem to the phase fluctuations of a two dimensional superconductor.
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1. INTRODUCTION

Fermionic systems which undergo a zero temperature phase transition as a function of some experimental parameter exhibit unusual physical properties. The phase transitions which are driven by quantum rather than thermal fluctuations have been studied intensively theoretically and experimentally during the last few years. While significant progress in the understanding of low dimensional spin systems could be achieved the physics of itinerant electrons coupled to the low energy collective fluctuations is far less understood.

One of the problems studied most intensively in this context is itinerant electron magnetism. The interplay between superconductivity and spin fluctuations in nearly ferromagnetic metals has been first studied in nearly ferromagnetic metals. Berk and Schrieffer[1] and Doniach[2] used the term "paramagnons" to describe the long-lived and long-range spin fluctuations in a

*This paper is dedicated to Peter Wölfle on the occasion of his 60th birthday.

nearly ferromagnetic metal. The exchange of long-lived and long-range ferromagnetic spin fluctuations has been argued to mediate an unusual type of superfluidity in ^{3}He. The nonlinear feedback of spin-fluctuations has been used successfully to explain the stability of the "Anderson-Brinkmann-Morel" superfluid phase. However, by now it has become clear that ^{3}He is closer to localization than to a ferromagnetic transition[3]. In recent years it has been proposed that in the high temperature superconductors with their magnetic parent compounds the exchange of antiferromagnetic spin fluctuations may lead to d-wave superconductivity [4,5]. Some experimental features like the the unusual relaxation rates in the NMR experiments have been understood using a *phenomenological approach* to the spin fluctuations[6]. Various re-summation schemes, like the fluctuation-exchange approximation (FLEX) and other more complicated schemes like Parquet re-summation[7], have been used to calculate properties in the "nearly antiferromagnetic phase" and to compare it to more *microscopic* approaches. Already in 1976 Hertz showed how to generalize the concepts of classical phase transitions to a zero temperature quantum phase transition for itinerant electrons[8]. While thermodynamic properties of the electronic system can be calculated close to the phase transition the spectral properties of the electrons have been calculated only in approaches basically relying on the assumption of Gaussian order parameter fluctuations[9]. Very little is known about the physics of the electronic degrees of freedom in the non-Gaussian regime. The purpose of the paper is to draw attention to the fact that the non-Gaussian order parameter fluctuations drastically modify the electronic properties. This is particularly relevant for the *pseudo-gap regime.* The paper is organized as follows. First we briefly review the theory of *quantum phase transitions* by Hertz and Millis. We then explain the physics of the non-Gaussian regime using a one-dimensional example. Finally we show how to generalize the one-dimensional example to the problem of phase fluctuations in a two-dimensional superconductor and calculate the tunneling density of states in the fluctuation regime.

2. QUANTUM PHASE TRANSITIONS

The partition function, Z, of an interacting electron gas with incipient order can be expressed as a functional integral over a field Φ which represents the order-parameter density of the incipient order, and the electronic degrees of freedom, ψ [10]:

$$Z = Z_0 \int \mathcal{D}[\Phi] \int \mathcal{D}[\psi] \exp(-S[\psi, \Phi]) \tag{1}$$

The last integral defines an effective action, $S_{\text{eff}}[\Phi]$, for the bosonic field Φ:

$$S_{\text{eff}}[\Phi] = \int \mathcal{D}[\psi] \exp(-S[\psi, \Phi]) \tag{2}$$

The electronic degrees of freedom can be integrated out, since they only appear quadratic in the action. An external field $h_n(q)$ can be coupled to the field Φ via

$$S_{\text{eff}}^{(ext)} = \beta \sum_{i\omega_n, q} h_n(q) \cdot \Phi_{-n}(-q) \tag{3}$$

Integrating out the electronic degrees of freedom and expanding in the field Φ the action $S[\Phi]$ can be written as

$$S_{\text{eff}}[\Phi] = S_{\text{eff}}^{(0)} + S_{\text{eff}}^{(2)}[\Phi] + S_{\text{eff}}^{(4)}[\Phi] + \ldots \tag{4}$$

as shown in Fig. 1. The zig-zag line represents the field Φ and the solid line the electron propagator.

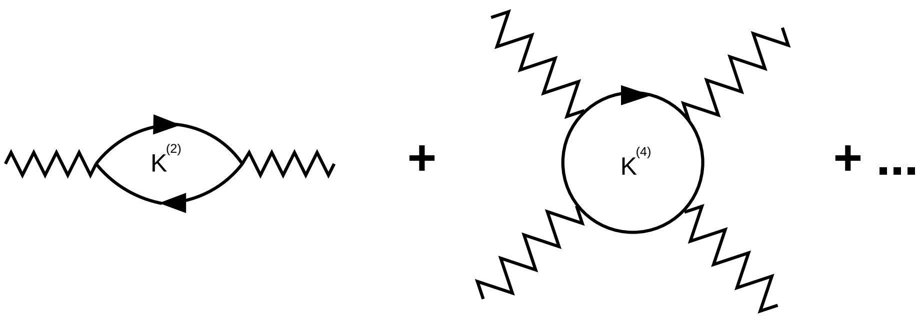

Fig. 1. Expansion of the partition function Z in terms of the Hubbard-Stratanovich fields.

The second order term is given by: $S^{(2)}[\Phi] = \beta \sum_{1,2} K^{(2)}(1,2)\Phi(1)\Phi(2)$ where 1 represents $(q_1, i\omega_1, \alpha_1)$ and so on. The sum over the bosonic Matsubara frequencies $i\omega$ is multiplied with the inverse temperature β. $K^{(2)}(1,2)$ can be calculated explicitely, $K^{(2)}(1,2) = \delta_{\omega_1+\omega_2}\delta_{q_1+q_2}\delta_{\alpha,\alpha'}U/\left(1 - U\chi_0(q_1, i\omega_1)\right)$ where $\chi_0(q_1, i\omega_1)$ is the electronic polarization and U is the coupling strength of the electrons to Φ.

$$\chi_0(q, i\omega) = -\sum_p \frac{f(\epsilon_{p+q}) - f(\epsilon_p)}{\epsilon_{p+q} - \epsilon_p - i\omega} \tag{5}$$

where $f(\epsilon_p)$ is the Fermi distribution function. In a paramagnon type of theory only $K^{(2)}$ is considered and the interaction of the the bosonic fields is neglected. In the self-consistent renormalized (SCR) approach by Moriya[11] the interaction of the bosonic modes is taken into account by renormalizing $K^{(2)}$. The SCR is therefore an effective Gaussian theory. The effects we are considering here are due to the interaction of the bosonic modes which is given by the next term in the series for $S_{\rm eff}$.

The fourth order term obviously depends on four bosonic fields and is given by: $S^{(4)}[\Phi] = \beta \sum_{1,2,3,4} K^{(4)}(1,2,3,4)\Phi(1)\Phi(2)\Phi(3)\Phi(4)$. If the Fermi surface is not nested and the ordering wave vector of the incipient order is not an extremal spanning vector of the Fermi surface then the complicated fourth order term might be approximated by a constant. The effective action including the fourth order term was first studied by Hertz[8] and subsequently by Millis[9] using renormalization group. The resulting phase diagram for a two dimensional system is sketched in Fig. 2. We briefly summarize the

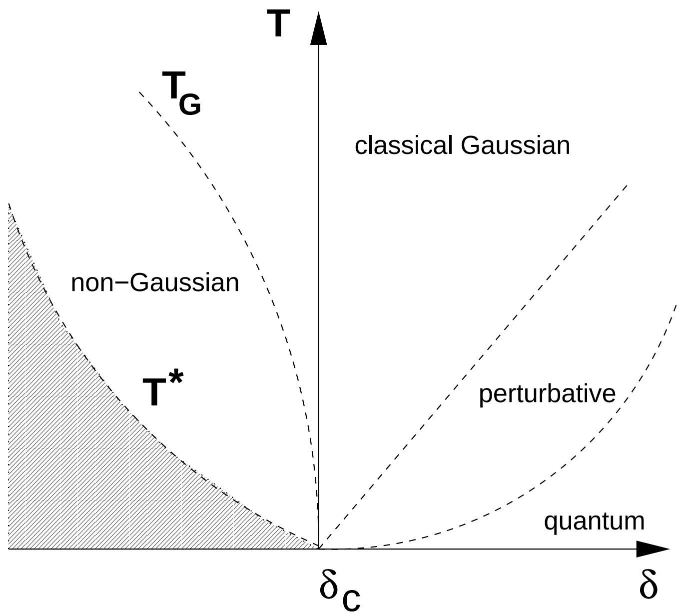

Fig. 2. The phase diagram for an itinerant electronic system close to a quantum phase transition controlled by a parameter δ. The dashed lines refer to cross-overs. The region relevant for this paper is located to the left of δ_c.

results by Millis relevant for this paper. To the left of the quantum critical point the phase diagram is dominated by three regions. On lowering the temperature one first enters a regime which is dominated by classical order parameter fluctuations. Below the doted line which indicates the Ginzburg temperature classical non-Gaussian order parameter fluctuations occur. Decreasing the temperature further the behavior of the model depends on the symmetry class of the fluctuations and whether the fermions are fully or partly gapped. Paramagnon like theories are often used in a parameter regime close to a 3D transition which is intercepting the low temperature regime of the quantum phase transition. It is often assumed that the order parameter fluctuations are still Gaussian. However, in a regime where the electronic density of states is already substantially suppressed like in the pseudogap regime this is a questionable assumption. The purpose of this paper is to draw attention to the fact that the non-Gaussian fluctuations modify the electronic properties drastically compared to the Gaussian fluctuations.

3. A QUASI-ONE-DIMENSIONAL PROBLEM

To illustrate the effect of the non-Gaussian fluctuations, we discuss a model system for which most properties can be calculated without further approximation. To be specific we consider a one-dimensional charge density system with a metallic phase at high temperatures and an insulating phase at zero temperature. Contrary to the assumption in previous work [12,13], it is *not* sufficient to describe the order parameter fluctuations by the *variance* and *correlation length* only, but one needs to consider higher moments of the order parameter correlator. This becomes intuitively clear if one considers the situation depicted in Fig. 3. If the order parameter varies smoothly, as in the Gaussian regime, regions where the order parameter is suppressed are smeared out over the correlation length. The electronic wavefunction is spread out over a length comparable with the correlation length. The kinetic energy is low, and consequently many states can be found at low energy even when the correlation length is large. On the other hand, if the order parameter is established and only suppressed over a length scale much shorter than the correlation length of the potential, as in the non-Gaussian regime, the electronic wavefunction decays over a distance v_F/Δ, where v_F is the Fermi velocity of the electrons and Δ is the amplitude of the orderparameter, and has a large kinetic energy. For the *same* correlation length and variance of the order parameter the electronic wavefunction is much stronger suppressed for non-Gaussian fluctuations. The overlap of parts of the wavefunction lo-

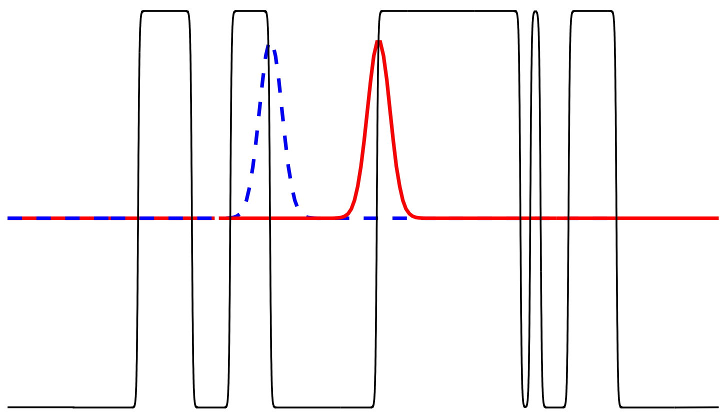

Fig. 3. Typical order parameter configuration in the non-Gaussian regime. The electronic wave function is localized in the regions where the order-parameter is small. The overlap between electronic wave functions localized in different regions is exponentially small.

cated at different regions where the order parameter is exponentially small. In dimension d the electron wave function will be constrained to a $d-1$ dimensional manifold. If the dimension is greater than one the regions where the order parameter is small form a "network" in which the electrons can move and one has to consider "quantum-percolation".

To be specific we consider here only the most simple case namely a one-dimensional system close to a CDW transition. The dispersion of the electrons close to the Fermi energy can be assumed to be linear. The Hamiltonian of the electrons has the form:

$$\hat{H} = -iv_F(R^\dagger \partial_x R - L^\dagger \partial_x L) + \Delta(x) R^\dagger L + \Delta^*(x) L^\dagger R, \tag{6}$$

where the operators $R^\dagger$ and $L^\dagger$ create left and right moving electrons respectively. The classical order parameter field $\Delta(x)$ is determined by a Ginzburg Landau action given below, v_F is the Fermi velocity.

Next we consider the order parameter fluctuations. For commensurate fluctuations, the low energy electronic density of states is dominated by the Dyson singularity which only exists in one dimension [14,15]. For the more general case, the order parameter fluctuations are complex and the Dyson singularity is absent. Therefore we will restrict our discussion to complex order parameters. Here we assume that the *classical* complex order parameter fluctuations, $\Delta(x)$, are described by the Ginzburg-Landau action:

$$F[\Delta(x)] = \frac{1}{k_B T} \int_0^L dx/\xi_0 \left(\xi_0^2 |\partial_x \Delta|^2 + \alpha |\Delta|^2 + \beta |\Delta|^4 \right) \tag{7}$$

In the purely one-dimensional case integrating out the electrons introduces singular terms in the order-parameter action which are cut off by the curvature of the Fermi-surface. Close to the mean field phase transition α varies linearly with the temperature $\alpha = \alpha'(T/T_c^{MF} - 1)$, whereas β and ξ_0 are nearly temperature independent. In principle, the coefficients ξ_0, α and β have to be determined self consistently from the electronic properties. The correlator for the order parameter fluctuations always decays exponentially, $< \Delta(x)\Delta(0) >=< \Delta^2 > \exp(-|x|/\xi)$ since the 1D system is disordered above the 3D ordering temperature, T_c^{3D}. Nevertheless, the action Eq. (7) has two different regimes: if $\alpha(T)$ is positive and large, the order parameter fluctuations are centered around zero and basically Gaussian. For $\alpha(T)$ negative and large the amplitude of the order parameter is given by $\sqrt{< \Delta^2 >}$, and only the phase fluctuations play a role.

The density of states of the electrons in an order parameter potential given by Eq. (7) can be calculated exactly numerically using the transfer-matrix formalism for the order-parameter fluctuations[16]. The Schrödinger equation for the right moving and left moving electrons, with the wavefunction $u(x)$ and $v(x)$ respectively, reads:

$$\begin{aligned} -iv_F\partial_x u(x) + \Delta\ (x)\ v(x) &= \epsilon\, u(x) & (8)\\ +iv_F\partial_x v(x) + \Delta^*(x)\ u(x) &= \epsilon\, v(x) & (9) \end{aligned}$$

where ϵ is the single-particle energy. The logarithms of $u(x)$ and $v(x)$ obey the following equation of motion:

$$\begin{aligned} -iv_F\partial_x \log(u(x)) &= \epsilon - \Delta\ (x)u(x)/v(x)\\ +iv_F\partial_x \log(v(x)) &= \epsilon - \Delta^*(x)v(x)/u(x) \end{aligned}$$

Where one has to keep in mind choosing the correct branch for $\log(z)$. Adding the two equations we obtain an equation for the ratio $r(x) = u(x)/v(x)$:

$$-iv_F\partial_x \log(r(x)) = 2\left[\epsilon - \Delta(x)r(x) - \Delta^*(x)r^{-1}(x)\right] \qquad (10)$$

With the ansatz $r(x) = \exp(i\varphi(x))$ and $\Delta(x) = |\Delta(x)|e^{i\Phi}$ we finally obtain the equation of motion for the $\varphi(x)$:

$$\partial_x\varphi(x) = 2\left[\epsilon - |\Delta(x)|\cos(\varphi(x) + \Phi(x))\right] \qquad (11)$$

Note that $\varphi(x)$ is the scattering phase of the wavefunction. Surprisingly the phase information alone is quite sufficient to obtain all the thermodynamic information. The integrated density of states, $\mathcal{N}(\epsilon)$, can be related to the phase by[17]

$$\mathcal{N}(\epsilon) = \lim_{L\to\infty}\frac{\varphi(L)}{2L}, \qquad (12)$$

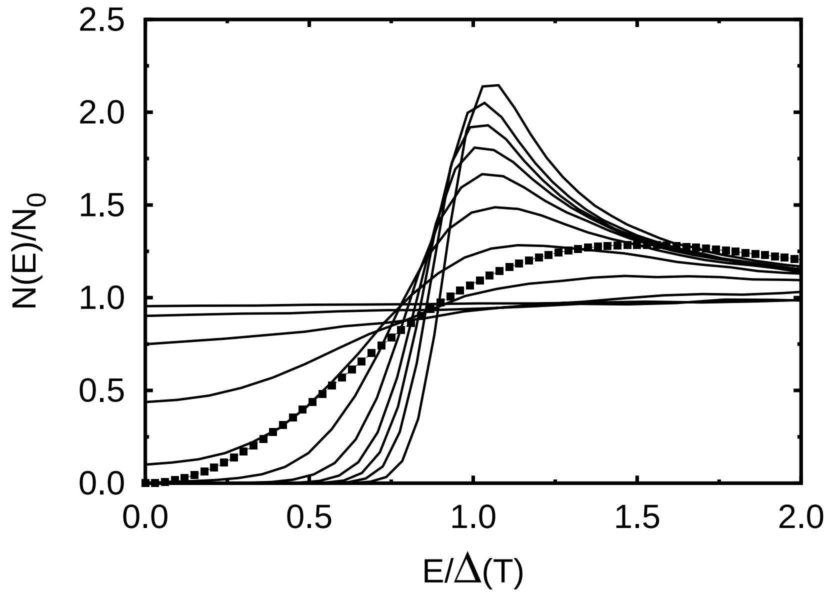

Fig. 4. The electronic density of states as a function of temperature. The temperatures are 0.1, 0.2, 0.3 ... $1.0 \times T_c^{MF}$. The Ginzburg temperature is set to $T_G = 0.1 T_c^{MF}$. The square boxes are the result of the Gaussian calculation in the limit correlation length going to infinity. N_0 is the bare density of states.

where L is the length of the system. The density of states can then be obtained by numerically differentiating $\mathcal{N}(\epsilon)$ with respect to ϵ. Calculating $\varphi(x)$ for a particular configuration of the order-parameter field amounts to integrating a one-dimensional differential equation with a random potential $\Delta(x)$.

The remaining problem is to generate a typical configuration of $\Delta(x)$ and sum over all configurations with the correct statistical weight. In principle this can be done using a classical Monte-Carlo simulation. It turns out that there is a much more efficient way for this problem since eigenfunctions of the transfer matrix for the free energy function Eq. (7) can be calculated easily. Using the transfer matrix formalism, this problem can be mapped to a Langevin equation for $\Delta(x)$:

$$\frac{\partial \Delta}{\partial x} = \exp(-i\Phi) f(|\Delta|) + \eta \tag{13}$$

where f is the "guiding function" of the random walk and η is complex Gaussian white noise. If $f(|\Delta|)$ is a linear function then Eq. 13 just describes an Orenstein-Uhlenbeck process with a Gaussian spatial correlation. It has been shown that f can be obtained from the transfer-matrix of the Eq. 7.

The exact result for the density of states of the electrons as a function of temperature is shown in Fig. 4 and compared with the result of the calculation assuming Gaussian fluctuations with a very long correlation length [13]. Whereas the Gaussian model still allows many states in the mean-field gap, the non-Gaussian fluctuations remove the states much more effectively. The artefact in the Gaussian model that the density of states behaves like $N(\epsilon) \sim \epsilon^2$ even if the correlation length is infinite is due to the fact that in the Gaussian model the most probable value for the order parameter is $|\Delta| = 0$ which is not true in the non-Gaussian model. In the Gaussian theories the suppression of the electronic states is due to the large amplitude of the order parameter fluctuations which are strongly overestimated if one would like to obtain the same loss of spectral weight as in the non-Gaussian model. Since the paramagnon theories are Gaussian, the naive application to the pseudogap regime is highly questionable[18,19].

4. QUASIPARTICLES IN A TWO-DIMENSIONAL SUPERCONDUCTOR

In this section we apply the methods developed in the previous chapter to the thermodynamic properties of a quasi-particle in a two-dimensional superconductor. It has been claimed that the thermal and transport properties of a high temperature superconductor above the transition are mostly determined by the phase-fluctuations of the preformed superconducting pairs. We will apply the quasi-classical approximation which is not really justified if the length scale of the phase fluctuations of the order parameter is comparable to the lattice spacing. The main drawback of the quasiclassical approach is that it neglects the effect of vortices which have been argued to dominate this regime in approximate treatments of the Z_2 gauge theories[20,21] and QED_3 theories[22,23]. We first present the quasiclassical calculation and then outline how vortices might be taken into account.

It has been noted by Schopohl[24] that the quasi-classical Eilenberger equation of a superconductor can be mapped to the linearized Bogoliubov-DeGennes (BdG) equation. If we identify u and v with particle and hole excitations in a superconductor Eq. (8, 9) can be viewed as a BdG equation. With the phase equation, Eq. (11), it is then feasible to calculate the density of states of an inhomogeneous superconductor. We have applied this method to calculate the density of states of a quasiparticle put into a two-dimensional superconductor. We assume that the order parameter

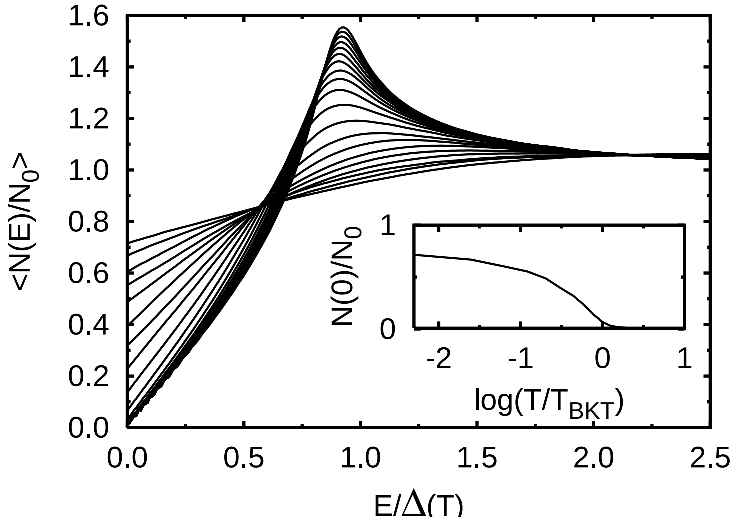

Fig. 5. Density of states of a quasiparticle in a two-dimensional $d_{x^2-y^2}$ superconductor. The inverse temperature $\beta = 1/T$ is varied from 0.1 to 2.0 in steps of 0.1. The BKT transition is located approximately at $J\beta_c \approx 0.7$, where J is the coupling of the phases. The energy is measured in terms of the amplitude of the order parameter. The inset shows the density of states at zero energy as a function of $\log(T/T_{BKT})$.

amplitude is already fixed. The phase fluctuations are then described by an xy-model. The classical xy-model can be simulated efficiently even close to the Bereshinskii-Kosterlitz-Thouless (BKT) transition using the Wolff algorithm[25]. We used a 128 x 128 grid for the xy - model. For each thermal configuration the phase equation is solved and the density of states is calculated. Finally we assume a $d_{x^2-y^2}$ gap - which is the relevant gap structure for the high temperature superconductors. The result of the calculation is shown in Fig. 5. The temperature is varied from much below the BKT transition to very high temperatures. The surprising fact is that the BKT transition has very little effect on the equilibrium electronic degrees of freedom. At very high temperatures one does recover most of the density of states although the order parameter is already established. At very low temperatures one recovers the usual d-wave density of states for a $d_{x^2-y^2}$ superconductor, which is linear at low energies[26,27]. It would be interesting to apply the quasi-classical approach to the transport properties in the phase-fluctuation regime. However, for transport vortices have a highly nontrivial effect on the electrons[22,23]. In these calculations the vortices were taken into account by using a singular gauge transformation. Recently interfering paths in the quasiclassical approach have been studied by Ozana and Shelankov[28]. This approach might be promising to examine the transport of a quasiparticle in a two-dimensional d-wave superconductor close to the transition. Another question which arises naturally in this context is how impurities affect single particle properties. This question has been studied mostly in the superconducting state[29]. The nodes in the d-wave gap have a profound effect - making the system more one-dimensional and thus more susceptible to localization of the remaining quasiparticles close to the quantum phase transition (see e.g. Vojta et al.[30]).

5. CONCLUSIONS

Paramagnon-like theories have been used extensively to study electronic properties of itinerant electronic systems close to a phase transition. These theories amount to using a Gaussian approximation for the incipient order parameter field. In this paper we have discussed the effect of non-Gaussian order parameter fluctuations on the electronic properties. The non-Gaussian order parameter fluctuations have been shown to be relevant for the electronic properties of a two-dimensional itinerant system close to a quantum phase transition. For a one-dimensional system close to a charge-density-wave transition the electronic properties can be calculated exactly. The suppression of the density of states is much more dramatic than in Gaussian models. Finally we have investigated a quasiparticle in a two-dimensional superconductor and mapped the problem to a one-dimensional BdG equation. Using this method the electronic contribution to thermodynamic properties in the fluctuation regime of a two dimensional superconductor can be calculated easily. Whereas the effect of the BKT transition is small on the thermodynamic properties it is clear the the topological excitations have a profound effect on the transport. It will be interesting to see how a quasiclassical theory can be modified to include effects of vortex excitations.

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