

Microscopic theory of the pseudogap and Peierls transition in quasi-one-dimensional materials

Ross H. McKenzie*

School of Physics, University of New South Wales, Sydney, New South Wales 2052, Australia

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The problem of deriving from microscopic theory a Ginzburg-Landau free-energy functional to describe the Peierls or charge-density-wave transition in quasi-one-dimensional materials is considered. Particular attention is given to how the thermal lattice motion affects the electronic states. Near the transition temperature the thermal lattice motion produces a pseudogap in the density of states at the Fermi level. Perturbation theory diverges and the traditional quasiparticle or Fermi-liquid picture breaks down. The pseudogap causes a significant modification of the coefficients in the Ginzburg-Landau functional from their values in the rigid lattice approximation, which neglects the effect of the thermal lattice motion.

I. INTRODUCTION

A. Motivation

A wide range of quasi-one-dimensional materials undergo a structural transition, known as the Peierls or charge-density-wave (CDW) transition, as the temperature is lowered.¹⁻⁴ A periodic lattice distortion, with wave vector, $2k_F$, twice that of the Fermi wave vector, develops along the chains. Anomalies are seen in the electronic properties, due to the opening of an energy gap over the Fermi surface.

Over the past decade, due to the development of high-quality samples and higher resolution experimental techniques, data have become available which allow a quantitative comparison of experiment with theory. The most widely studied material is the blue bronze, $K_{0.3}MoO_3$. There is a well-defined three-dimensional transition at $T_P = 183$ K and careful measurements have been made of thermodynamic anomalies⁵ and CDW coherence lengths⁶ at the transition. The critical region, estimated from the Ginzburg criterion⁷ is only a few percent of the transition temperature and so the transition should be described by an anisotropic three-dimensional Ginzburg-Landau free-energy functional, except close to the transition temperature. The challenge is to derive from a microscopic theory the coefficients in the Ginzburg-Landau free energy, so that a quantitative comparison can be made between theory and experiment. Inspiration is provided by the case of superconductivity. The superconducting transition is well described by Ginzburg-Landau theory and the coefficients can be calculated from BCS theory⁸ and depend on microscopic parameters, such as the normal state density of states, Debye frequency, and the electron-phonon coupling. This program is so successful that one can even consider refinements to BCS theory, such as strong coupling effects, in order to get better agreement between experiment and theory.⁹ However, the problem

of the CDW transition is more difficult, because of the large fluctuations, due to the quasi-one-dimensionality.

B. Ginzburg-Landau theory

The Peierls transition is described by an order parameter, which is proportional to the $2k_F$ lattice distortion along the chains. The order parameter is complex if the lattice distortion is incommensurate with the lattice. For a commensurate lattice distortion (e.g., a half-filled band), the order parameter is real. I recently considered the general problem of Ginzburg-Landau theory for a three-dimensional phase transition, described by a complex order parameter, in a system of weakly coupled chains.¹⁰ The key results of that study are now summarized, partly to put this paper in a broader context.

The Ginzburg-Landau free-energy functional $F_1[\phi]$ for a *single* chain with a complex order parameter $\phi(z)$, where z is the coordinate along the chain, is

$$F_1[\phi] = \int dz \left[a|\phi|^2 + b|\phi|^4 + c \left| \frac{\partial \phi}{\partial z} \right|^2 \right]. \quad (1)$$

Near the single-chain mean-field transition temperature T_0 , the second-order coefficient $a(T)$ can be written

$$a(T) = a' \left(\frac{T}{T_0} - 1 \right). \quad (2)$$

Due to fluctuations in the order parameter, this one-dimensional system cannot develop long-range order at finite temperature.^{11,12} To describe a finite-temperature phase transition, consider a set of weakly interacting chains. If $\phi_i(z)$ is the order parameter on the i th chain, the free-energy functional for the system is

$$F[\phi_i(z)] = \sum_i F_1[\phi_i(z)] - \frac{J}{4} \sum_{\langle i,j \rangle} \int dz \operatorname{Re}[\phi_i(z)^* \phi_j(z)], \quad (3)$$

where J describes the interchain interactions between nearest neighbors. A mean-field treatment of this functional will only give accurate results if the width of the three-dimensional critical region is much smaller than T_0 . This requires that the width of the one-dimensional critical region $\Delta t_{1D} \equiv (bT_0)^{2/3}/a'c^{1/3}$ be sufficiently small that

$$\Delta t_{1D} \ll \left(\frac{J}{a'}\right)^{2/3}. \quad (4)$$

If this is not the case one can integrate out the one-dimensional fluctuations to derive a Ginzburg-Landau functional with renormalized coefficients,

$$\tilde{F}[\Phi(x, y, z)] = \frac{1}{a_x a_y} \int d^3x \left[A|\Phi|^2 + B|\Phi|^4 + C_x \left| \frac{\partial \Phi}{\partial x} \right|^2 + C_y \left| \frac{\partial \Phi}{\partial y} \right|^2 + C_z \left| \frac{\partial \Phi}{\partial z} \right|^2 \right], \quad (5)$$

where a_x and a_y are the lattice constants perpendicular to the chains. The order parameter $\Phi(x, y, z)$, is proportional to the average of $\phi_i(z)$ over neighboring chains. The three-dimensional mean-field temperature T_{3D} is defined as the temperature at which the coefficient $A(T)$ changes sign. Close to T_{3D} ,

$$A = A' \left(\frac{T}{T_{3D}} - 1 \right). \quad (6)$$

The transition temperature T_{3D} and the coefficients A' , B , C_x , C_y , and C_z can be written in terms of the interchain interaction J and the coefficients a , b , and c of a single chain. The coefficients in (5) determine measurable quantities associated with the transition, such as the specific heat jump, coherence lengths, and width of the critical region.

Most of the physics is determined by a *single* dimensionless parameter,

$$\kappa \equiv \frac{2(bT)^2}{|a|^3 c}, \quad (7)$$

which is a measure of the fluctuations along a single chain. It was assumed that the coefficients a , b , and c were independent of temperature and the measurable quantities at the transition were determined as a function of the interchain coupling. The transition temperature increases as the interchain coupling increases. The coherence length and specific heat jump depends only on the single-chain coherence length, $\xi_0 \equiv (c/|a|)^{1/2}$, and the interchain coupling. The width of the critical region, estimated from the Ginzburg criterion, was virtually parameter independent, being about 5–8% of the transition temperature for theory should be valid over a broad temperature range.

This paper uses a simple model to demonstrate some of the difficulties involved in deriving the coefficients a , b , c , and J from a realistic microscopic theory.

C. Microscopic theory

The basic physics of quasi-one-dimensional CDW materials is believed to be described by a Hamiltonian, due to Fröhlich,¹³ which describes electrons with a linear coupling to phonons. Even in one dimension, this is a highly nontrivial many-body system and must be treated by some approximation scheme. The simplest treatment^{13–15} is a rigid-lattice one, in which the phonons associated with the lattice distortion are treated in the mean-field approximation and the zero point and thermal lattice motions are neglected. The resulting theory is mathematically identical to BCS theory.¹⁵ An energy gap opens at the Fermi surface at a temperature $T_{RL} \simeq 1.14 E_F e^{-1/\lambda}$, where E_F is the Fermi energy and λ is the dimensionless electron-phonon coupling. T_{RL} is related to the zero-temperature energy gap $\Delta_{RL}(0)$ by

$$\Delta_{RL}(0) = 1.76 k_B T_{RL}. \quad (8)$$

In this approximation, the coefficients in the single-chain Ginzburg-Landau free-energy functional (1) are¹⁵

$$a_{RL}(T) = \frac{1}{\pi v_F} \ln \left(\frac{T}{T_{RL}} \right), \quad (9)$$

$$b_{RL}(T) = \frac{1}{\pi v_F} \frac{7\zeta(3)}{(4\pi T)^2}, \quad (10)$$

$$c_{RL}(T) = \frac{1}{\pi v_F} \frac{7\zeta(3)v_F^2}{(4\pi T)^2}, \quad (11)$$

where v_F is the Fermi velocity and $\zeta(3)$ is the Riemann ζ function. If $4t_{\perp}$ is the electronic bandwidth perpendicular to the chains [see (57)], then the interchain coupling is given by^{16,17}

$$J_{RL} = \left(\frac{4t_{\perp}}{v_F} \right)^2 c_{RL}(T). \quad (12)$$

It might be hoped that the transition in real materials can be described by the mean-field theory of the functional (1), with the coefficients (9)–(11). However, this is not the case for several reasons. (i) The width of the critical regime given by the one-dimensional Ginzburg criterion¹⁸ is very large: $\Delta t_{1D} = 0.8$,¹⁶ suggesting that fluctuations are important because condition (4) is not satisfied. (ii) A rigid-lattice treatment predicts a metallic density of states at all temperatures above T_{RL} . In contrast, magnetic susceptibility,^{19–21} optical conductivity,^{22–27} and photoemission^{28–30} measurements suggest that there is a gap or pseudogap in the density of states for a broad temperature range above T_P . (iii) The transition temperature, specific heat jump, and coherence lengths are inconsistent with rigid-lattice predictions (Table I). This failure should not be surprising, given that recent work has shown that in the

TABLE I. Comparison of experimental values for $K_{0.3}MoO_3$ of various dimensionless ratios with the predictions of two simple microscopic models. The three-dimensional transition temperature is $T_P = 183$ K. The zero-temperature energy gap $\Delta(0)$ is estimated from optical conductivity data (Ref. 22). A Fermi velocity of $v_F = 2 \times 10^5$ cm/sec was estimated from band structure calculations (Ref. 66). ΔC is the specific heat jump at the transition (Ref. 5) and γT_P is the normal state electronic specific heat that has been calculated from the density of states estimated from magnetic susceptibility measurements (Ref. 20) well above the transition temperature. The longitudinal coherence length ξ_{0z} has been estimated from x-ray scattering experiments (Ref. 6). In both models the dimensionless ratios are independent of any parameters, except for $\Delta(0)/k_B T_P$ in Schulz's model, which is described in Appendix A. The rigid lattice theory (Refs. 15 and 16) involves a mean-field treatment of the single-chain Ginzburg Landau functional (1), with the coefficients (9–11).

Dimensionless ratio	Experimental value	Schulz model	Rigid lattice theory
$\frac{\Delta(0)}{k_B T_P}$	5 ± 1		1.76
$\frac{\Delta C}{\gamma T_P}$	5 ± 1	3.4	1.43
$\frac{\xi_{z0} T_P}{v_F}$	0.18 ± 0.04	0.23	0.23

three-dimensionally ordered Peierls state the zero-point and thermal lattice motions must be taken into account to obtain a quantitative description of the optical properties.^{22,23,31–33}

The next level of approximation is to use the coefficients (9 and 10) and take into account the intrachain order parameter fluctuations and the interchain coupling and use results similar to those in Ref. 10. This is the approach that has been taken previously.^{16,34,35} There are two problems with this approach. First, if the dimensionless parameter κ , given by (7), is evaluated using the expressions (9–11), the result is

$$\kappa_{RL}(T) = \frac{7\zeta(3)}{8|\ln(T/T_{RL})|^3}. \quad (13)$$

Hence, the temperature dependence is quite different from the dependence $\kappa \sim T^2$ that was assumed in Refs. 10, 35, and 36 and the analysis there needs to be modified. The second and more serious problem is one of self-consistency. The coefficients a , b , and c are calculated neglecting fluctuations in the order parameter, which will modify the electronic properties which in turn will modify the coefficients. In this paper, a simple model is used to demonstrate that the fluctuations have a significant effect on the single-chain coefficients. An alternative microscopic theory, due to Schulz,¹⁶ and which takes into account fluctuations in only the phase of the order parameter is briefly reviewed in Appendix A.

D. Overview

Discrepancies between phonon rigid-lattice theory and the observed properties of the Peierls state well below the transition temperature T_P were recently resolved,^{31,32} by taking into account the effect of the zero-point and thermal lattice motion on the electronic properties. It was shown that the lattice fluctuations have an effect similar to a Gaussian random potential. This mapping breaks down near the transition temperature, because of the phonon dispersion, due to the softening of the phonons near $2k_F$. In this paper, this dispersion is taken into account and the effect of the large thermal lattice motion near the transition temperature is studied.

The thermal lattice motion has the same effect on the electronic properties as a static random potential with finite correlation length. Close to the transition temperature, the problem reduces to a simple model, corresponding to a single classical phonon, which can be treated exactly (Sec. II). This model was first studied by Sadovskii.³⁷ It was recently used in the description of the destruction of spin-density-wave states by high magnetic fields.³⁸ The one-electron Green's function is calculated in Sec. III. There is a pseudogap in the density of states (Fig. 1). The complexity of this simple model is indi-

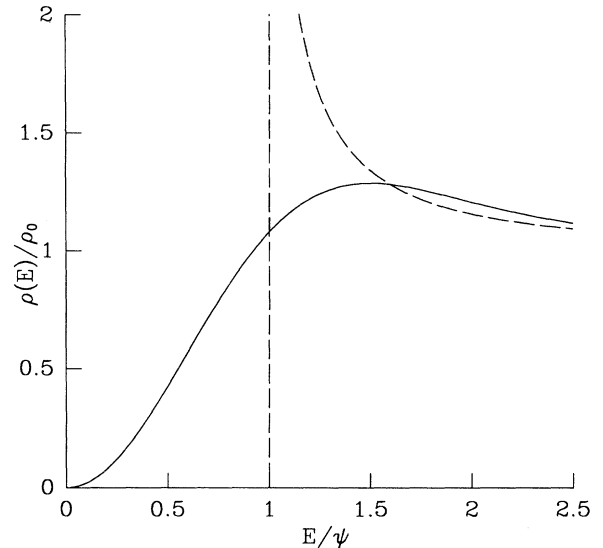


FIG. 1. Pseudogap in the density of states near the three-dimensional transition temperature T_P . Perturbative treatments (dotted line, compare Refs. 34 and 41) give an absolute gap ψ at the transition temperature, whereas the exact treatment (solid line) gives only a pseudogap. The energy E is relative to the Fermi energy and the density of states is normalized to the free-electron value ρ_0 . The density of states is symmetrical about $E = 0$. This result is only valid sufficiently close to T_P that the longitudinal CDW correlation length $\xi_{||} \gg v_F/\psi$. As the temperature increases above T_P , $\xi_{||}$ decreases and the density of states at the Fermi energy increases, i.e., the pseudogap gradually fills in (see Figs. 5 and 6 in Ref. 48).

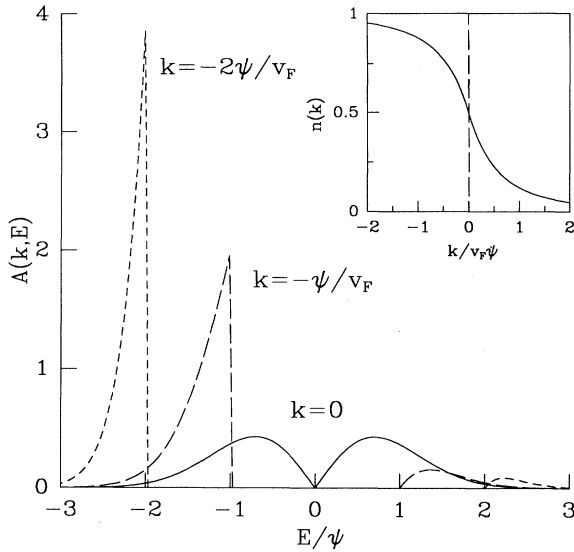


FIG. 2. Breakdown of the quasiparticle picture. The electronic spectral function is shown for several different momenta k , relative to the Fermi momentum k_F . As the momentum approaches k_F the spectral function broadens significantly, similar to the behavior of a Luttinger liquid. Inset: Momentum dependence of the occupation function $n(k)$. The dashed line is the result in the absence of a pseudogap, i.e., a noninteracting Fermi gas.

cated by two nontrivial many-body effects: (i) Perturbation theory diverges but is Borel summable. (ii) The traditional quasiparticle picture breaks down (Fig. 2), reminiscent of behavior seen in Luttinger liquids.³⁹ To illustrate that calculations based on perturbation theory can be unreliable, it is shown that a predicted scaling relation between the specific heat and the temperature derivative of the magnetic susceptibility⁴⁰ does not hold if the *exact*, rather than approximate, density of states is used in the calculation. Using this model the coefficients a , b , and c are calculated in Appendix B. The coefficients deviate significantly from the rigid-lattice values if the pseudogap is comparable to or larger than the transition temperature. In Sec. VI, experimental data are used to estimate the pseudogap in $\text{K}_{0.3}\text{MoO}_3$.

E. Previous work on fluctuations and the pseudogap

To put this paper in context some important earlier work is briefly reviewed. Lee, Rice, and Anderson³⁴ considered how fluctuations in the order parameter produce a pseudogap in the density of states. It is important to be aware of the assumptions made in their calculation. Although their results describe much of the physics on a qualitative level, for the reasons described below, their results cannot be expected to give a quantitative description of the density of states near the CDW transition. The starting point of Lee, Rice, and Anderson was the one-dimensional Ginzburg-Landau functional (1)

with a *real* order parameter and with the coefficients derived from rigid-lattice theory [see Eqs. (9–11)]. Earlier, Scalapino, Sears, and Ferrell¹² evaluated the correlation length $\xi_{\parallel}(T)$ for one-dimensional Ginzburg-Landau theory, with an exact treatment of the fluctuations in the order parameter; $\xi_{\parallel}(T)$ only diverges as $T \rightarrow 0$. The results of this calculation were used by Lee, Rice, and Anderson as input in a random potential with correlations given by

$$\langle \Delta(z)\Delta(z') \rangle = \Delta_{\text{RL}}(T)^2 \exp[-|z - z'|/\xi_{\parallel}(T)], \quad (14)$$

where $\Delta_{\text{RL}}(T)$ is the rigid-lattice (BCS) order parameter and the average is over the thermal fluctuations of the order parameter. The electronic Green's function was calculated using Eq. (14) and a formula originally used for liquid metals (essentially, second-order perturbation theory for the random potential). They found a gradual appearance of a gap as the temperature decreased. For $T_P < 0.25T_{\text{RL}}$, an absolute gap of magnitude $\Delta_{\text{RL}}(0)$ appears. Lee, Rice, and Anderson suggested that a three-dimensional transition occurs for $T_P \simeq 0.25T_{\text{RL}}$ based on the temperature at which $\xi_{\parallel}(T)$ becomes extremely large. There are several problems with trying to use these results to give a quantitative description of the CDW transition, because of the following assumptions. (i) *A real order parameter*. Most CDW transitions are described by a complex order parameter, for which quantitatively distinct behavior occurs. For example, the transition to very large correlation lengths for $T_P \simeq 0.25T_{\text{RL}}$ does not occur for a complex order parameter. (See Fig. 6 in Ref. 12.) (ii) *Rigid-lattice coefficients*. It is shown in this paper that the pseudogap, due to the thermal lattice motion, causes the Ginzburg-Landau coefficients to deviate significantly from their rigid-lattice values (Fig. 4). (iii) *Perturbation theory*. It is demonstrated in this paper that this is unreliable. In particular as $\xi_{\parallel}(T) \rightarrow \infty$ in (14), only a pseudogap rather than an absolute gap develops in the density of states (Fig. 1).

Rice and Strässler⁴¹ calculated the contribution of the phonon fluctuations to the electronic self-energy in the Migdal approximation, i.e., second-order perturbation theory. Interchain interactions were included through an anisotropic phonon dispersion. They found a pseudogap in the density of states above the transition temperature. At T_P , there is an absolute gap whose magnitude is determined by the electron-phonon coupling and the interchain interactions. They equated the observed transition temperature with the single-chain mean-field transition temperature T_0 , which they found to be significantly reduced below the rigid-lattice value T_{RL} and to vanish as the interchain coupling vanishes.

In the limit of weak interchain interactions, the analytic form of the density of states is identical to that of Lee, Rice, and Anderson.³⁴ However, it is not commonly appreciated that the origin of the pseudogap in the two calculations is quite different. The magnitude of the Rice and Strässler pseudogap is proportional to the thermal lattice motion (compare Sec. II A), while the pseudogap studied by Lee, Rice, and Anderson pseudogap is by assumption equal to the rigid-lattice gap $\Delta_{\text{RL}}(T)$.

Calculations similar to that of Rice and Strässler have been performed by Bjeliš and Barišić,⁴² Suzumura and Kurihara,⁴³ Patton and Sham,⁴⁴ and Chandra.⁴⁰ The main problem with these calculations is that they are based on perturbation theory.

II. MODEL HAMILTONIAN

The starting point for this paper is the following one-dimensional model. The states in an electron gas with Fermi velocity v_F are described by spinors $\Psi(z)$. The upper and lower components describe left and right moving electrons, respectively. The phonons are described by the field

$$\Delta(z) = g \sum_q \sqrt{\frac{\hbar}{2M\omega_{2k_F+q}}} (b_{2k_F+q} + b_{-2k_F-q}^\dagger) e^{iqz}, \quad (15)$$

where b_s destroys a phonon of momentum s and frequency ω_s and g is the linear electron-phonon coupling. The dimensionless electron-phonon coupling λ is defined by

$$\lambda = 2g^2 a_z / \pi v_F \omega_Q, \quad (16)$$

where a_z is the lattice constant along the chains. The electronic part of the Hamiltonian is⁴⁵

$$H_{el} = \int dz \Psi^\dagger(z) \left[-iv_F \sigma_3 \frac{\partial}{\partial z} + \frac{1}{2} [\Delta(z) \sigma_+ + \Delta(z)^* \sigma_-] \right] \Psi(z), \quad (17)$$

where σ_3 and $\sigma_\pm \equiv \sigma_1 \pm i\sigma_2$ are Pauli matrices.

This paper focuses on the following model, where $\Delta(z)$ is replaced with a random potential with zero mean and finite length correlations:

$$\langle \Delta(z) \rangle = 0, \quad \langle \Delta(z) \Delta(z')^* \rangle = \psi^2 \exp(-|z - z'| / \xi_{||}). \quad (18)$$

$\xi_{||}$ is the CDW correlation length along the chains. In most of this paper, ψ will be treated as a parameter. It is central to this paper, being a measure of the thermal lattice motion and a measure of the pseudogap in the density of states. This paper focuses on behavior near T_P and so the limit $\xi_{||} \psi / v_F \rightarrow \infty$ is taken. A rough argument is now given to justify using this model to describe thermal lattice motion near the phase transition.

A. Thermal lattice motion

In rigid-lattice theory, $\Delta(z)$ is replaced by its expectation value $\langle \Delta(z) \rangle = \Delta_0$. To go beyond this, the effect of the quantum and thermal lattice fluctuations in the Peierls state was recently modeled^{31,32,46} by treat-

ing $\Delta(z)$ as a static random potential with mean Δ_0 and correlations

$$\langle \Delta(z) \Delta(z')^* \rangle = \Delta_0^2 + \gamma \delta(z - z'), \quad (19)$$

where

$$\gamma = \frac{1}{2} \pi \lambda v_F \omega_{2k_F} \coth\left(\frac{\omega_{2k_F}}{2T}\right). \quad (20)$$

This model is expected to be reliable, except near the transition temperature, where there is significant dispersion in the phonons. This dispersion is now taken into account.

Near the transition temperature, the phonons can be treated *classically*, since in most materials, the frequencies of the phonons with wave vector near $2k_F$ are much smaller than the transition temperature (Table II). Following Rice and Stässler⁴¹ renormalized phonon frequencies $\Omega(q, T)$ are used in the expression for the correlations of the random potential,

$$\langle \Delta(z) \Delta(z')^* \rangle = \lambda \pi T \frac{v_F}{a_z} \sum_q \frac{\omega_Q^2}{\Omega(q, T)^2} e^{iq(z-z')}. \quad (21)$$

At the level of the Gaussian approximation the phonon dispersion relation can be written in the form

$$\Omega(q, T)^2 = \Omega(T)^2 [1 + (q - 2k_F)^2 \xi_{||}(T)^2]. \quad (22)$$

Evaluating (21) then gives (18), where

$$\psi^2 = \lambda \pi T \left(\frac{\omega_Q}{\Omega(T)} \right)^2 \frac{v_F}{2\xi_{||}(T)}. \quad (23)$$

TABLE II. Parameters for several quasi-one-dimensional materials. The observed transition temperature T_P is always much smaller than the rigid-lattice transition temperature T_{RL} . The phonons near $2k_F$, which soften at the transition, can be treated classically, since they have frequencies of the order of $\Omega(0)$ (estimated from Raman and neutron scattering), which is much smaller than T_P . The zero-temperature gap $\Delta(0)$, estimated from the peak in the optical absorption was used to calculate T_{RL} [$T_{RL} = \Delta(0)/1.76k_B$].

	T_P (K)	$\Delta(0)$ (meV)	T_P/T_{RL}	$\Omega(0)$ (K)
$K_{0.3}MoO_3$	183	90 ^a	0.31	80 ^b
$(TaSe_4)_2I$	263	200 ^c	0.20	130 ^d
$K_2Pt(CN)_4Br_{0.3}$	120 ^e	100 ^f	0.18	58 ^g
TSeF-TCNQ	29	10 ^h	0.42	

^aReference 22.

^bJ. P. Pouget, B. Hennion, C. Escribe-Filippini, and M. Sato, Phys. Rev. B **43**, 8421 (1991).

^cReference 27.

^dS. Sugai, M. Sato, and S. Kurihara, Phys. Rev. B **32**, 6809 (1985).

^eComplete ordering does not occur (Ref. 4).

^fReference 26.

^gReference 4.

^hFrom activation energy of dc conductivity, Ref. 19.

Note that this expression together with (18) is then quite different from (14) used by Lee, Rice, and Anderson.³⁴ In the limit $\xi_{\parallel} \rightarrow 0$, i.e., the phonons become dispersionless and the sum in (21) becomes a δ function and giving (19) (with $\Delta_0 = 0$) and (20).

The rms fluctuations δu in the positions of the atoms, due to thermal lattice motion, is related to the Debye-Waller factor and given by

$$(\delta u)^2 = kT \sum_{\vec{q}} \frac{1}{M\Omega(\vec{q}, T)^2}. \quad (24)$$

This is related to $\psi = (2M\omega_Q)^{1/2} g \delta u$. Hence, ψ is proportional to the thermal lattice motion.

If ψ is defined by (23), it diverges as $T \rightarrow T_P$, because as $T \rightarrow T_P$, $\Omega(T) \rightarrow 0$,

$$\xi_{\parallel}(T) \rightarrow \infty \text{ with } \Omega(T)\xi_{\parallel}(T) \text{ finite.} \quad (25)$$

However, in a real crystal, the phonons are three-dimensional and the thermal lattice motion is finite. We define

$$\psi^2 = \lambda\pi T \frac{v_F}{a_x} \sum_{\vec{q}} \frac{\omega_Q^2}{\Omega(\vec{q}, T)^2} \quad (26)$$

and write the three-dimensional dispersion relation (for a tetragonal crystal) in the form

$$\Omega(\vec{q}, T)^2 = \Omega(T)^2 [1 + (q_{\parallel} - 2k_F)^2 \xi_{\parallel}(T)^2 + (q_{\perp} - Q_{\perp})^2 \xi_{\perp}(T)^2], \quad (27)$$

where $\vec{Q} = (Q_{\perp}, 2k_F)$ is the nesting vector associated with the three-dimensional CDW transition [see Eq. (56)]. Due to the quasi-one-dimensionality of the crystal, the dispersion perpendicular to the chains is small and $\xi_{\perp} \ll \xi_{\parallel}$. Let a_x denote the lattice constant perpendicular to the chains. Performing the integral over the wave vector in (26) gives⁴⁷

$$\psi^2 = \lambda\pi T \left(\frac{\omega_Q}{\Omega(T)} \right)^2 \frac{a_x^2 v_F}{\pi^2 \xi_{\parallel}(T) \xi_{\perp}(T)^2} \times \left[\sqrt{1 + (\rho_c \xi_{\perp}(T))^2} - 1 \right] \quad (28)$$

where ρ_c is a wave vector cutoff perpendicular to the chains. If $\rho_c = \pi/a_x$, this expression reduces to (23) in the one-dimensional limit $\xi_{\perp} \ll a_x$. Near the transition, $\xi_{\perp}(T) \rightarrow \infty$, giving

$$\psi(T_P)^2 = \lambda\pi T \left(\frac{\omega_Q}{\Omega(T)} \right)^2 \frac{a_x v_F}{\pi \xi_{\parallel}(T) \xi_{\perp}(T)}. \quad (29)$$

From (25) and the fact that $\xi_{\parallel}(T)/\xi_{\perp}(T)$ is finite, it follows that ψ is finite as $T \rightarrow T_P$. Note that the magnitude of this quantity is dependent on the choice of the momentum cutoff ρ_c . The above treatment is quite similar to Schulz's discussion of fluctuations in the order parameter in the Gaussian approximation.¹⁶

Although the expressions (23), (28), and (29) for ψ in the different regimes look very different, ψ is actually weakly temperature dependent and does not vary much in magnitude. To see this, (28) can be written as

$$\psi^2 = (\psi(T_P))^2 \frac{1}{\rho_c \xi_{\perp}(T)} \left[\sqrt{1 + (\rho_c \xi_{\perp}(T))^2} - 1 \right]. \quad (30)$$

The postfactor is a slowly varying function of $\rho_c \xi_{\perp}(T)$. Since well above T_P , $\rho_c \xi_{\perp}(T) \sim 1$ [e.g., for $\text{K}_{0.3}\text{MoO}_3$ $\xi_{\perp}(300 \text{ K}) \sim 4 \text{ \AA}$ (Ref. (6))] the postfactor does not vary by more than a factor of 2, although $\rho_c \xi_{\perp}(T)$ varies by several orders of magnitude. Johnston²⁰ used a crude method of estimating the pseudogap and found it to be weakly temperature dependent above T_P for $\text{K}_{0.3}\text{MoO}_3$.

B. Solution of the model

Sadovskii⁴⁸ solved the one-dimensional model (17) and (18) exactly. He calculated the one-electron Green's function in terms of a continued fraction by finding a recursion relation satisfied by the self energy. He found³⁷ that the Green's function reduced to a simple analytic form in the limit of large correlation lengths ($\xi_{\parallel} \gg v_F/\psi$). This can be seen by the following rough argument. In the limit $\xi_{\parallel} \rightarrow \infty$, the moments of the random potential $\Delta(z)$ are independent of position:

$$\langle \Delta(z) \rangle = 0, \quad \langle \Delta(z) \Delta(z')^* \rangle = \psi^2. \quad (31)$$

This means that the random potential has only one nonzero Fourier component, i.e., the one with zero wave vector.

The potential can be written $\Delta(z) = v\psi$, where v is a complex random variable with a Gaussian distribution. Averages over the random potential can then be written

$$\langle A[\Delta(z)] \rangle = \int \frac{dv dv^*}{\pi} e^{-vv^*} A[v\psi]. \quad (32)$$

It is then a straightforward exercise to evaluate the averages of different electronic Green's functions.

III. ONE-ELECTRON GREEN'S FUNCTION NEAR T_P

The matrix Matsubara Green's function, defined at the Matsubara energies $\epsilon_n = (2n+1)\pi T$, for the Hamiltonian (17) with (31) is

$$\hat{G}(i\epsilon_n, k) = \int \frac{dv dv^*}{\pi} e^{-vv^*} \hat{G}(i\epsilon_n, k, v), \quad (33)$$

where

$$\hat{G}(i\epsilon_n, k, v) = \frac{-[i\epsilon_n - kv_F\sigma_3 - \psi(v\sigma_+ + v^*\sigma_-)]}{\epsilon_n^2 + (kv_F)^2 + vv^*\psi^2} \quad (34)$$

is the matrix Green's function for the Hamiltonian (17) with $\Delta(z) = v\psi$. The off-diagonal (anomalous) terms vanish when the integral over v is performed, indicating

there is no long range order. The integral over the phase of v can be performed and variables changed to $\varphi = vv^*$ and

$$\hat{G}(i\epsilon_n, k) = -(i\epsilon_n - kv_F\sigma_3) \int_0^\infty d\varphi \frac{e^{-\varphi}}{\epsilon_n^2 + (kv_F)^2 + \varphi\psi^2} \quad (35)$$

is obtained. Sadvskii³⁷ obtained the same expression by diagrammatic summation. For the case of a half-filled band, v is strictly real and the resulting expressions are the same as those obtained by Wonneberger and Lautenschläger.⁴⁹ Expanding (35) in powers of ψ gives

$$\hat{G}(i\epsilon_n, k) = \hat{G}_0(i\epsilon_n, k) \int_0^\infty d\varphi e^{-\varphi} \sum_{n=0}^\infty \left[\frac{-\varphi\psi^2}{\epsilon_n^2 + (kv_F)^2} \right]^n, \quad (36)$$

where $\hat{G}_0 = (i\epsilon_n - kv_F\sigma_3)^{-1}$ is the free-electron Green's function. Performing the integral over φ gives

$$\hat{G}(i\epsilon_n, k) = \hat{G}_0(i\epsilon_n, k) \sum_{n=0}^\infty n! \left[\frac{-\psi^2}{\epsilon_n^2 + (kv_f)^2} \right]^n. \quad (37)$$

This is a *divergent* series and asymptotic expansion. However, it is Borel summable.⁵⁰ This divergence suggests that perturbation theory as used in Refs. 34, 40–44 may give unreliable results. This can be seen in Fig. 1 and Sec. III E.

A. Density of states

The electronic density of states is calculated directly from the imaginary part of the one-electron Green's function (35). The result is

$$\rho(E) = \rho_0 \int_0^\infty d\varphi e^{-\varphi} \frac{E}{[E^2 - \varphi\psi^2]^{1/2}} \theta(|E|^2 - \varphi\psi^2) \quad (38)$$

$$= 2\rho_0 \left| \frac{E}{\psi} \right| \exp \left[- \left(\frac{E}{\psi} \right)^2 \right] \operatorname{erfi} \left(\frac{E}{\psi} \right), \quad (39)$$

where $\rho_0 = 1/\pi v_F$ is the free-electron density of states and erfi is the error function of imaginary argument.⁵¹ Figure 1 shows the energy dependence of the density of states. It vanishes at zero energy (the Fermi energy) and is suppressed over an energy range of order ψ , i.e., there is a pseudogap. It has the asymptotic behavior:

$$\rho(E) \simeq 2\rho_0 \left(\frac{E}{\psi} \right)^2 \quad \text{for } E \ll \psi, \quad (40)$$

$$\rho(E) \simeq \rho_0 \quad \text{for } E \gg \psi.$$

Figure 1 shows that the exact result (39) (solid line) deviates significantly from the result of second-order perturbation theory in Refs. 34 and 41 (dashed line),

$$\rho(E) = \rho_0 \frac{E}{[E^2 - \psi^2]^{1/2}} \theta(E^2 - \psi^2). \quad (41)$$

This latter form has been assumed in much earlier work.^{17,20,44,52}

The above expressions for the density of states are all for infinite correlation length ($\xi_{\parallel}\psi/v_F \rightarrow \infty$), i.e., very close to the three-dimensional transition temperature T_P . What happens *above* T_P as the intrachain correlation length decreases? This problem was considered in detail by Sadvskii.⁴⁸ [He calculated the density of states for the random potential (18) with finite ξ_{\parallel} exactly.] As the correlation length decreases, the density of states at the Fermi energy increases, i.e., the pseudogap fills in. How quickly this happens depends on the dimensionless ratio $v_F/(\psi\xi_{\parallel})$. [See Eq. (48) below and Figs. 5 and 6 in Ref. 48.] Sadvskii showed that perturbation theory^{34,40–44} only gives reliable results for $|E| < \psi$, when $\xi_{\parallel} < v_F/\psi$, i.e., well above T_P .

What happens *below* T_P as the intrachain correlation length decreases? In Ref. 31 it was shown that in the three dimensionally ordered Peierls state, well below T_P , there is an absolute gap with a subgap tail that increases substantially as the temperature becomes larger than the phonon frequency. A smooth crossover to the pseudogap discussed here is expected. It is an open problem to construct a single theory that can describe the density of states over the complete temperature range.

B. Spectral function

The spectral function for right moving electrons of momentum k is given by

$$\begin{aligned} A(k, E) &= -\frac{1}{\pi} \operatorname{Im} G_{11}(k, E + i\eta) \\ &= \int_0^\infty d\varphi e^{-\varphi} \left\{ \delta \left[E - \sqrt{(kv_F)^2 + \varphi\psi^2} \right] \right. \\ &\quad \left. + \delta \left[E + \sqrt{(kv_F)^2 + \varphi\psi^2} \right] \right\} \\ &= \frac{|E|}{\psi^2} \exp \left(\frac{(kv_F)^2 - E^2}{\psi^2} \right) \theta \left[E^2 - (kv_F)^2 \right], \end{aligned} \quad (42)$$

where the momentum k is relative to the Fermi momentum k_F . Note that this form is very different from the Lorentzian form associated with the quasiparticle picture and perturbation theory.⁵³ The spectral function is asymmetrical, very broad, and has a significant high energy tail. Figure 2 shows how the quasiparticle weight is reduced near the Fermi momenta, i.e., the quasiparticles are not well defined. This was first pointed out by Wonneberger and Lautenschläger⁴⁹ for the corresponding model for a half-filled band. This is strictly a nonperturbative effect. In perturbation theory, the quasiparticles are well defined. This breakdown of the quasiparticle picture is similar to the properties of a Luttinger liquid.³⁹

The momentum distribution function $n(k)$ at $T = 0$ for right moving electrons is given by

$$\begin{aligned}
n(k) &\equiv \int_{-\infty}^0 dEA(k, E) \\
&= \frac{1}{2} \left\{ 1 - \sqrt{\pi} \left(\frac{kv_F}{\psi} \right) \right. \\
&\quad \left. \times \exp \left[\left(\frac{kv_F}{\psi} \right)^2 \right] \left[1 - \operatorname{erf} \left(\frac{kv_F}{\psi} \right) \right] \right\}, \quad (43)
\end{aligned}$$

where erf is the error function. The inset to Fig. 2 shows how the momentum distribution $n(k)$ at $T = 0$ is smeared over a momentum range $\delta k \sim \psi/v_F$. The absence of a step at $k = k_F$ indicates that there is no clearly defined Fermi surface. However, this is *not* like in a Luttinger liquid, but solely due to disorder. In fact, in an ordinary metal with mean free path ℓ , similar behavior is seen; disorder smears out $n(k)$ over a momentum range $\delta k \sim 1/\ell$.

C. Electronic specific heat

The electronic specific heat $C_e(T)$ is related to the density of states $\rho(E)$ by

$$C_e(T) = -\frac{4}{T} \int_0^\infty dEE^2 \rho(E) \frac{\partial f}{\partial E}, \quad (44)$$

where $f(E)$ is the Fermi-Dirac distribution function. In the absence of a pseudogap, $C_e(T) = \frac{2\pi^2}{3} \rho_0 T \equiv C_0(T)$. If the expression (39) is used for the density of states in the presence of a pseudogap, then $C_e(T)/C_0(T)$ only

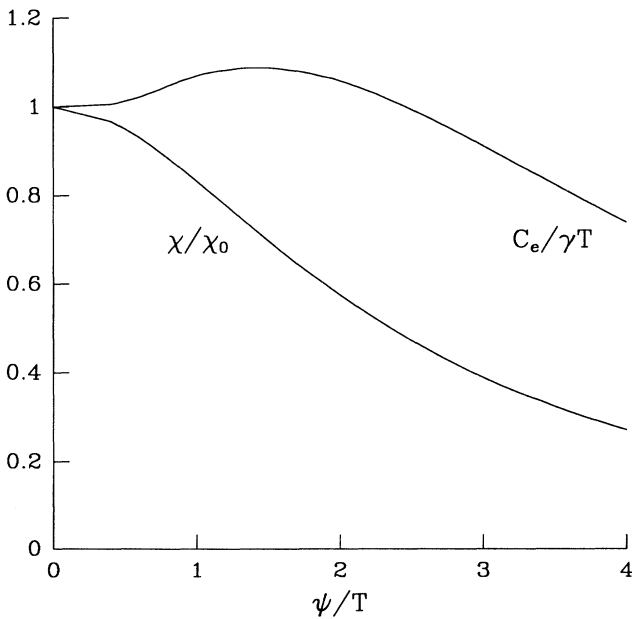


FIG. 3. Modification of the electronic specific heat $C_e(T)$ and the Pauli spin susceptibility $\chi(T)$ by the pseudogap. Both are normalized to their values in the absence of the pseudogap.

depends on ψ/T and is shown in Fig. 3. A similar result was recently used³⁸ to explain the temperature dependence of the electronic specific heat near a spin-density-wave phase boundary of the organic conductor $(\text{TMTSF})_2\text{ClO}_4$. Note that when $\psi \sim T$, $C_e(T)$ can be slightly larger than $C_0(T)$, because $E^2 \frac{\partial f}{\partial E}$ has a maximum near $E \sim T$ and for $E \sim \psi$, $\rho(E)$ is larger than ρ_0 (Fig. 1).

D. Pauli spin susceptibility

The Pauli spin susceptibility $\chi(T)$ is related to the density of states $\rho(E)$ by

$$\chi(T) = -\mu_B^2 \int_0^\infty dE \rho(E) \frac{\partial f}{\partial E}, \quad (45)$$

where $f(E)$ is the Fermi-Dirac distribution function and μ_B is a Bohr magneton.⁵⁴ In the absence of a pseudogap, $\chi(T) = \mu_B^2 \rho_0 \equiv \chi_0$, which is independent of temperature. If the expression (39) is used for the density of states in the presence of a pseudogap, then $\chi(T)/\chi_0$ only depends on ψ/T and is shown in Fig. 3. This result will be used in Sec. VI to provide an estimate of the pseudogap in $\text{K}_{0.3}\text{MoO}_3$.

E. Chandra's scaling relation

The effect of thermal lattice fluctuations on the temperature dependence of $\chi(T)$ was first considered by Lee, Rice, and Anderson.³⁴ They argued that as the temperature is lowered towards T_P the intrachain correlation length increases, more of a pseudogap opens in the density of states and $\chi(T)$ decreases. This problem was recently reconsidered by Chandra⁴⁰ who derived a scaling relation between the derivative $d\chi/dT$ and the specific heat C_P in the critical region. I now repeat the essential features of her argument. She calculated the electronic self-energy in the Born approximation, taking into account the interchain interactions and the finite mean free path of the electrons. She assumed that the pseudogap is much larger than the transition temperature ($\psi \gg T_P$; it will be shown in Sec. VI that this is a poor approximation for $\text{K}_{0.3}\text{MoO}_3$), so that $\chi(T) \simeq \mu_B^2 \rho(0)$. Chandra also assumed that the temperature dependence of the density of states at the Fermi energy is determined solely by the temperature dependence of $\xi_{\parallel}(T)$. Moreover, based on the Born approximation, she found

$$\rho(0) \sim \frac{1}{\xi_{\parallel}(T)}. \quad (46)$$

Defining $t \equiv |T - T_P|/T_P$ then gives the scaling relation

$$\frac{d\chi(T)}{dT} \sim \frac{d}{dT} \frac{1}{\xi_{\parallel}(T)} \sim \frac{d}{dT} t^{1/2} \sim C_P, \quad (47)$$

where use has been made of the temperature dependence of $\xi_{\parallel}(T)$ and C_P in the Gaussian approximation.¹⁸

This same scaling relation was suggested earlier by

Horn, Herman, and Salomon.⁵⁵ They claimed to have found the critical exponent for $d\chi/dT$ to be -0.5 for TTF-TCNQ. Kwok, Grüner, and Brown⁵⁶ claim to have observed a scaling between $d(T\chi)/dT$ and C_P within a 30 K region about $T_P = 183$ K for $K_{0.3}\text{MoO}_3$. However, Mozurkevich has argued that the Gaussian approximation is not valid in this temperature range.⁵⁷ Chung *et al.*⁵⁸ found that $d\chi/dT$ was comparable to C_P when a background contribution was subtracted from the latter. Brill *et al.*⁵ found that χ was proportional to the entropy (evaluated from integrating the specific heat) between 140 and 220 K. (This is equivalent to a scaling between $d\chi/dT$ and C_P .) They show that this is what is expected if χ and C_P are derived from a free energy functional in which the complete magnetic field dependence is contained in the field dependence of T_P .

Chandra's derivation of the scaling relationship (47) is not valid. It depends on (46) which is a direct result of the perturbative treatment of the lattice fluctuations. The exact Green's function calculated by Sadovskii⁴⁸ gives different results. He found that for $\xi_{\parallel}(T) \gg v_F/\psi$,

$$\frac{\rho(0)}{\rho_0} \simeq (0.54 \pm 0.01) \left(\frac{v_F}{\psi \xi_{\parallel}(T)} \right)^{1/2}, \quad (48)$$

(see Fig. 6 in Ref. 48) rather than (46). This will give

$$\frac{d\chi(T)}{dT} \sim t^{-3/4} \quad (49)$$

and so the scaling relation (47) does not hold. It should be stressed that this result assumes $\psi \gg T_P$, a condition that is poorly satisfied in most materials (Sec. VI).

IV. PROPERTIES OF THE GINZBURG-LANDAU COEFFICIENTS

In Appendix B, the coefficients a , b , and c in the Ginzburg-Landau free energy (1) describing the Peierls transition are evaluated in the presence of the random potential (31), which is used here to model the thermal lattice motion. The calculation is based on a linked cluster expansion similar to that used to derive the Ginzburg-Landau functional for superconductors.⁵⁹ The results are

$$a(T) = \frac{1}{\pi v_F} \left[\ln \left(\frac{T}{T_{RL}} \right) + \pi T \sum_{\epsilon_n} \left(\frac{1}{|\epsilon_n|} - \int_0^{\infty} d\varphi e^{-\varphi} \frac{\epsilon_n^2}{(\epsilon_n^2 + \varphi \psi^2)^{3/2}} \right) \right], \quad (50)$$

$$b(T) = \frac{T}{4v_F} \sum_{\epsilon_n} \int_0^{\infty} d\varphi e^{-\varphi} \left(\frac{\epsilon_n^2}{(\epsilon_n^2 + \varphi \psi^2)^{5/2}} - \frac{5\varphi(\psi \epsilon_n)^2}{(\epsilon_n^2 + \varphi \psi^2)^{7/2}} \right), \quad (51)$$

$$c(T) = \frac{v_F T}{4} \sum_{\epsilon_n} \epsilon_n^2 \int_0^{\infty} \frac{d\varphi e^{-\varphi}}{(\epsilon_n^2 + \varphi \psi^2)^{5/2}}. \quad (52)$$

The integrals over φ in the above expressions can be written in terms of error functions and incomplete γ functions.⁵¹ However, for both numerical and analytical calculations it is actually more convenient to use the expressions above. As $\psi \rightarrow 0$, the above expressions reduce to the rigid-lattice values (9–11).

Single-chain mean-field transition temperature. T_0 is determined by the temperature at which the second-order Ginzburg-Landau coefficient (50) vanishes:

$$a(T_0) = 0. \quad (53)$$

This defines relations between T_0/T_{RL} and ψ/T_0 , shown in Fig. 4. (The inset shows T_0/T_{RL} versus ψ/T_{RL} .) The pseudogap suppresses the transition temperature. At a crude level, this is because in the presence of a pseudogap opening a gap due to a Peierls distortion causes a smaller decrease in the electronic energy than in the absence of a pseudogap. In most materials $T_P < 0.4T_{RL}$ (Table II) and so the inset of Fig. 4 implies $\psi \sim T_{RL}$ which is comparable to the zero-temperature gap. Rice and Strässler⁴¹ found from second-order perturbation theory that for $T_0 \ll T_{RL}$, $\psi \simeq 1.05T_{RL}$. Thus, the single-chain mean-field transition temperature can be quite different from T_{RL} , defined by (8), and often referred to as the mean-field transition temperature, and so no experimen-

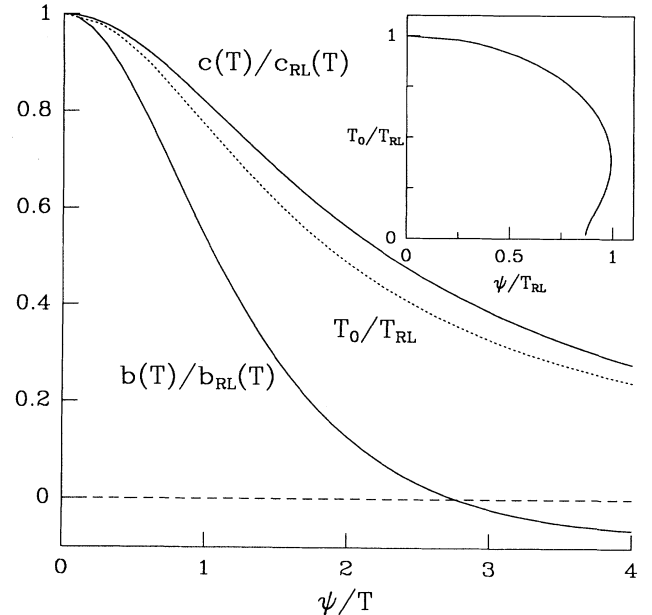


FIG. 4. The pseudogap, due to thermal lattice motion, has a significant effect on the coefficients in the Ginzburg-Landau free energy (1) for a single chain. The ratio of the single-chain mean-field transition temperature T_0 and the coefficients b and c to their rigid-lattice values [given by (9–11)] are shown as a function of the ratio of the pseudogap ψ to the temperature. For $\psi > 2.7T$, the coefficient b becomes negative and the transition will be first order (Sec. IV). Inset: Relationship between T_0/T_{RL} and ψ/T_{RL} .

tal signatures are expected at $T = T_{\text{RL}}$.

Fourth-order coefficient. The ratio of the fourth-order coefficient b to its rigid-lattice value as a function of the ratio of the pseudogap ψ to the temperature is shown in Fig. 4. Note that b is negative for $\psi/T > 2.7$. This will change the nature of the phase transition. One must then include the sixth-order term in the free energy. If it is positive (I have calculated it and found it to be positive for this parameter range), then the transition will be *first order*. A complete discussion of such a situation is given by Toledano and Toledano.⁶⁰ Imry and Scalapino have discussed the effect of one-dimensional fluctuations for this situation.⁶¹ At the mean-field level, there is a coexistence of phases for the temperature range defined by

$$0 < a(T) < \frac{b(T)^2}{3d(T)}, \quad (54)$$

where $d(T)$ is the sixth-order coefficient. Hysteresis will be observed in this temperature range. I recently suggested that the first-order nature of the destruction by high magnetic fields of spin-density-wave states in organic conductors is due to similar effects.³⁸ If at low temperatures the electron-phonon coupling λ is varied, then $\psi/T_{\text{RL}} \sim \lambda e^{1/\lambda}$. According to the inset of Fig. 4, there will be a critical coupling below which the CDW phase will be destroyed. This transition will be first order. It is interesting that Altshuler, Ioffe, and Millis⁶² recently obtained a similar result for a two-dimensional Fermi liquid (with a quasi-one-dimensional Fermi surface), using a very different approach.

However, it should be pointed out that when b is small, corrections due to other effects such as a finite correlation length and interchain coupling, will be important and could make b positive. It is unclear whether this unexpected behavior is only a result of the simplicity of the model or actually is relevant to real materials. The three-dimensional transition occurs when the parameter κ , defined by (7), becomes sufficiently small.¹⁰ Generally this is assumed to be due to the temperature becoming sufficiently low. However, I speculate that the transition could alternatively be driven by b becoming sufficiently small. The fact that $\psi \sim (2-3)T_P$ in $\text{K}_{0.3}\text{MoO}_3$ (Sec. VI) is consistent with b being small.

The coefficient of the longitudinal gradient term is given by (52). It can be shown that $c(T)/c^{\text{RL}}(T)$ is a universal function of ψ/T (see Fig. 4) and that the pseudogap reduces the value of c .

Interchain coupling. Consider a crystal with tetragonal unit cell of dimensions $a_x \times a_x \times a_z$, where the z axis is parallel to the chains. For a tight-binding model the electronic band structure is given by the dispersion relation,

$$E(k) = -2t_{\perp} [\cos(k_x a_x) + \cos(k_y a_x)] - 2t_{\parallel} \cos(k_z a_z). \quad (55)$$

Assume the band structure is highly anisotropic, i.e., $t_{\parallel} \gg t_{\perp}$. The Fermi velocity v_F is defined by $v_F = 2t_{\parallel} a_z \sin(k_F a_z)$. Horovitz, Gutfreund, and Weger¹⁷ have

shown that imperfect nesting of the Fermi surface [i.e., $E(k) \simeq -E(k+Q)$] occurs for the nesting vector,

$$\vec{Q} = (\pi/a_x, \pi/a_x, 2k_F). \quad (56)$$

To calculate the interchain coupling J in the Ginzburg-Landau functional (3), it is assumed that the one-dimensional Green's function (34) can simply be replaced with the corresponding one with the anisotropic band structure, given by Eq. (55). The calculation is then essentially identical to the rigid-lattice calculation of Horovitz, Gutfreund, and Weger¹⁷ and so only the result is given [compare (12)]:

$$J = \left(\frac{4t_{\perp}}{v_F} \right)^2 c(T). \quad (57)$$

Since the pseudogap reduces the value of the longitudinal coefficient c , it will also reduce the interchain coupling.

V. MEAN-FIELD THEORY OF A SINGLE CHAIN

The single-chain Ginzburg-Landau functional with the coefficients discussed in the previous section is now considered. In particular, it is shown that the one-dimensional fluctuations can be much smaller than for the functional with the rigid-lattice coefficients. The first step is to consider the temperature dependence of the second-order coefficient $a(T)$ near T_0 , the mean-field transition temperature. This is difficult because, to be realistic, the temperature dependence of the parameter ψ must be included. This is done at a crude level, using the simple model based on the discussion of thermal lattice motion in Sec. II A. This is then used to evaluate a' , defined by (2), and needed to evaluate physical quantities associated with the transition: the specific heat jump, the coherence length, and width of the critical region.

The jump in the specific heat at T_0 is

$$\Delta C_{1\text{D}} = \frac{(a')^2}{2 b T_0}. \quad (58)$$

An important length scale is the coherence length ξ_0 , defined by

$$\xi_0 = \left(\frac{c}{a'} \right)^{1/2}. \quad (59)$$

The one-dimensional Ginzburg criterion⁷ provides an estimate of the temperature range, $\Delta T_{1\text{D}}$, over which critical fluctuations are important

$$\Delta t_{1\text{D}} \equiv \frac{\Delta T_{1\text{D}}}{T_0} = \left(\frac{b T_0}{a'^{3/2} c^{1/2}} \right)^{2/3} = \frac{1}{(2\xi_0 \Delta C_{1\text{D}})^{2/3}}. \quad (60)$$

A. Self-consistent determination of the pseudogap

At the level of the Gaussian approximation, the phonon dispersion is related to the Ginzburg-Landau co-

efficients by

$$\Omega(q, T)^2 = \lambda\omega_Q^2 [a(T) + c(T)(q - 2k_F)^2 + Ja_x^2(q_\perp - Q_\perp)^2]. \quad (61)$$

Hence, the phonon dispersion depends on the pseudogap ψ . However, it was shown in Sec. IIA that ψ depends on the dispersion. Hence, ψ must be determined self-consistently. Equation (29) gives the dependence of the pseudogap at T_0 on the phonon dispersion. Equation (52) gives the dependence of the coefficient $c(T)$ on the pseudogap. These can be combined with (57) to give

$$1 = t_\perp \psi^2 \sum_{\epsilon_n} \epsilon_n^2 \int_0^\infty \frac{d\varphi e^{-\varphi}}{(\epsilon_n^2 + \varphi\psi^2)^{5/2}}. \quad (62)$$

It follows that ψ/T is a universal function of t_\perp/T .

Dependence of T_0 on the interchain interactions. The self-consistent equation for the pseudogap (62) can be solved simultaneously with the equations for T_0 , and (57) to give the single-chain mean-field transition temperature, as a function of the interchain interactions. The transition temperature is then a monotonic increasing function of the interchain hopping. A similar procedure was followed by Rice and Strässler.⁴¹ The transition temperature tends to zero as the interchain coupling tends to zero, consistent with the fact that there are no finite-temperature phase transitions in a strictly one-dimensional system.¹¹

B. Evaluation of a'

It is now assumed that the temperature dependence of the pseudogap ψ is given implicitly by Eq. (62). Implicit differentiation then gives

$$\frac{d}{dT} \left(\frac{\psi}{T} \right) = \frac{\psi}{2T^2} \frac{X(T)}{Y(T)}, \quad (63)$$

where

$$X(T) = \sum_{\epsilon_n} \epsilon_n^2 \int_0^\infty \frac{d\varphi e^{-\varphi}}{(\epsilon_n^2 + \varphi\psi^2)^{5/2}}, \quad (64)$$

$$Y(T) = \sum_{\epsilon_n} \epsilon_n^2 \int_0^\infty \frac{d\varphi e^{-\varphi} \varphi}{(\epsilon_n^2 + \varphi\psi^2)^{5/2}}. \quad (65)$$

Note that since the right-hand side of (63) is positive, ψ/T is always an increasing function of temperature. A lengthy calculation gives

$$a' = \frac{1}{\pi v_F} \left(1 + \frac{3}{2} \psi^2 \pi T \sum_{\epsilon_n} \epsilon_n^2 \int_0^\infty \frac{d\varphi e^{-\varphi}}{(\epsilon_n^2 + \varphi\psi^2)^{5/2}} \right). \quad (66)$$

This is larger than the rigid-lattice value $a'_{\text{RL}} \equiv 1/\pi v_F$. This enhancement will enhance the specific heat jump (58) and reduce the coherence length (59).

C. Specific heat jump

The specific heat jump ΔC at the transition temperature is calculated from Eq. (58). It is shown in Fig. 5. Note that the jump is much larger than the rigid-lattice value of $1.43\gamma T_P$. The trend shown in Fig. 5 can be explained by a rough argument correlating the sizes of $\Delta C/\gamma T_P$ and $\Delta(0)/k_B T_P$. Simply put, if $\Delta(0)/k_B T_P$ is large, then $\Delta(T)^2$ will have a large slope at T_P . It has previously been noted experimentally⁶³ that the order parameter has a BCS temperature dependence with $\Delta(0)$ and T_P treated as independent parameters. Some theoretical justification was recently provided for such a temperature dependence well away from T_P .³¹ Close to T_P the BCS form gives

$$\Delta(T) \simeq 1.74\Delta(0) \left(1 - \frac{T}{T_P} \right)^{1/2}. \quad (67)$$

Within a BCS type of framework, the specific heat discontinuity is given by⁶⁴

$$\Delta C \sim -\rho_0 \left. \frac{d\Delta^2}{dT} \right|_{T_P} = 3.03\rho_0 \frac{\Delta(0)^2}{T_P}. \quad (68)$$

Using $\Delta(0) = 1.76k_B T_{\text{RL}}$ and $\gamma = 2\pi^2\rho_0/3$ gives

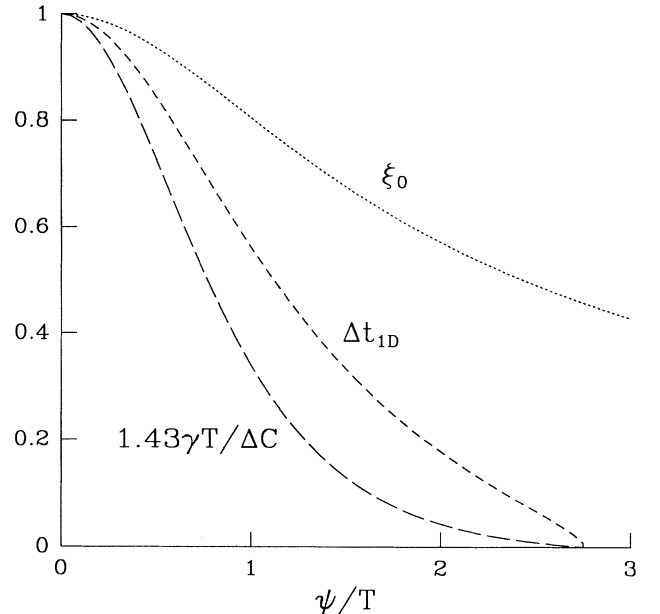


FIG. 5. Dependence on the pseudogap of physical quantities associated with mean-field theory of a single chain. The plot shows the coherence length ξ_0 , the width of the one-dimensional critical region Δt_{1D} , and the inverse of the specific heat jump ΔC . All quantities are normalized to their rigid-lattice values. For $\psi > 2.7T$ the coefficient b becomes negative and the transition will be first order (Sec. IV). The large reduction of Δt_{1D} below the rigid-lattice value of 0.8 means that a mean-field treatment of the single-chain Ginzburg-Landau functional may be justified.

$$\frac{\Delta C}{1.43\gamma T_P} \sim \left(\frac{T_{RL}}{T_P} \right)^2. \quad (69)$$

This simple argument gives the correct trend that as the fluctuations increase, the enhancement of the specific heat jump increases.

D. Width of the one-dimensional critical region

The width of the one-dimensional critical region is calculated from Eq. (60), with the Ginzburg-Landau coefficients in the presence of the pseudogap. It is shown in Fig. 5, normalized to the rigid-lattice value $\Delta t_{1D} = 0.8$. The large reduction is very important, because it means that even for weak interchain coupling, it may be possible for condition (4) to be satisfied and for a mean-field treatment of a single-chain functional, such as that used in this section, to be justified.

VI. ESTIMATE OF THE PSEUDOGAP IN $K_{0.3}MOO_3$

Optical conductivity, magnetic susceptibility, and photoemission experiments all suggest that near $T_P = 183$ K, there is a pseudogap in the density of states.

Optical conductivity. Sadovskii has calculated the optical conductivity $\sigma(\omega)$ for the model introduced in Sec. II.³⁷ For small frequencies, $\sigma(\omega)$ is linear in ω and has a peak at about $\omega \simeq 3\psi$. The data in Refs. 22 and 24 then imply $\psi \sim 40$ meV and $\psi/T_P \sim 2.5$. On a less rigorous level, ψ can be estimated based on the analysis contained in the inset of Fig. 4. If the single-chain mean-field transition temperature $T_0 < 0.4T_{RL}$ then $\psi \sim T_{RL}$. Using the BCS relation (8) and the estimate $\Delta(0) \simeq 80$ meV for the zero-temperature gap from the optical conductivity²² gives $\psi \sim 45$ meV and $\psi/T_P \sim 3$.

Magnetic susceptibility. The data of Refs. 5 and 20 give $\chi(T_P)/\chi(300 \text{ K}) \simeq 0.5$. Assuming that $\chi(300 \text{ K}) \simeq \chi_0$ and using Fig. 3 gives $\psi/T_P \sim 2.4$. Note that all of the above three estimates for ψ/T_P are consistent with one another and are all in the regime where the fourth-order coefficient b is small (Fig. 4).

Photoemission. Recent high resolution photoemission measurements²⁸⁻³⁰ on $K_{0.3}MoO_3$ and $(TaSe_4)_2I$ have several puzzling features: (1) There is a suppression of spectral weight over a large energy range (of the order of 200 meV for $K_{0.3}MoO_3$) near the Fermi energy. (2) The spectrum is very weakly temperature dependent. The suppression occurs even for $T \sim 2T_P$. (3) At T_P the spectrum does not just shift near E_F , due to the opening of the Peierls gap, but also at energies of order 0.5 eV from E_F .

These features *cannot* be explained using the model presented in this paper. The photoemission data suggest that the pseudogap is about $\psi \sim 130$ meV. Clearly this estimate is inconsistent with the estimates ($\psi \sim 40-50$ meV) given above from the optical conductivity and magnetic susceptibility. Furthermore, in the model presented

here the pseudogap occurs only when $\xi_{||}(T) \gg v_F/\psi$, i.e., fairly close to T_P . The temperature dependence of the Pauli spin susceptibility and the optical conductivity^{22,23} suggest that the pseudogap disappears for $T > 2T_P$ [in contrast to (2) above]. Dardel *et al.*²⁸ speculate that the anomalous behavior that they observe may arise, because the photoemission intensity $I(E)$ might be related to the density of states $\rho(E)$ by $I(E) = Z\rho(E)$ and the quasiparticle weight Z vanishes, due to Luttinger liquid effects. This suggestion has been examined critically by Voit,³⁹ who concludes that the photoemission data are only quantitatively consistent with a Luttinger liquid picture if very strong long-range interactions are involved. Kopietz, Meden, and Schönhammer⁶⁵ have recently considered such models.

VII. CONCLUSIONS

In this paper, a simple model has been used to illustrate some of the difficulties involved in constructing from microscopic theory a Ginzburg-Landau theory of the CDW transition. The main results are (1) the large thermal lattice motion near the transition temperature produces a pseudogap in the density of states. (2) Perturbation theory diverges and gives unreliable results. This is illustrated by showing that a predicted⁴⁰ scaling relation between the specific heat and the temperature derivative of the susceptibility does not hold. (3) The pseudogap significantly alters the coefficients in the Ginzburg-Landau free energy. The result is that one-dimensional order parameter fluctuations are less important, making a mean-field treatment of the single-chain Ginzburg-Landau functional more reasonable.

This work raises a number of questions and opportunities for future work. (a) The most important problem is that there is still no microscopic theory that can make reliable quantitative predictions about how dimensionless ratios, such as $\Delta(0)/k_B T_P$, $\Delta C/\gamma T_P$, and $\xi_{0z} T_P/v_F$ depend on parameters such as v_F , the electron-phonon coupling λ , T_P and the interchain coupling. (b) Is the change of the sign of the fourth-order coefficient b of the single-chain Ginzburg-Landau functional for $\psi > 2.7T_P$ an important physical effect or merely a result of the simplicity of the model considered here? (c) Calculation of the contribution of the sliding CDW to the optical conductivity in the presence of the short-range order associated with the pseudogap.^{24,25}

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APPENDIX A: SCHULZ'S MODEL

For completeness an alternative microscopic model is discussed. Schulz¹⁶ considered only thermal fluctuations in the phase of the order parameter. He assumed that the temperature was sufficiently low that fluctuations in the amplitude of the order parameter were not significant. (However, in real materials the amplitude fluctuations *are* important.³¹) Fluctuations along the chain were treated exactly and the interchain interactions were treated in the mean-field approximation. He derived a free-energy functional of the form (5). The coefficients in a tetragonal crystal ($a_x = a_y$) are

$$A = \frac{2}{J} - \frac{2v_F}{\pi T^2}, \quad (\text{A1})$$

$$B = \frac{7v_F^3}{\pi^3 T^6}, \quad (\text{A2})$$

$$C_x = \frac{a_x^2}{2J}, \quad (\text{A3})$$

$$C_z = \frac{2v_F^3}{\pi^3 T^4}. \quad (\text{A4})$$

The coefficient $A(T)$ vanishes at the three-dimensional transition temperature,

$$T_{3D} = \left(\frac{Jv_F}{\pi} \right)^{1/2}. \quad (\text{A5})$$

Thus, the ratio $\Delta(0)/k_B T_{3D}$ is not a universal quantity. The specific heat jump at the transition is

$$\Delta C = \frac{1}{a_x^2} \frac{(A')^2}{2BT_{3D}} = \frac{16\pi T_{3D}}{7a_x^2} = \frac{24}{7} \gamma T_{3D}, \quad (\text{A6})$$

where $\gamma T = 2\pi T/3v_F a_x^2$ is the normal state electronic specific heat. The coherence length parallel to the chains is

$$\xi_{z0} = \left(\frac{C_z}{A'} \right)^{1/2} = \frac{v_F}{\sqrt{2\pi T_{3D}}}. \quad (\text{A7})$$

Equations (A6) and (A7) then give the ratios given in Table I.

APPENDIX B: EVALUATION OF THE GINZBURG-LANDAU COEFFICIENTS

The Ginzburg-Landau free-energy functional (1) is related to the partition function Z , by the functional integral,

$$\frac{Z}{Z_0} = \int [d\phi(z)] \exp(-\beta F[\phi]), \quad (\text{B1})$$

where Z_0 is the partition function in the absence of interactions.

The phonon field in the Hamiltonian (17) is treated classically. For the Hamiltonian,

$$H = \int dz \left\{ \Psi^\dagger(z) \left[-iv_F \sigma_3 \frac{\partial}{\partial z} + \frac{1}{2} [\Delta(z) \sigma_+ + \Delta(z)^* \sigma_-] \right] \times \Psi(z) + \frac{\Delta(z)^2}{\lambda \pi v_F} \right\}, \quad (\text{B2})$$

the partition function is given by

$$Z = \int d\Delta(z) \exp \left(-\beta \int dz \frac{\Delta(z)^2}{\lambda \pi v_F} \right) \times \left\langle T \exp \left(-\int_0^\beta d\tau \int dz \Psi^\dagger(z, \tau) \left[-iv_F \sigma_3 \frac{\partial}{\partial z} + \frac{1}{2} [\Delta(z) \sigma_+ + \Delta(z)^* \sigma_-] \right] \Psi(z, \tau) \right) \right\rangle. \quad (\text{B3})$$

The goal is to get this expression into a form comparable to (B1), so the coefficients a , b , and c can be extracted.

The linked cluster or cumulant expansion⁶⁷ can be used to rewrite the time-ordered product in (B3). In general, if the Hamiltonian is separated according to

$$H = H_0 + H_1 \quad (\text{B4})$$

and

$$\langle S \rangle \equiv \left\langle T \exp \left(-\int_0^\beta d\tau H_1(\tau) \right) \right\rangle_0 = \frac{Z}{Z_0}, \quad (\text{B5})$$

where $\langle \rangle_0$ denotes a thermal average with respect to H_0 , then the linked cluster theorem states that

$$\langle S \rangle = \exp(\langle S \rangle_{0, \text{conn}}) - 1, \quad (\text{B6})$$

where $\langle S \rangle_{0, \text{conn}}$ denotes the set of connected terms in the diagrammatic expansion of S .

The important question is how to make the separation (B4)? A rigid-lattice treatment of the phonons neglects the effect of the thermal lattice motion on the electronic states. The Hamiltonian is separated according to

$$H_{0, \text{RL}} = \int dz \Psi^\dagger(z) \left[-iv_F \sigma_3 \frac{\partial}{\partial z} \right] \Psi(z), \quad (\text{B7})$$

$$H_{1, \text{RL}} = \frac{1}{2} \int dz \Psi^\dagger(z) [\Delta(z) \sigma_+ + \Delta(z)^* \sigma_-] \Psi(z). \quad (\text{B8})$$

The resulting free-energy functional is

$$F_{\text{RL}}[\phi] = \int dz \left\{ \frac{\phi(z)^2}{\lambda \pi v_F} \right\} + \frac{1}{\beta} \left[\left\langle T \exp \left(-\frac{1}{2} \int dz \phi(z) \times \int_0^\beta d\tau \Psi^\dagger(z, \tau) \sigma_+ \Psi(z, \tau) - \text{H.c.} \right) \right\rangle_{0, \text{RL, conn}} - 1 \right], \quad (\text{B9})$$

where $\Delta(z)$ has been equated with $\phi(z)$ in the functional integral. Expanding to fourth order in $\phi(z)$ gives the rigid-lattice coefficients given by (9–11).¹⁵

To improve on this rigid-lattice treatment, we want to expand relative to a Hamiltonian, which includes at least some of the effects of lattice fluctuations. The rigid-lattice expression (B9) is modified in the following way:

$$F[\phi] = \int dz \left\{ \frac{\phi(z)^2}{\lambda v_F} \right\} + \frac{1}{\beta} \left[\left\langle \left\langle T \exp \left(-\frac{1}{2} \int dz \phi(z) \int_0^\beta d\tau \Psi^\dagger(z, \tau) \sigma_+ \times \Psi(z, \tau) - \text{H.c.} \right) \right\rangle \right\rangle_{\text{conn}} - 1 \right], \quad (\text{B10})$$

where the expectation value of an operator A is defined by

$$\langle\langle A \rangle\rangle = \int \frac{dv dv^*}{\pi} \exp(-vv^*) \text{Tr} [A \exp(-\beta H_0[v])], \quad (\text{B11})$$

with the Hamiltonian H_0 ,

$$H_0[v] = \int dz \left\{ \Psi^\dagger(z) \left[-iv_F \sigma_3 \frac{\partial}{\partial z} + \frac{1}{2} \psi (v \sigma_+ + v^* \sigma_-) \right] \Psi(z) \right\}. \quad (\text{B12})$$

It is now possible to evaluate analytically the free-energy functional (B10). The Fourier transform

$$\phi(z) = \frac{1}{\sqrt{L}} \sum_q \phi_q e^{iqz} \quad (\text{B13})$$

is performed and the free energy (B10) expanded to fourth order in ϕ . The result is

$$F[\phi] = \sum_q a(q) \phi_q \phi_q^* + \frac{1}{L} \sum_{q_1, q_2, q_3} b(q_1, q_2, q_3) \phi_{q_1}^* \phi_{q_2}^* \phi_{q_3} \phi_{q_1+q_2-q_3}, \quad (\text{B14})$$

where the coefficients $a(q)$ and $b(q_1, q_2, q_3)$ are given by

$$a(q) = \frac{1}{\pi v_F \lambda} + \pi T \sum_{\epsilon_n} \int \frac{dv dv^*}{\pi} e^{-vv^*} \int \frac{dk}{2\pi} \times \text{Tr} \left[\sigma_+ \hat{G}(k+q, \epsilon_n, v) \sigma_- \hat{G}(k, \epsilon_n, v) \right], \quad (\text{B15})$$

$$b(q_1, q_2, q_3) = \pi T \sum_{\epsilon_n} \int \frac{dv dv^*}{\pi} e^{-vv^*} \int \frac{dk}{2\pi} \times \text{Tr} \left[\sigma_- \hat{G}(k+q_1, \epsilon_n, v) \sigma_- \times \hat{G}(k+q_1+q_2, \epsilon_n, v) \sigma_+ \hat{G}(k+q_1+q_2-q_3, \epsilon_n, v) \sigma_+ \hat{G}(k, \epsilon_n, v) \right], \quad (\text{B16})$$

and the electronic Green's function $\hat{G}(k, \epsilon_n, v)$ is defined in Eq. (34).

Expanding $a(q)$ in powers of q^2 gives the Ginzburg-Landau coefficients $a(T)$ and $c(T)$:

$$a(q) = a(T) + c(T)q^2 + \dots \quad (\text{B17})$$

The fourth-order coefficient is $b = b(0, 0, 0)$. The coefficients a, b , and c are given in terms of ψ in Eqs. (50)–(52).

* Electronic address: ross@newt.phys.unsw.edu.au

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