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 us 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 [1,2] have been used to describe the physics of the suppression of electronic density of states due to antiferromagnetic or superconducting fluctuations [3–6]. Here we present a method which allows us to describe the crossover from the Gaussian regime dominated by amplitude fluctuations to the non-Gaussian regime dominated by phase fluctuations. We solve the problem originally posed by Lee, Rice, and Anderson [1] 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 such as $K_{0.3}MoO_3$ 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 $T_c^{\mathrm{MF}} \gg T \gg T_c^{\mathrm{3D}}$ 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 [1,2,7–9] assume Gaussian order parameter amplitude fluctuations. Recent calculations [10–12] corrected a technical mistake in the original paper by Sadovskii [2] but confirmed that the density of states, $N(\epsilon)$, of the electrons behaves as $N(\epsilon) \sim \epsilon^2$ 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 [11,12]. Models taking into account phase fluctuations only [13], 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

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

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. Contrary to the assumption in previous work, it is *not* sufficient to describe the order parameter fluctuations by the *variance* and *correlation length* only. In fact it is necessary 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 wave function 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 wave function decays over a distance v_F/Δ and has a large kinetic energy. For the *same* correlation length and variance of the order parameter the electronic wave function 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

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exists in only one dimension [11,12]. 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

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

Close to the mean-field phase transition a varies linearly with the temperature $a(T) = a'(T/T_c^{\mathrm{MF}} - 1)$, whereas b and c (and therefore the length scale, $\xi_0 = \sqrt{c/a'}$) 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_c^{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 $\sqrt{\langle \Delta^2 \rangle}$ 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, $\exp(-F[\Delta(x)]/k_B T_c)$. 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 [14] has to be adopted to avoid critical slowing down close to T_c^{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 [15] 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 ξ_0, the size of the order parameter in units of $\Delta_0 = \sqrt{a'/2b}$, and the temperature in units of T_c^{MF}, $\tau = T/T_c^{\mathrm{MF}} - 1$. The reduced Ginzburg temperature, $\Delta\tau$, at which the fluctuations start to dominate is $\Delta\tau = (a'^2/b k_B T_c^{\mathrm{MF}})^{-2/3}$ (note the factor of 2 between our definition and Ref. [15]). The relevant physical parameters are the bare length scale, ξ_0, the gap scale, Δ_0, the mean-field critical temperature, T_c^{MF}, and the size of the fluctuation regime, $\Delta\tau$.

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

$$\frac{\hat{H}}{k_B T_c} = \sqrt{\Delta\tau}\left[-\frac{1}{2}\nabla^2 + \frac{1}{2}\frac{\tau}{\Delta\tau}|\vec{\Delta}|^2 + \frac{1}{4}|\vec{\Delta}|^4 \right], \quad (3)$$

where $\vec{\Delta}$ is a two-dimensional vector of the real order parameter components, $\Delta = \Delta' + i\Delta''$ and $\vec{\Delta} = (\Delta', \Delta'')$. The Nabla 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 [16] where the ground state wave function is the *distribution function* of the spatial coordinate of the Schrödinger equation. The "spatial" coordinate of the transfer Hamiltonian is the order parameter fluctuation Δ and the imaginary time corresponds to the spatial coordinate along the chain x. To see this, we introduce the wave function, ψ, as a ratio $\psi(\Delta, x) = \Phi(\Delta, x)/\psi_0(\Delta, x)$ of an auxiliary function Φ and ψ_0 the ground state wave function of the anharmonic oscillator for given parameters a, b, and c. The function Φ obeys the following equation of motion:

$$\frac{\partial \Phi}{\partial x} = -\frac{1}{2}\nabla^2\Phi + \nabla \cdot \left(\frac{\nabla\psi_0}{\psi_0}\Phi \right). \quad (4)$$

This is nothing but a diffusion equation for Φ. The diffusion of the order parameter, Δ, can thus be described by the Langevin equation

$$\frac{\partial \vec{\Delta}}{\partial x} = -\frac{\nabla\psi_0}{\psi_0} + \vec{\eta}\,, \quad (5)$$

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

The Langevin equation (5) is nonlinear but can be simulated very easily (see, e.g., [17]). The distribution function of the order parameter Δ is given by the ground state wave function of the transfer Hamiltonian by construction. The key observation now is that the order parameter fluctuations which can be *locally* generated from the Langevin equation (5) have precisely the statistics given by the action Eq. (2). The Langevin equation (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 [16]. Because the "guiding function," ψ_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, $\langle|\Delta|^2\rangle$, and the correlation length ξ and compare to the exact results by Scalapino *et al.* [15] in Fig. 1. It is obvious that even for a relative short chain the calculated variance and correlation length are basically identical to the exact results. The differences are due to the numerical evaluation of the drift function $\nabla\psi_0/\psi_0$. We solve the Schrödinger equation (1) numerically and approximate the logarithmic derivative of the ground state wave function by a fourth

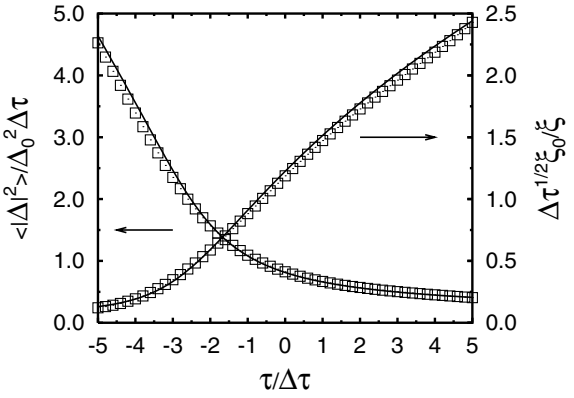

FIG. 1. Variance and correlation length of the order parameter fluctuations as a function of reduced temperature τ generated using Eq. (5) (marked by □) for a finite system with length $L = 10^6$ compared to the exact results by Scalapino *et al.* [15] (solid line).

order polynom in $|\vec{\Delta}|$, which apparently is a very good representation of $|\nabla\psi_0|/\psi_0(|\vec{\Delta}|)$. As an aside we remark that for the case of Gaussian order parameter fluctuations the drift term $|\nabla\psi_0|/\psi_0(|\vec{\Delta}|)$ is linear and corresponds to the Ornstein-Uhlenbeck process considered in Ref. [12].

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 [18], 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

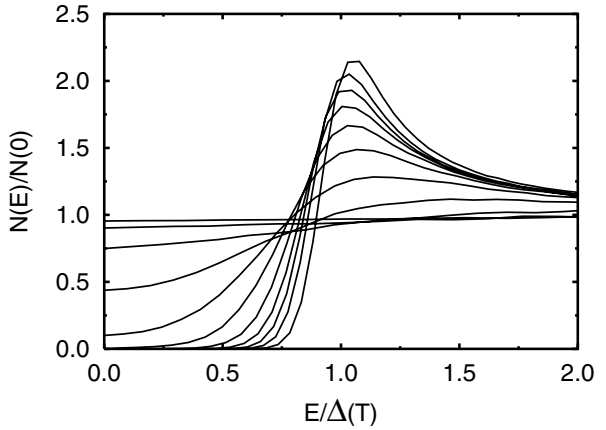

FIG. 2. The density of states normalized to the bare density of states, $N(0)$, as a function of energy, $E/\Delta(T)$, and reduced temperature τ. The temperature varies from $\tau/\Delta\tau = -10\ldots0$ in steps of one. As the temperature is decreased below the mean-field transition the density of states is strongly suppressed.

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 Δ_0 and the size of the fluctuation regime, $\Delta\tau$. A comparison of the theoretically calculated susceptibility and the experimental data is shown in Fig. 4. Apparently excellent agreement can be achieved with the experimentally determined Ginzburg temperature 20 K 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 $(TaSe_4)_2I$, respectively].

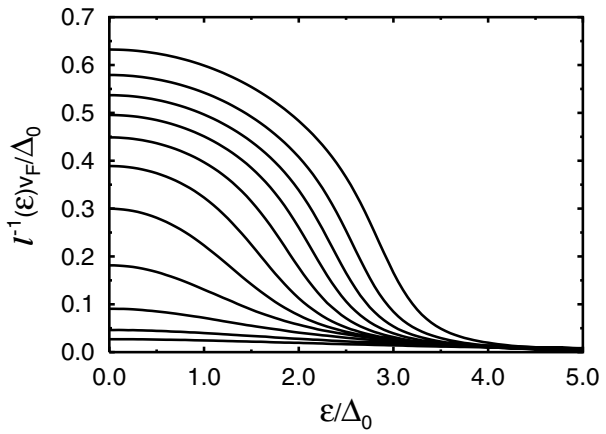

FIG. 3. The inverse localization length as a function of frequency for reduced temperature. τ varies from $\tau/\Delta\tau = -10\ldots0$ in steps of one. The localization length increases with decreasing temperature. The lower curve corresponds to the highest temperature and the topmost to the lowest temperature.

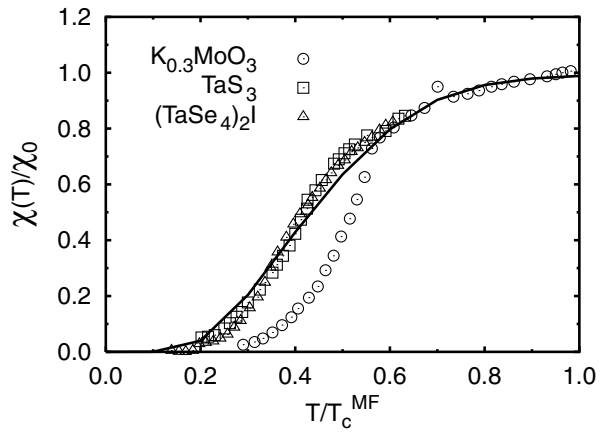

FIG. 4. Experimentally determined static spin susceptibilities $\chi_0(T)$ for a number of materials from Ref. [19] and a tentative fit (solid line) using the calculated density of states. The parameters are $\Delta_0 = 2T_c^{\mathrm{MF}}$ and $\Delta\tau = 0.1$.

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 us to study the electronic properties in the 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 generally, 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, such as the Parquet approximation [21], or self-consistent approaches such as the self-consistent renormalization 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 is necessary.

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