Classical Phase Fluctuations in Incommensurate Peierls Chains

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In the pseudogap regime of one-dimensional incommensurate Peierls systems, fluctuations of the phase of the order parameter prohibit the emergence of long-range order and generate a finite correlation length. For classical phase fluctuations, we present exact results for the average electronic density of states, the mean localization length, the electronic specific heat and the spin susceptibility at low temperatures. Our results for the susceptibility give a good fit to experimental data.

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Continuous symmetries in one-dimensional electronic systems are not spontaneously broken at any finite temperature. The mean-field prediction of a finite critical temperature $T_{c}^{MF}$ is incorrect in this case. The experimentally observed Peierls transition at a finite temperature $T_{c}^{3D} \ll T_{c}^{MF}$ in many quasi one-dimensional conductors is due to weak interchain coupling which triggers a crossover to three-dimensionality. In the intermediate temperature regime $T_{c}^{3D} \lesssim T \lesssim T_{c}^{MF}$, the physical properties of Peierls chains are dominated by one-dimensional order parameter fluctuations. This is the so-called pseudogap regime where mean-field theory is not even qualitatively correct.

In this work, we shall present an exact solution of an effective model for the low temperature thermodynamics of incommensurate Peierls chains. For incommensurate chains, the order parameter $\Delta(x)$ is complex, so that in the pseudogap regime the generalized Ginzburg-Landau potential has the form of a “Mexican hat”. It is then a good approximation to ignore amplitude fluctuations of $\Delta(x) = |\Delta(x)|e^{i\theta(x)}$ and focus on the gapless fluctuations of the phase $\theta(x)$. At long wavelengths and low energies, the thermodynamics of phase fluctuations can be described by a classical Hamiltonian which is formally identical with the kinetic energy of a superfluid. However, the calculation of the electronic properties amounts to solving a one-dimensional random problem with colored noise. Usually, problems of this type cannot be solved exactly. At low energies, the electronic degrees of freedom can be described by the Hamiltonian of the so-called fluctuating gap model (FGM)

$$H_{d} = -iv_{F}\partial_{x}\sigma_{3} + \Delta(x)\sigma_{+} + \Delta^{*}(x)\sigma_{-},$$

where $v_{F}$ is the Fermi velocity, $\sigma_{i}$ are the usual Pauli matrices, with $\sigma_{\pm} = \frac{1}{2}(\sigma_{1} \pm i\sigma_{2})$. In the pseudogap regime, the gapped amplitude fluctuations are frozen out, so that we may set $\Delta(x) = \Delta_{s}e^{i\theta(x)}$, where $\Delta_{s}$ is determined by the local minimum of the generalized Ginzburg-Landau functional. From Eq. (1), it is then easy to show that

$$\langle \Delta(x)\Delta^{*}(x') \rangle = \Delta_{s}^{2}e^{-|x-x'|/\xi},$$

where $\langle \ldots \rangle$ denotes the thermodynamic average with respect to the Hamiltonian $H_{d}$ given in Eq. (1), and the order parameter correlation length is $\xi = n_{s}/(2m^{*}T)$. In this work, we shall calculate the average electronic density of states (DOS) $\rho(\omega) = \langle \text{Tr} \delta(\omega - H_{d}) \rangle$ of the model defined via Eqs. (1)–(3) exactly for arbitrary $\xi$.

Previously, the DOS of the FGM has been calculated assuming a Gaussian distribution of $\Delta(x)$ with covariance given by Eq. (3). Although in this case the problem is not exactly solvable, a sophisticated algorithm has been developed which produces an expression for $\rho(\omega)$ which is reasonably close to the exact numerical result for Gaussian disorder. However, as explained above, the assumption of a Gaussian distribution of $\Delta(x)$ centered at $\Delta = 0$ is rather unphysical in the pseudogap regime. It is therefore not surprising that in this regime the true behavior of $\rho(\omega)$ (to be discussed below) is very different from the DOS for Gaussian disorder.

The electronic contribution to the thermodynamic properties of our system can be obtained from the disorder-averaged free energy

$$F_{el} = -T \int_{-\infty}^{\infty} d\omega \int_{0}^{L} dx \langle \rho(x,\omega) \rangle \ln(1 + e^{-\omega/T}) .$$

The local DOS $\rho(x,\omega)$ can be expressed as $\rho(x,\omega) = -\pi^{-1}\text{Im} \text{Tr} \mathcal{G}(x, x, \omega + i0^{+})$, where the Green function $\mathcal{G}(x, x', \omega + i0^{+})$ satisfies

$$[\omega - H_{d}] \mathcal{G}(x, x', \omega + i0^{+}) = \delta(x - x')\sigma_{0} .$$

Here, $\sigma_{0}$ is the $2 \times 2$ unit matrix. For periodic boundary conditions, the average $\langle \rho(x,\omega) \rangle$ is independent of $x$ and can be identified with the average DOS $\rho(\omega)$.
Following Ref. [10], we eliminate the phase of the order parameter \( \Delta(x) = \Delta e^{i\phi(x)} \) via a gauge transformation,

\[
\mathcal{G}(x, x', \omega) = e^{i\tau_3 \phi(x)} \mathcal{G}(x, x', \omega) e^{-i\tau_3 \phi(x')} .
\]  

(6)

The transformed Green function \( \mathcal{G} \) satisfies an equation of the form (3), but with \( H_{el} \) replaced by

\[
\hat{H}_{el} = -iv_F \partial_x \sigma_3 + V(x) \sigma_0 + \Delta_4 \sigma_1 ,
\]

(7)

where \( V(x) = \frac{\pi}{\tau} \partial_x \phi(x) \). Eq. (3) is a chiral transformation that eliminates the phase of \( \Delta(x) \) in favor of a forward scattering random potential \( V(x) \). The local DOS is invariant under this transformation, so that we may replace \( \mathcal{G} \to \mathcal{G} \) in all expressions involving the DOS. The crucial point is now that with \( H_{el} \) given by Eq. (3), the probability distribution of \( V(x) \) is determined by Gaussian white noise, with zero average and covariance \( \langle V(x)V(x') \rangle = v_F^2 (2\xi)^{-1} \delta(x-x') \). Due to the Gaussian white noise statistics of \( V(x) \), the average DOS of our model can be calculated exactly in the thermodynamic limit. Several methods of obtaining the exact \( \rho(\omega) \) are available. Actually, Eq. (3) is a special case of the class of random Hamiltonians discussed by Hayn and Mertschinger [11], who calculated the average DOS by means of the supersymmetry method [12]. Alternatively, the DOS can be calculated within the phase formalism [14]. In Ref. [13] a modification of this formalism [15] is used to directly obtain the integrated Green function \( \Gamma(\omega) \) defined via \( \partial_x \Gamma(\omega) = \text{Tr} \langle \mathcal{G}(x_0, x_0 + \tau^+) \rangle \) from the solution of a Fokker-Planck equation. For \( L \to \infty \), only the stationary solution is needed, and we obtain

\[
\Gamma(\omega) = \ell^{-1}(\omega) - i\pi N(\omega) = \pi \rho_0 \Delta \Gamma_{\nu}(g)/I_{\nu}(g) ,
\]

(8)

where \( \rho_0 = (\tau^+ v_F)^{-1} \) is the DOS for \( \Delta = 0 \), and \( I_{\nu}(g) \) is a modified Bessel function with imaginary index \( iv \). The dimensionless parameters \( g \) and \( \nu \) are

\[
g = \frac{4\Delta_4 \xi}{v_F} = \frac{2n_s}{m^* v_F} \Delta s , \quad \nu = \frac{4\omega \xi}{v_F} = \frac{\omega}{\Delta s} .
\]

(9)

Note, that the imaginary part of \( \Gamma(\omega) \) is proportional to the integrated average DOS \( N(\omega) \) which satisfies \( \partial_\omega N(\omega) = \rho(\omega) \) while, according to Thouless [14], the real part of \( \Gamma(\omega) \) can be identified with the inverse mean localization length \( \ell^{-1}(\omega) \), i.e. the Lyapunov exponent [9]. Using a Wronskian relation for \( I_{\nu}(g) \) [13] we get

\[
N(\omega) = \rho_0 v_F \sinh((\pi \nu)/4 \xi^2 |I_{\nu}(g)|^2 .
\]

(10)

For the inverse mean localization length we get

\[
\ell^{-1}(\omega) = \frac{\Delta s}{v_F} \frac{\partial}{\partial g} \ln |I_{\nu}(g)| .
\]

(11)

We now discuss the behavior of the average DOS. Because \( \rho(\omega) \) is an even function of \( \omega \), we restrict ourselves to \( \omega \geq 0 \). Using [15] \( |I_{\nu}(0)|^2 = (\pi \nu)^{-1} \sin(\pi \nu) \) one easily verifies that \( N(\omega) \sim \rho_0 \omega \) for \( g \to 0 \), so that in this limit we recover the result for free electrons with linearized energy dispersion. While for small \( g \), the leading corrections can be calculated perturbatively in powers of \( g \). In the pseudogap regime \( g \gg 1 \), the behavior of the average DOS is quite complicated. It is convenient to measure frequencies in units of \( \Delta_4 \), and to express Eq. (4) in terms of the Bessel function \( J_{\nu}(g \omega) \) with imaginary index and argument, using \( I_{\nu}(g) = e^{\pi \nu/2} J_{\nu}(g \omega) \) [13]. Defining \( \omega = \omega/\Delta_4 = \nu/g \), we may write

\[
\rho(\omega) = \frac{\rho_0}{2\pi g} \frac{\partial}{\partial \omega} |J_{\nu}(g \omega)|^2 .
\]

(12)

In Fig. 4 we show a graph of Eq. (12) for several values of \( \nu \). For a more quantitative analysis, we use the uniform asymptotic expansion of \( J_{\nu}(\nu g) \) for large \( g \) and fixed \( \omega \) [13] which reveals three different regimes: First of all, for \( 1 - \omega \gg g^{-2/3} \) (i.e. for frequencies sufficiently far below \( \Delta_4 \), the average DOS in the pseudogap regime \( g \gg 1 \) can be approximated by

\[
\rho(\omega)/\rho_0 \approx 2g(1 - \omega^2)^{1/2} \exp[-2gQ(\omega)] \times [1 + e^{-2g\omega}] \pi \text{arcsec}(\omega) ,
\]

(13)

where \( Q(\omega) = (1 - \omega^2)^{1/2} \) and \( \text{arcsec}(\omega) \). In particular, for small \( \omega \), we may expand \( Q(\omega) \approx 1 - \frac{\omega^2}{2} + \frac{\omega^4}{2} \), so that

\[
\rho(\omega)/\rho_0 \approx 2\pi g e^{-2g\omega} \cosh[\pi g \omega] e^{-\omega^2/2}, \quad \omega^2 \lesssim 1 .
\]

(14)

Hence, for \( \omega = 0 \), the DOS is exponentially small, \( \rho(0)/\rho_0 \approx 2\pi g e^{-2g} \). As shown in Fig. 2, such a strong suppression of the DOS at the Fermi energy is a unique feature for classical phase fluctuations, which is neither reproduced within the Born approximation [13] (which predicts \( \rho(0) \propto g^{-1} \)), nor for Gaussian disorder [13] (where \( \rho(0) \propto g^{-\nu} \), with \( \nu \approx 0.64 \)). The approximation (13) breaks down when \( 1 - \omega \) becomes comparable with \( g^{-2/3} \). Note that \( Q(1 - \epsilon) \approx \epsilon^{2/3} g^{-2/3} \) for \( \epsilon \ll 1 \), so that \( gQ(\omega) = O(1) \) when Eq. (13) ceases to be valid. In this case, we have to go back to our exact result (12) which implies for \( |1 - \omega| \lesssim g^{-2/3} \ll 1 \)

\[
\rho(\omega)/\rho_0 \approx a_1 g^{1/3}[1 - a_2 g^{1/3}(\omega - 1)^2] .
\]

(15)

Here, \( a_1 = 2^{-4/3} \pi^{-1} c_2 / c_1 \approx 0.7306 \) and \( a_2 = 2^{2/3} [3(c_2/c_1)^2 - 1] / c_1 \approx 0.3534 \), with \( c_1 = A_i(0) = \{3^{2/3} \Gamma(2/3)\}^{-1} \) and \( c_2 = -A_i(0) = \{3^{2/3} \Gamma(1/3)\}^{-1} \), where \( A_i(x) \) is the Airy function. From Eq. (15), we conclude that, leading order in \( g \gg 1 \), the average DOS exhibits a maximum precisely at \( \omega = \Delta_s \), with a height that diverges as \( g^{-2/3} \propto \xi^{1/3} \propto T^{-1/3} \) for \( T \to 0 \). Finally, for \( \omega - 1 \gg g^{-2/3} \), our exact result (12) reduces to the well known expression for the DOS in the presence of a static gap, \( \rho(\omega)/\rho_0 \approx \omega/\sqrt{\omega^2 - 1} \). At \( \omega - 1 \approx g^{-2/3} \), this expression smoothly matches with the parabola (13).
In Fig. 8 we show the exact inverse localization length $\ell^{-1}(\omega)$ given in Eq. (11) for several values of $g$. For $g \gg 1$ we obtain the following approximations: $\ell^{-1}(\omega) \approx (\Delta_s/v_F)(1 - \omega^2)^{1/2}$ for $1 - \omega \gtrsim g^{-2/3}$, where $\Delta_s \approx 2^{-2/3}c_2/c_1 \approx 0.4592$; finally, for $\omega \gtrsim g^{-2/3}$ the leading behavior is $\ell^{-1}(\omega) \approx (\Delta_s/v_F)[2g(\omega^2 - 1)]^{-1}$.

Let us now consider the electronic contribution to the free energy $F_{el}$ defined in Eq. (3). For the FGM with a linearized energy dispersion, Eq. (3) is ultraviolet divergent, because then the DOS approaches a constant for $|\omega| \to \infty$. However, physical quantities involve derivatives of $F_{el}$, which at low temperatures depend only on the low-energy part of the spectrum and are finite. For convenience, we regularize Eq. (3) by subtracting from $F_{el}$ the free energy $F_{el}^{\xi=\infty}$ for an infinite correlation length, where the gap is static. After an integration by parts, we express the integral in Eq. (4) in terms of a fermionic Matsubara sum and obtain

$$F_{el} - F_{el}^{\xi=\infty} = \frac{2L\Delta_s T}{v_F} \sum_{n=0}^{\infty} \left[ 1 + \frac{\omega_n^2}{\omega_n^2} \right]$$

where $\omega_n = \pi(2n + 1)/\Delta_s$. For large $\omega_n$, the term in the square bracket vanishes as $\omega_n^{-2}$, so that the sum converges. In the pseudogap regime $g \gg 1$, we may use the uniform asymptotic expansion of $I_{\omega_n}(g)$ for large $g$ [13] to obtain an expansion of Eq. (11) in powers of $g^{-1} \propto \xi^{-1} \propto T$. For $T \ll \Delta_s$ the leading terms are

$$F_{el} - F_{el}^{\xi=\infty} = \frac{L}{16\xi} \left[ \Delta_s - \frac{v_F}{12\pi \xi} + O(\xi^{-2}) \right].$$

The physical interpretation of this result is simple: Because $\xi$ is roughly the size of domains where the order parameter is spatially constant, the prefactor $L/\xi$ in Eq. (17) can be identified with the number of locally ordered domains in a system of size $L$. At distances of the order of $\xi$, the phase fluctuations distort the order parameter, which leads to an increase of the energy. In the limit $\Delta_s \xi/v_F \to \infty$, the energy scale associated with a twist in the order parameter is set by $\Delta_s$. For finite $\xi$ this energy scale decreases, because the time $\xi/v_F$ it takes for electrons to propagate over the distance $\xi$ is finite. This gives rise to the second term in Eq. (17). We emphasize that our exact result (14) gives the change in the free energy due to phase fluctuations for arbitrary $\xi$.

The low-temperature behavior of the specific heat $C_{el} = -\partial^2 F_{el}/\partial T^2$ can be calculated analytically. Keeping in mind that $\xi = n_s/(2m*^2)$, we see that the leading contribution to $C_{el}$ is due to the first correction term (involving the energy $v_F/\xi$) in Eq. (17).

$$C_{el} \sim (\pi^2/24)(n_0/n_s)^2 \rho_0 LT,$$

where $n_0 = m*^2/v_F$, and we have used the fact that the contribution from $F_{el}^{\xi=\infty}$ is exponentially small due to the static gap. Thus, in the pseudogap regime, the electronic specific heat of Peierls chains is linear in $T$, just as the specific heat for non-interacting electrons in one dimension, $C_{el}^{(0)} \sim \frac{\pi^2}{3} \rho_0 LT$. Note that $C_{el}/C_{el}^{(0)} = \frac{1}{3}(n_0/n_s)^2$ for $T \to 0$. In general, we expect that $n_s/n_0$ is a number of the order of unity for $T \ll T_c^{MF}$ [16], so that $C_{el}/C_{el}^{(0)} = O(1)$. In the same regime, we find from Eq. (14) that $\rho(0)/\rho_0 \sim 4\frac{\pi^2}{3} \frac{\rho_0}{\rho} \exp[-\frac{1}{2}\frac{\pi^2}{3} \frac{n_0}{\rho}]$, i.e. the average DOS at the Fermi energy is exponentially small (see the dashed line in Fig. 4).

Given $\rho(\omega)$, we may also calculate the spin susceptibility $\chi = T^{-1} \int_0^\infty d\omega \rho(\omega) \cosh^{-2}(\omega/2T)$. A graph of $\chi$ as a function of $T/T_c^{MF}$ is shown in Fig. 4 (solid line). The low-temperature behavior can again be calculated analytically. If $g \gg 1$ but $n_s/n_0 \ll 1$, we find $\chi \sim \frac{1}{2} \rho(0)$ (assuming now $n_s = 2$ for spin degeneracy [3]). On the other hand, for $n_s/n_0 \gg 1$ the frequency integral is dominated by a new saddle point at $\omega = \cos \rho$, where $r = \frac{n_0}{\rho}$. Using Eq. (13), we obtain

$$\chi/\rho_0 \sim 2(2\pi)^{1/2} \pi^2(\Delta_s/T)^{3/2} \exp[-\Delta_s/T],$$

where $\Delta_s = \frac{\sin \rho \Delta_s}{2\rho_0}$ and $\chi_0 = 2\rho_0$ is the susceptibility of free electrons. $n_s/n_0 > \frac{1}{2}$ implies $r < \frac{n_0}{\rho}$, so that at low temperatures the ratio $\chi/2\rho(0)$ is exponentially large, $\chi/2\rho(0) \propto \exp[(1 - \sin \rho)\Delta_s/(rT)]$. Our graph of $\chi(T)$ in Fig. 4 is quite similar to the corresponding graph given by Lee, Rice, and Anderson [16]. Note, however, that these authors assumed a real order parameter and an exponentially large correlation length at low temperatures. Because incommensurate Peierls chains are characterized by a complex order parameter and a correlation length that diverges only as a power law, $\xi \propto T^{-1}$, the agreement between the theory of Ref. [16] and experiments for incommensurate chains [17] seems to be accidental. Here, we have shown that the susceptibility data for incommensurate Peierls chains can be explained by a non-perturbative treatment of classical phase fluctuations. The exponential variation with temperature is due to the fact that in the pseudogap regime $-\ln \chi \propto T^{-1}$. Keeping in mind that our model is strictly one-dimensional and ignores amplitude fluctuations (which become important at temperatures of order $T_c^{MF}$), our theoretical curve for $\chi(T)$ shown in Fig. 4 agrees reasonably well with the susceptibility data [17].

In summary, we have presented exact results for the average DOS, the mean localization length, the susceptibility and the low-temperature thermodynamics of disordered incommensurate Peierls chains in the pseudogap regime, where only phase fluctuations are important. In particular, we have derived the exact frequency-dependence of $\rho(\omega)$ which can be measured by means of angular integrated photoemission; we predict that at low temperatures $\rho(\omega)$ exhibits a maximum at $\omega = \Delta_s$, the height of which scales as $T^{-1/3}$.

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FIG. 1. Frequency-dependence of the DOS given in Eq. (12) for $g = 4\Delta_s \xi / v_F = 0.4, 1.2, 4.0, 12, 40$ and $\infty$.

FIG. 2. The solid line is a graph of the density of states $\rho(0)$ at the Fermi energy for classical phase fluctuations as a function of $1/g = v_F / 4\Delta_s \xi$. For a comparison, the dashed line shows the result found in the leading order Born approximation [5] and the diamonds give the DOS for Gaussian statistics [9,13].

FIG. 3. Graph of the inverse localization length for $g = 4\Delta_s \xi / v_F = 0.4, 1.2, 4.0, 12, 40$ and $\infty$.

FIG. 4. Graph of the susceptibility $\chi(T)$ calculated for $\xi(T) = n_s(T)/2m^* T$ with $n_s(T)$ given in Ref. [16] and $\Delta_s(T)$ determined by minimizing a generalized Ginzburg-Landau functional. The symbols represent susceptibility data from Ref. [17]. The dashed line is the DOS at the Fermi energy.