Exact Results for the Crossover from Gaussian to Non-Gaussian Order Parameter Fluctuations in Quasi One-Dimensional Electronic Systems

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The physics of quasi one-dimensional Peierls systems is dominated by order parameter fluctuations. We present an algorithm which allows for the first time to exactly calculate physical properties of the electrons gas coupled to classical order parameter fluctuations. The whole range from the Gaussian regime dominated by amplitude fluctuations to the non-Gaussian regime dominated by phase fluctuations is accessible. Our results provide insight into the ‘pseudogap’ phenomenon occurring in underdoped high-$T_c$ superconductors, quasi one-dimensional organic conductors and liquid metals.

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Pseudogaps have been discussed recently in the context of the high temperature superconductors. Methods which were originally designed for studying the quasi one-dimensional problems \cite{1,2} have been used to describe the physics of the suppression of electronic density of states due to antiferromagnetic or superconducting fluctuations.\cite{3,4,5,6}. Here we present a method which allows to describe the crossover from the Gaussian regime dominated by amplitude fluctuations to the non-Gaussian regime dominated by phase fluctuations without any approximation. We solve the problem originally posed by Lee, Rice and Anderson\cite{7,8,9} in 1973 exactly.

Although the pseudogap problem is more general, it first appeared in the context of the charge density wave (CDW) systems. The Peierls transition of quasi one-dimensional electronic systems like K$_{0.3}$MoO$_3$ is due to the coupling of a particular phonon mode to the electrons. This coupling would lead to a mean field phase transition at some temperature $T_c^{MF}$. However, the phase transition of the one-dimensional system to the charge density wave phase, which would break a continuous symmetry is prevented by order parameter fluctuations. Only at some lower temperature, $T_c^{3D}$, determined by the three-dimensional coupling of the one-dimensional systems the charge density wave phase is established. The Kohn anomaly leads to a softening of the phonon so that at some temperature close to the mean field Peierls transition temperature, $T_c^{MF}$ the phonon mode can be viewed as a static lattice distortion. The properties of the electrons in the intermediate temperature regime $T_c^{MF} \gg T \gg T_c^{3D}$ are determined by the coupling to 1D CDW order parameter fluctuations, which the mean-field theory does not describe even qualitatively. All attempts to describe the electronic properties in this regime starting with Lee, Rice and Anderson\cite{7,8,9} assume Gaussian order parameter amplitude fluctuations. Recent calculations\cite{10,11,12} corrected a technical mistake in the original paper by Sadovskii\cite{13} but confirmed that the density of states, $N(\epsilon)$, of the electrons behaves like $N(\epsilon) \sim \epsilon^2$ below the mean field gap for large correlation lengths in the Gaussian model which is completely unphysical. On the other hand, even a modest suppression of the density of states, i.e. a pseudogap, requires an enormous correlation length in a Gaussian model\cite{10,12}. Models taking into account phase fluctuations only\cite{14}, which should contain the right physics far below $T_c^{MF}$, tend to overestimate the suppression of the electronic density at the Fermi surface and cannot describe the physics above the mean field transition. Thus a more sophisticated approach is needed.

We begin by defining the problem. The dispersion of the electrons close to the Fermi energy can be assumed to be linear. The Hamiltonian of the electrons has the form:

$$\hat{H} = -i v_F (R^{1 \dagger} \partial_x R - L^{1 \dagger} \partial_x L) + \Delta(x) R^{1 \dagger} L + \Delta^*(x) L^{1 \dagger} R,$$

where the operators $R^{1}$ and $L^{1}$ 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. Contrary to the assumption in previous work, it is not sufficient to describe the order parameter fluctuations by the variance and correlation length only, but that one needs to consider higher moments of the order parameter correlator. This becomes intuitively clear if one considers two cases. 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 off at a distance $v_F/\Delta$ 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.
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. 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. The classical complex order parameter fluctuations, $\Delta(x)$ are described by the Ginzburg-Landau functional:

$$F[\Delta(x)] = \int_0^L dx / \xi_0 (c|\partial_x \Delta|^2 + a|\Delta|^2 + b|\Delta|^4)$$

(2)

Close to the mean field phase transition $a$ varies linearly with the temperature $a(T) = a^0(T/T_c^{MF} - 1)$, whereas $b$ and $c$ (and therefore the length scale, $\xi_0 = \sqrt{c/a^0}$) are nearly temperature independent. In principle, the coefficients $a$, $b$, and $c$ have to be determined self consistently from the electronic properties. The 1D system is disordered above the 3D ordering temperature, $T^{3D}$. Nevertheless the action Eq. (2) has two different regimes: if $a(T)$ is positive and large, the order parameter fluctuations are centered around zero and basically Gaussian. For $a(T)$ negative and large the amplitude of the order parameter is given by $\sqrt{<\Delta^2>}$ and only the phase fluctuations play a role.

Here we would like to sum over all configurations of the order parameter with the Boltzmann weight, $\exp(-F[\Delta(x)])/kBT_c$. The technical problem is how to generate a sufficiently large configuration of the order parameter (typically lengths of a chain: $L \sim 10^7 \xi_0$) in the intermediate regime so that the electronic properties can be calculated reliably. A Monte Carlo simulation of such a large system can in principle be done (a more sophisticated algorithm like the Wolff algorithm has to be adopted to avoid critical slowing down close to $T^{MF}$) but it turns out that there is a much simpler way to perform the calculation. The method presented here is based on the transfer matrix formalism first used by Scalapino, Sears and Ferrell to calculate the thermodynamic properties of classical order parameter fluctuations in one dimension exactly. It is useful to write the free energy in units where the length is measured in units of $\xi_0$, the size of the order parameter in units of $\Delta_0 = \sqrt{a^0/2b}$ and the temperature in units of $T^{MF}_c$, $\tau = T/T^{MF}_c - 1$. The reduced Ginzburg temperature, $\Delta \tau$, at which the fluctuations start to dominate is $\Delta \tau = (a^0 2/kBT^{MF}_c)^{-2/3}$ (note the factor of 2 between our definition and Ref.[13]). The relevant physical parameters are the bare length scale, $\xi_0$, the gap scale, $\Delta_0$, the mean field critical temperature, $T^{MF}_c$, and the size of the fluctuation regime, $\Delta \tau$.

The transfer Hamiltonian for Eq. (2) is given in appropriate units by:

$$\frac{\hat{H}}{k_B T_c} = \sqrt{\Delta \tau} \left[ -\frac{1}{2} \nabla^2 + \frac{1}{2} \frac{\tau}{\Delta \tau} |\Delta|^2 + \frac{1}{4} |\Delta|^4 \right]$$

(3)

where $\vec{\Delta}$ is a two dimensional vector of the real order parameter components, $\Delta = \Delta' + i \Delta''$ and $\Delta = (\Delta', \Delta'')$. The Nabl operator is defined as $\nabla = (\partial_{\Delta'}/\partial_{\Delta'})$. The prefactor of the Hamiltonian, $\sqrt{\Delta \tau}$, can be absorbed in the length scale. This Schrödinger equation in imaginary time is equivalent to a stochastic random walk where the groundstate wavefunction is the distribution function of the spatial coordinate of the Schrödinger equation. The “spatial” coordinate of the transfer Hamiltonian is the order parameter fluctuation $\Delta$ and the imaginary time corresponds to the spatial coordinate along the chain $x$. To see this, we introduce the wavefunction, $\psi$, as a ratio $\psi(\Delta, x) = \Phi(\Delta, x)/\psi_0(\Delta, x)$ of an auxiliary function $\Phi$ and $\psi_0$ the ground state wave function of the anharmonic oscillator for given parameters $a$, $b$ and $c$. The function $\Phi$ obeys the following equation of motion:

$$\frac{\partial \Phi}{\partial x} = -\frac{1}{2} \nabla^2 \Phi + \nabla \cdot \left( \frac{\nabla \psi_0}{\psi_0} \Phi \right).$$

(4)

This is nothing but a diffusion equation for $\Phi$. The diffusion of the order parameter, $\Delta$, can thus be described by a Langevin equation:

$$\frac{\partial \vec{\Delta}}{\partial x} = -\nabla \psi_0 / \psi_0 + \vec{\eta},$$

(5)

where $\vec{\eta} = (\eta', \eta'')$, is uncorrelated Gaussian noise in the complex plane which can be generated easily.

The Langevin equation Eq. (5) is nonlinear but can be simulated very easily (see e.g. [17]). The distribution of the order parameter fluctuations $\Delta$ is given by construction by the ground state wave function of the transfer Hamiltonian. The key observation now is that the order parameter fluctuations which can be locally generated from the Langevin equation Eq. (5) have precisely the statistics given by the action Eq. (2). The Langevin equation, Eq. (5) can be viewed as an extremely efficient way to generate typical order parameter fluctuations.

The method presented here is related to the path integral Monte Carlo algorithm in which the solution of the Schrödinger equation is obtained by simulating the kinetic energy with a diffusion equation and the potential energy using a von Neumann rejection to implement importance sampling [10]. Because the “guiding function”, $\psi_0$, is the solution of the transfer Hamiltonian Schrödinger equation “paths” (configurations) in the order parameter space are generated according to their weight in the partition function. In some sense we have inverted the path integral Monte Carlo method to generate the paths according to their statistical weight.

As a first test, we use Eq. (5) to generate a configuration of a chain with length $L = 10^6$ and calculate the average of the square of the order parameter fluctuation, $<|\Delta|^2>$, and the correlation length $\xi$ and compare to the exact results by Scalapino et al. [13] in Fig. 1. It is obvious that even for a relative short chain the calculated
FIG. 1: Variance and correlation length of the order parameter fluctuations as a function of reduced temperature, $\tau$ generated using Eq. (5) (marked by ◦) for a finite system with length $L = 10^6$ compared to the exact results by Scalapino et al. [15] (dashed line).

The density of states of Eq. (1) for a given order parameter configuration can be calculated by various methods, for example by using a lattice version of the Hamiltonian Eq. (1) and exact diagonalization [11] or some more sophisticated method based on the phase formalism which has been developed recently in Ref. [12] (for a detailed description see [18]). We calculate the density of states with the Langevin equation for the order parameter, Eq. (5) which contains amplitude and phase fluctuations. In this way only local information is needed to calculate the properties of the electrons. The requirement for storage is minimal compared to a full simulation of the classical field. The density of states can be obtained by differentiating numerically the integrated density of states. The resulting density of states as a function of energy is shown in Fig. 2. The energy scale at a fixed temperature is $\Delta(T) = \sqrt{\langle |\Delta|^2 \rangle}$.

The calculated density of states shown in Fig. 2 has several features which apparently resolve some of the problems of the approximations made in previous calculations. One of the problems of the Gaussian approximations is that only for very large correlation lengths of the order parameter fluctuations a pseudogap appears. Here we see that already for relatively modest correlation lengths much above the mean field transition the density of states at zero frequency is strongly suppressed. Our calculation smoothly interpolates between the amplitude fluctuation dominated regime and the phase fluctuation dominated regime.

The localization length can be calculated from the Thouless relation [12], and is presented in Fig. 3. For increasing temperatures the localization length decreases and approaches zero uniformly. The localization length at a given energy is a monotonic function of temperature which is different from the phase fluctuation only model [13]. This might be due to the fact that in those
models the variation of the gap scale as a function of temperature is not taken into account.

Finally we discuss the implication of our calculation for experiments. As an example, we calculate the temperature dependence of the electronic spin susceptibility as a function of temperature. The relevant parameters are the size of the gap fluctuations $\Delta_0$ and the size of the fluctuation regime, $\Delta\tau$. Apparently excellent agreement can be achieved with the experimentally determined Ginzburg temperature 20K for $K_{0.3}MoO_3$ [20]. At a lower temperature, $T_{3D}$, three-dimensional ordering sets in ($T_{3D}/T_{MF} = 0.4$, 0.6 and 0.26 for TaS$_3$, $K_{0.3}MoO_3$ and (TaSe$_4$I)$_2$, respectively). The departure from the purely 1D behavior can be most clearly noted for $K_{0.3}MoO_3$.

To summarize, we have developed a new algorithm for studying the electronic properties of the quasi-one-dimensional Peierls systems which allowed for the first time to study the electronic properties in crossover regime from the Gaussian to the non-Gaussian regime of the order parameter fluctuations without further approximations. Similar problems appear in the study of the pseudogap phenomenon in the High Temperature Superconductors. More general the question of what happens to an electronic system coupled to soft classical degrees of freedom is relevant not only for the pseudogap but also for the question of how to describe the moment formation in an itinerant electronic system. These questions have been discussed in terms of sophisticated perturbation theories, like the Parquet approximation [21], or self consistent approaches like the SCR theory by Moriya [22]. Our calculation basically demonstrates that it is not possible to describe the moment formation by Gaussian fluctuations (or perturbation theory), but that a self consistent theory which takes into account the non-Gaussian fluctuations into account is necessary.

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