I. INTRODUCTION

A. Motivation

Crystals consisting of linear molecular chains can have highly anisotropic electronic properties. Many of these quasi-one-dimensional materials undergo finite temperature phase transitions. Detailed experimental studies in the 1970’s of the charge-density-wave (CDW) transition in materials such as KCP and TTF-TCNQ[1] stimulated work on the theoretical description of phase transitions in quasi-one-dimensional materials[2–7]. Unfortunately, due to the limited quality of samples it was not possible to make a quantitative comparison of experiment with theory. In the past decade, a whole new range of quasi-one-dimensional materials, many in high-purity single crystals, have been synthesized[8]. Examples of new materials are the CDW material K$_{0.3}$MoO$_3$ (blue bronze), the Bechgaard salt (TMTSF)$_2$PF$_6$[9], that undergoes a spin-density-wave (SDW) transition, thin wires of superconducting lead[10], and an inorganic compound CuGeO$_3$ that undergoes a spin-Peierls transition[11]. Furthermore, high-quality experimental data[12–14] on these crystals opens the possibility of making a quantitative comparison of experiment with theory. For example, recently anomalies in the specific heat, Young’s modulus, thermal expansion, and magnetic susceptibility close to the three-dimensional CDW transition in K$_{0.3}$MoO$_3$ were all precisely measured on the same single crystal[13].

Fluctuations in the order parameter are extremely important in these materials. In a strictly one-dimensional system with short-range interactions there are no phase transitions at finite temperature because fluctuations in the order parameter destroy long range order[15,16]. Consequently in a real quasi-one-dimensional material a finite-temperature phase transition only occurs as a result of the weak interchain interactions. Hence, a complete theory must treat fluctuations along the chain carefully and also include the interchain interactions. On the other hand, in most materials the three-dimensional transition temperature, $T_{3D}$, is clearly defined and the width of the critical region is only a few percent of $T_{3D}$. Hence, a three-dimensional Ginzburg-Landau theory should accurately describe the transition, except in a narrow temperature range.

The purpose of the present paper is to provide a complete derivation of a Ginzburg-Landau theory describing the three-dimensional ordering transition of a quasi-one-dimensional system with a complex (i.e., two-component) order parameter. Such an order parameter describes superconductors, charge- and spin-density waves (which are incommensurate with the lattice), and a spin-Peierls system in a large magnetic field. Particular attention is given to examining the validity of the assumptions and approximations made in previous work[3–7]. This work is the continuation of a larger program of examining the effect that lattice fluctuations have on electronic properties of CDW compounds. Recently, the role of order parameter fluctuations in the blue bronze and the Bechgaard salts was considered by Castella, Baeriswyl, and Maki[20]. Schulz and Bourbonnais have considered quantum fluctuations in the phase of the order parameter in quasi-one-dimensional superconductors[21].
B. Overview

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

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

In this paper the coefficients \( a, b, \) and \( c \) will be treated as phenomenological parameters. For a specific system these coefficients can be calculated from microscopic theory.

Due to fluctuations in the order parameter this system cannot develop long-range order at finite temperature. Furthermore, the values for the coefficients \( a, b, \) and \( c \) given by the simplest microscopic theories predict that the fluctuations are important over a temperature range comparable to the single chain mean-field transition temperature. To describe a finite-temperature phase transition, a set of weakly interacting chains are considered. If \( \phi_i(z) \) is the order parameter on the \( i \)-th chain the free energy functional for the system is

\[
F[\phi_i(z)] = \sum_i F_1[\phi_i(z)] - \sum_{i,j} J_{ij} \int dz \text{Re}[\phi_i(z)\phi_j(z)]
\] (2)

where \( J_{ij} \) describes the interchain interactions. In most of this paper it will be assumed that the interchain interaction \( J_{ij} \) is non-zero only for nearest neighbour chains and that its value is \( J_x/4 \) and \( J_y/4 \) in the \( x \) and \( y \) directions respectively. A mean-field treatment of this functional will not give accurate results due to the large intrachain fluctuations (see Section III). This problem is solved by integrating out these fluctuations to derive a new Ginzburg-Landau free energy functional with renormalized coefficients\( \tilde{F} \) respectively.

The correlation and coherence lengths perpendicular to the chains are given by similar expressions.

The specific heat jump per unit volume is \( \Delta C \)

\[
\Delta C = \frac{(A')^2}{2BT_{3D}}.
\] (5)

The specific heat jump per chain at the transition is given by

\[
\Delta C_{3D} \equiv \Delta C/(a_xa_y).
\]

In the Gaussian approximation the correlation length parallel to the chains is given by

\[
\xi_z = \sqrt{\frac{C_z}{A'}} = \xi_{0z} \left( \frac{T}{T_{3D}} - 1 \right)^{-1/2}
\] (6)

where \( \xi_{0z} \) is the longitudinal coherence length defined as

\[
\xi_{0z} = \sqrt{\frac{C_z}{A'}}.
\] (7)

The correlation and coherence lengths perpendicular to the chains are given by similar expressions.

The Ginzburg criterion gives a rough estimate of the width, \( \Delta T_{3D} \), of the 3D critical region.

\[
\Delta t_{3D} \equiv \frac{\Delta T_{3D}}{T_{3D}} = \frac{1}{32\pi \Delta C_{3D}\xi_x\xi_y\xi_{0z}^2}
\] (8)
This paper establishes the striking result that most of the physics is determined by a single dimensionless parameter

\[ \kappa = \frac{2(bT)^2}{|a|^3 c}. \]  

A brief argument is now given to show that \( \kappa \) is a measure of the fluctuations along a single chain. The rms fluctuation in the single chain order parameter \( \langle |\phi|^2 \rangle \), calculated in the Gaussian approximation, is \( T(2|c|a)^{1/2} \). The magnitude of the order parameter, calculated in the mean-field approximation, \( \phi_0 \), is given by \( \phi_0^2 = |a|/2b \). Hence, \( \kappa = 2 \langle |\phi|^2 \rangle / \phi_0^2 \) and so is a measure of the importance of fluctuations. The strength of the interchain interactions determines the value of \( \kappa \) at the three-dimensional transition temperature.

The general approach that has been taken previously when deriving a Ginzburg-Landau functional for the three-dimensional transition is to treat the interchain interactions in the mean-field approximation and then solve the resulting one-dimensional problem treating the fluctuations along the chain in the lowest-level approximation (see Section A.2 for a definition). In this paper the interchain interactions are also treated in the mean-field approximation but the fluctuations along the chain are treated exactly. This paper is confined to a mean-field analysis of the functional \( \mathcal{L} \). In Section IV it is shown that this is justified except in a narrow temperature range very close to \( T_{3D} \). However, it should be pointed out that one could perform a sophisticated renormalization group analysis for the functional \( \mathcal{L} \) such as that due to Chen and which has been recently used in the analysis of specific heat measurements on the CDW compound \( K_{0.3}\text{MoO}_3 \). The free energy functional that derived here could be used as the input to such an analysis.

The outline of the paper is as follows. Table I contains a summary of the symbols for the important quantities for a single chain and for a three-dimensional system of weakly interacting chains. Section II describes an exact treatment of the fluctuations in a strictly one-dimensional system. Section III contains a complete derivation of the coefficients \( \kappa_0 \) for a definition). In this paper the interchain interactions are also treated in the mean-field approximation and then solve the resulting one-dimensional problem treating the fluctuations along the chain in the lowest-level approximation (see Section A.2 for a definition). In this paper the interchain interactions are also treated in the mean-field approximation but the fluctuations along the chain are treated exactly. This paper is confined to a mean-field analysis of the functional \( \mathcal{L} \). In Section IV it is shown that this is justified except in a narrow temperature range very close to \( T_{3D} \). However, it should be pointed out that one could perform a sophisticated renormalization group analysis for the functional \( \mathcal{L} \) such as that due to Chen and which has been recently used in the analysis of specific heat measurements on the CDW compound \( K_{0.3}\text{MoO}_3 \). The free energy functional that derived here could be used as the input to such an analysis.

The outline of the paper is as follows. Table I contains a summary of the symbols for the important quantities for a single chain and for a three-dimensional system of weakly interacting chains. Section II describes an exact treatment of the fluctuations in a strictly one-dimensional system. Section III contains a complete derivation of the coefficients in the Ginzburg-Landau functional \( \mathcal{L} \). In Section IV it is assumed that the single chain coefficients \( a, b, \) and \( c \) are temperature independent. The three-dimensional transition temperature is calculated as a function of the interchain coupling (Figure 1). The values derived for the coefficients \( A', B, C_x, C_y, \) and \( C_z \) are used to calculate the specific heat jump, coherence lengths, and width of the critical region at the three-dimensional transition (Figures 2 and 3). The striking result is established that the width of the critical region is fairly independent of any parameters, \( \Delta T_{3D} \approx 0.05 - 0.08 \). Sections II and III can be omitted by readers not interested in technical details. The Hartree, Hartree-Fock, and lowest-level approximations for the fluctuations that have been given in previous work are described in the Appendix. It is shown that the lowest-level approximation is only reliable for \( \kappa < 10^{-3} \) (Figures 4 and 5). In Table I very rough estimates of \( \kappa \) for various CDW materials give \( \kappa > 10^{-2} \), showing that they are well outside the regime of validity of the lowest-level approximation.

II. ONE-DIMENSIONAL GINZBURG-LANDAU THEORY

The mean-field treatment of one-dimensional Ginzburg-Landau theory is described before an exact treatment of the order-parameter fluctuations is given. For completeness the Appendix to the paper describes various approximate treatments of fluctuations that have been given in earlier work.

A. Mean-field treatment

Long-wavelength fluctuations associated with the gradient term in \( \mathcal{L} \) are neglected. One simply minimizes the potential

\[ V(\phi) = a \int |\phi|^2 + b \int |\phi|^4. \]  

The single chain mean-field transition temperature \( T_0 \) is defined by the temperature at which the coefficient \( a(T) \) vanishes. Close to \( T_0 \) it is convenient to write

\[ a(T) = (t-1)a' \]

where \( t = T/T_0 \). In the mean-field approximation there is a phase transition at \( T_0 \) and the magnitude of the order parameter for \( T < T_0 \), \( \phi_0 \), is

\[ \phi_0^2 = \frac{|a|}{2b}. \]
The free energy per unit length of the ordered state, relative to the disordered state is smaller by $V_0$, given by

$$V_0 \equiv -V[\phi_0] = \frac{a^2}{4b}. \quad (13)$$

The jump in the specific heat at the transition is

$$\Delta C_{1D} = \frac{(a')^2}{2bT_0}. \quad (14)$$

An important length scale is the coherence length $\xi_0$, defined by

$$\xi_0 = \left(\frac{c}{a'}\right)^{1/2} \quad (15)$$

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

$$\Delta t_{1D} = \Delta T_{1D} \equiv \Delta T_{1D} = \left(\frac{bT_0}{a'^{3/2}c^{1/2}}\right)^{2/3} = \frac{1}{(2\xi_0\Delta C_{1D})^{2/3}}. \quad (16)$$

There are several serious problems with a mean-field treatment. First, it predicts a finite temperature phase transition. Second, the simplest microscopic models give $\Delta t_{1D} \sim 1/7$, suggesting that the neglected fluctuations play an important role over a very broad temperature range. An exact treatment of these fluctuations is now given.

### B. Exact solution

The goal is to evaluate the functional integral for the partition function $Z$ of a system with the Ginzburg-Landau free energy (1),

$$Z = \int [d\phi(z)] \exp \left( -\frac{F_1[\phi(z)]}{T} \right) \quad (17)$$

It is convenient to rescale the order parameter $\phi(z) \rightarrow \phi(z)/\phi_0$ and write the functional (1) as

$$F_1[\phi] = V_0 \int dz \left[ -2 |\phi|^2 + |\phi|^4 + \frac{2c}{a'} |\frac{\partial \phi}{\partial z}|^2 \right] \quad (18)$$

assuming that $T < T_0$. Scalapino, Sears, and Ferrell showed that a transfer matrix method could be used to reduce the problem to that of diagonalizing a transfer matrix Hamiltonian $H_{tr}$. This involves a cylindrically symmetric Schrödinger-like equation with a single complex degree of freedom $s = \rho e^{i\varphi}$,

$$H_{tr} \Psi_m = \left[ -\kappa \left( \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} \right) - 2\rho^2 + \rho^4 \right] \Psi_m(\rho, \varphi) = \lambda_m \Psi_m(\rho, \varphi). \quad (19)$$

The eigenvalues $\lambda_m$ only depend on the dimensionless parameter $\kappa$.

As discussed in the introduction $\kappa$ is a measure of the size of the fluctuations in the order parameter, and defined by equation (9). $\kappa$ is central to this paper. It is shown in Section [IV] that the value of $\kappa$ at the three-dimensional transition temperature determines physically important quantities such as the specific heat jump. For the case of a real (i.e., one-component) order parameter the importance of $\kappa$ was emphasized previously by Bishop and Krumhansl ($\kappa$ corresponds to $2\mu^2$ in their paper) and Dieterich ($\kappa$ corresponds to $4/\alpha^2$ in his paper).

The partition function (17) for a system of length $L$ is

$$Z = \sum_m \exp(-LV_0\lambda_m/T) \quad (20)$$

Consequently, in the thermodynamic limit, the free energy per unit length equals $V_0\lambda_0$. The order parameter correlation function is
\[(\phi(z)\phi(0)^*) = \phi_0^2 \sum_m |< \Psi_m | s | \Psi_0 >|^2 \exp \left( -\frac{|z|}{T} V_0 (\lambda_m - \lambda_0) \right) \]  

(21)

which at large distances becomes

\[(\phi(z)\phi(0)^*) = \phi_0^2 |< \Psi_1 | s | \Psi_0 >|^2 \exp \left( -\frac{|z|}{\xi_1} \right) \]  

(22)

where \( \xi_1 \) is the correlation length given by the separation of the lowest two eigenvalues of the transfer matrix Hamiltonian

\[\xi_1 = \frac{T}{V_0 (\lambda_1 - \lambda_0)} = \left( \frac{c}{\alpha} \right)^{1/2} (8\kappa)^{1/2} \frac{1}{(\lambda_1 - \lambda_0)(\kappa)}. \]  

(23)

The Fourier transform of the correlation function defines the static linear susceptibility

\[\chi_1(q) = \frac{1}{T} \int dze^{-i q z} \langle \phi(z)\phi(0)^* \rangle. \]  

(24)

For small \( q \) it is of the form

\[\chi_1(q) = \frac{\chi_1(0)}{1 + (q\xi_1)^2}. \]  

(25)

where

\[\chi_1(0) = \frac{2\phi_0^2}{V_0} \sum_m |< \Psi_m | s | \Psi_0 >|^2 \lambda_m - \lambda_0 \equiv \frac{4}{\alpha} f(\kappa). \]  

(26)

and a dimensionless function, \( f(\kappa) \), that only depends on the fluctuation parameter \( \kappa \) has been introduced.

Due to the cylindrical symmetry of the potential \( V(s) \) the eigenfunctions can be written in the form

\[\Psi_{n,\ell}(\rho, \phi) = u_{n,\ell}(\rho) \sqrt{\frac{2}{\pi \rho}} \exp(i\ell\phi) \quad \ell = 0, \pm 1, \pm 2, \ldots \]  

(27)

Equation (19) reduces to the one-dimensional Schrödinger type equation

\[-\kappa \frac{d^2}{d\rho^2} + \frac{\kappa (\ell^2 - 1)}{\rho^2} - 2\rho^2 + \rho^4] u_{n,\ell}(\rho) = \lambda_{n,\ell} u_{n,\ell}(\rho). \]  

(28)

In order for the system wave function to be finite at the origin the radial wave function satisfies the boundary condition

\[u_{n,\ell}(0) = 0. \]  

(29)

Normalization of the wave function requires that

\[\int_0^\infty |u_{n,\ell}(\rho)|^2 d\rho = 1 \]  

(30)

The integrals over the angular variable \( \phi \) in the matrix elements in the susceptibility (26) can be performed explicitly. The function \( f(\kappa) \) in the susceptibility (26) then reduces to

\[f(\kappa) = \sum_n \frac{|< u_{n,1}| s | u_{0,0} >|^2}{\lambda_{n,1} - \lambda_{0,0}}. \]  

(31)

This expression has been evaluated numerically by solving the eigenvalue equation (28) numerically\(^2\). The results are shown in Figure [4]. To check the numerical results use was made of the sum rule

\[\frac{1}{2\kappa} \sum_n (\lambda_{n,1} - \lambda_{0,0}) |< u_{n,1}| s | u_{0,0} >|^2 = 1 \]  

(32)
which can be derived using standard arguments.

It is useful to consider the effect of an external potential \( \Phi \) on the system. Let \( \lambda(\Phi) \) be the energy of the lowest eigenstate of the transfer operator \( H_e + s \Phi + s^* \Phi \), where \( H_e \) is given by (14). Second-order perturbation theory shows that the static linear susceptibility \( \chi_1(0) \) is given by

\[
\chi_1(0) = -\frac{\phi_0^2}{V_0} \frac{\partial^2 \lambda(\Phi)}{\partial \Phi \partial \Phi^*} \bigg|_{\Phi=0}.
\]

The third-order nonlinear susceptibility is

\[
\chi_3 = -\frac{\phi_0^4}{4V_0^3} \frac{\partial^3 \lambda(\Phi)}{\partial \Phi^2 \partial \Phi^* \partial \Phi} \bigg|_{\Phi=0}.
\]

Expanding the Brillouin-Wigner perturbation theory expression for \( \lambda(\Phi) \) to fourth-order in \( |\Phi| \) gives

\[
\chi_3 = \frac{4\phi_0^4}{V_0} \sum_{m,n,p \neq 0} \frac{<\Psi_m|s|\Psi_n><\Psi_n|s|\Psi_p><\Psi_p|s|\Psi_0>}{(\lambda_m - \lambda_0)(\lambda_n - \lambda_0)(\lambda_p - \lambda_0)}
+ \frac{2\phi_0^4}{V_0} \sum_{m,n,p \neq 0} \frac{<\Psi_m|s|\Psi_n><\Psi_n|s|\Psi_{\bar{n}}><\Psi_{\bar{n}}|s|\Psi_0>}{(\lambda_m - \lambda_0)(\lambda_n - \lambda_0)(\lambda_{\bar{n}} - \lambda_0)}
- \frac{2\phi_0^2}{V_0} \chi_1(0) \sum_m \frac{|<\Psi_m|s|\Psi_0>|^2}{(\lambda_m - \lambda_0)^2} = \frac{16b}{a^4} g(\kappa).
\]

As for the linear susceptibility the above expression can be simplified by using the factorization of the wavefunction and performing the integrals over the angular variable \( \varphi \) in the matrix elements. The dimensionless function \( g(\kappa) \), defined in (33), only depends on the fluctuation parameter \( \kappa \) and is given by

\[
-g(\kappa) = 4 \sum_{n \neq 0,m,p} \frac{<u_{0,0}|\rho|u_{m,1}><u_{m,1}|\rho|u_{0,0}><u_{0,0}|\rho|u_{n,0}><u_{n,0}|\rho|u_{0,0}>}{(\lambda_{m,1} - \lambda_{0,0})(\lambda_{n,0} - \lambda_{0,0})(\lambda_{0,1} - \lambda_{0,0})}
+ 2 \sum_{m,n,p} \frac{<u_{0,0}|\rho|u_{m,1}><u_{m,1}|\rho|u_{n,2}><u_{n,2}|\rho|u_{0,1}><u_{0,1}|\rho|u_{0,0}>}{(\lambda_{m,1} - \lambda_{0,0})(\lambda_{n,2} - \lambda_{0,0})(\lambda_{0,1} - \lambda_{0,0})}
- 4f(\kappa) \sum_n \frac{|<u_{n,1}|\rho|u_{0,0}>|^2}{(\lambda_{n,1} - \lambda_{0,0})^2}.
\]

The functions \( f(\kappa) \) and \( g(\kappa) \) will appear in the expressions for the coefficients of the Ginzburg-Landau functional for the three-dimensional transition.

In summary, the free energy per unit length in the presence of an external field \( \Phi \), \( \tilde{F}_1[\Phi] \), is, to fourth-order in \(|\Phi|\)

\[
\tilde{F}_1[\Phi] = V_0 \lambda(0) - \chi_1(0) \left| \Phi \right|^2 - \chi_3 \left| \Phi \right|^4.
\]

If the external field is slowly varying in space \( \Phi(z) \) then the quadratic term is replaced with

\[
\Phi(z)^* \int dz' \chi_1(z - z') \Phi(z') = \Phi(z)^* \int \frac{dq}{2\pi} \chi_1(q) \Phi(q) e^{iqz} = \Phi(z)^* \int \frac{dq}{2\pi} \chi_1(0) \left( 1 - q^2 \xi_1^2 \right) \Phi(q) e^{iqz} = \chi_1(0) \Phi(z)^* \left( \Phi(z) + \xi_1^2 \frac{\partial^2 \Phi(z)}{\partial z^2} \right)
\]

where the long-wavelength expression (33) has been used.

### III. DERIVATION OF A THREE-DIMENSIONAL GINZBURG-LANDAU FUNCTIONAL

In this section a new three-dimensional Ginzburg-Landau free energy functional is derived by integrating out the order parameter fluctuations along the chain exactly and treating the interchain interactions in the mean-field approximation. Since this treatment (over)emphasizes the one-dimensional fluctuations its regime of validity is considered...
briefly in the Conclusions section. Before proceeding with the derivation a rough estimate is made of how small the interchain interactions must be in order for a mean-field treatment of the anisotropic functional \((\ref{eq:43})\) to be invalid. Taking the continuum limit of \((\ref{eq:43})\) and using the three-dimensional Ginzburg criterion gives

\[
\Delta t_{3D} \approx \frac{2}{\pi^2} (\Delta t_{1D})^3 \frac{(a')^2}{J_x J_y}.
\]  

(39)

Hence, if \(\Delta t_{1D} \sim 1\), as predicted by the simplest microscopic theories, and if \(J_x \sim J_y < 0.3a'\) (the regime considered in this paper) then \(\Delta t_{3D} > 1\) and a mean-field analysis will give poor results.

The treatment given here is similar to the derivation of the Ginzburg-Landau functional for the Ising model by Negele and Orland. The partition function for a set of chains is

\[
Z = \int \Pi_i [d\phi_i(z)] \exp \left( -F[\phi_i(z)]/T \right)
\]  

(40)

where the free energy functional \(F[\phi_i(z)]\) is given by \((\ref{eq:43})\). The interaction term is replaced with the following Gaussian integral

\[
\exp \left( \frac{1}{T} \sum_{i,j} J_{ij} \int dz \text{Re}[\phi_i(z)^* \phi_j(z)] \right)
\]

\[
= A \int \Pi_i [d\Phi_i(z)] \exp \left( -T \sum_{i,j} J_{ij}^{-1} \int dz \text{Re}[\Phi_i(z)^* \Phi_j(z)] + \sum_i \int dz \text{Re}[\phi_i(z)^* \Phi_i(z)] \right)
\]  

(41)

where \(A\) is a normalization constant. The new field \(\Phi_i(z)\) will be used below as the order parameter to describe the three-dimensional transition. It follows from \((\ref{eq:40})\) and \((\ref{eq:41})\) that

\[
\langle \Phi_i(z) \rangle = \frac{1}{T} \sum_j J_{ij} \langle \phi_j(z) \rangle
\]  

(42)

Hence, the new order parameter is the average of the single chain order parameter \(\phi_j(z)\) over neighbouring chains. The new expression for the partition function has the desirable feature that there are no interchain interactions involving the order parameter \(\phi_i(z)\). Consequently, the results of Section \(\ref{sec:2.1}\) can be used to integrate exactly over the fluctuations in \(\phi_i(z)\) along each chain. The partition function is now a functional integral over the new order parameter \(\Phi_i(z)\) which has a free energy functional \(\tilde{F}[\Phi_i(z)]\),

\[
Z = \int \Pi_i [d\Phi_i(z)] \exp \left( -\tilde{F}[\Phi_i(z)]/T \right)
\]  

(43)

where

\[
\tilde{F}[\Phi_i(z)] = \sum_i \tilde{F}_1[\Phi_i(z)] + T \sum_{i,j} J_{ij}^{-1} \int dz \text{Re}[\Phi_i(z)^* \Phi_j(z)]
\]  

(44)

and \(\tilde{F}_1[\Phi(z)]\) is the free energy of a single chain in the presence of an external field \(\Phi(z)\),

\[
\exp \left( -\tilde{F}_1[\Phi(z)]/T \right) = \int [d\phi(z)] \exp \left( -\frac{F_1[\phi(z)]}{T} + \sum_i \int dz \text{Re}[\phi(z)^* \Phi(z)] \right).
\]  

(45)

Up to this point the analysis is exact. A mean-field analysis of the functional integral \((\ref{eq:44})\) will now be given. In the next Section it is shown that this is justified except in a narrow temperature range very close to \(T_{3D}\). However, it should be stressed that one could perform a sophisticated renormalization group analysis of \((\ref{eq:44})\). The free energy functional that derived here could be used as the input to such an analysis.

Close to \(T_{3D}\), the three-dimensional transition temperature the new order parameter \(\Phi_i(z)\) will be small and slowly varying in space. Hence \(\tilde{F}_1[\Phi(z)]\) can be evaluated in a perturbation expansion in \(\Phi(z)\) and a gradient expansion.

Use is now made of the results from Section \(\ref{sec:2.2}\). Let \(\Lambda(\Phi)\) be the energy of the lowest eigenstate of the transfer operator \(H_{tr} + s\Phi^* + s^*\Phi\) where \(H_{tr}\) is given by \((\ref{eq:14})\). The free energy per unit length of a single chain in the presence of a slowly varying field \(\Phi(z)\) is
\[ F_1[\Phi(z)] = V_0\lambda(0) - \chi_1(0) \left( |\Phi|^2 - \xi_1^2 \frac{\partial \Phi}{\partial z} \right)^2 - \chi_3 |\Phi|^4 \]  

(46)

where \( \chi_1(0) \) is the static linear susceptibility of the system given by (26) and \( \chi_3 \) is the third-order nonlinear susceptibility given by (35).

Near the three-dimensional transition temperature the continuum limit perpendicular to the chains (\( \Phi_i(z) \rightarrow \Phi(x, y, z) \)) can be taken. Assume that the interchain interaction \( J_{ij} \) is non-zero only for nearest neighbour chains and that its value is \( J_x/4 \) and \( J_y/4 \) in the \( x \) and \( y \) directions respectively. Then the interchain interaction term in (44) becomes

\[
\sum_{i,j} J_{ij}^{-1} \int dz \text{Re}[\Phi_i(z)^* \Phi_j(z)] = 1 \frac{J_{xy}^a x + J_{xy}^a y}{4J^2} \int dx dy \left( |\Phi|^2 + \frac{a_x^2 J_x}{4J} |\frac{\partial \Phi}{\partial x}|^2 + \frac{a_y^2 J_y}{4J} |\frac{\partial \Phi}{\partial y}|^2 \right) \]  

(47)

where \( a_x \) and \( a_y \) are the lattice constants perpendicular to the chains and \( J \equiv \frac{1}{2}(J_x + J_y) \). The final free energy functional (44) is of the form (3) with coefficients

\[
A = \frac{1}{J} - \chi_1(0) 
B = -\chi_3 
C_x = \frac{a_x^2 J_x}{4J^2} 
C_y = \frac{a_y^2 J_y}{4J^2} 
C_z = \chi_1(0)\xi_1^2. 
\]  

(50)  
(51)  
(52)

The three-dimensional mean-field temperature \( T_{3D} \) is defined by the vanishing of the coefficient \( A \),

\[
1 = J\chi_1(0) 
\]  

(53)

where the right hand side depends on temperature. This equation can be written in the dimensionless form

\[
\frac{J}{|a|} = \frac{1}{4f(\kappa(T_{3D}))}. 
\]  

(54)

The relationship between the interchain coupling \( J \) and the value of \( \kappa \) at the three-dimensional transition defined by this equation is shown in Figure III.

**IV. MEASURABLE QUANTITIES AT THE THREE-DIMENSIONAL TRANSITION**

It will now be assumed that the coefficients \( a, b, \) and \( c \) are temperature independent and \( T_{3D} \ll T_0 \), so \( |a| \sim a' \). Consequently, the only temperature dependence in the fluctuation parameter \( \kappa \) is the factor of \( T^2 \) (compare equation (9)). Scalapino, Imry and Pincus, Manneville, and Dieterich also made this assumption. It is an open question as to how realistic this assumption is for different microscopic models of the CDW transition.

First, this assumption allows us to rewrite \( \kappa \) in terms of the width of the one-dimensional critical region \( \Delta t_{1D} \) and evaluate the three-dimensional transition temperature as a function of the interchain coupling (Figure III). Roughly

\[
\left( \frac{T_{3D}}{T_0} \right)^2 \sim \frac{1.5J}{|a|\Delta t_{1D}^3}. 
\]  

(55)

This is a useful relation because it gives a criterion

\[
J \ll |a|\Delta t_{1D}^3 
\]  

(56)
for how weak the interchain coupling must be in order for the three-dimensional transition temperature to be sub-
stantially less than the single-chain mean-field temperature $T_0$.

The coefficient $A'$ (which determines the specific heat jump and the coherence lengths) depends on the $\kappa$ dependence of $f(\kappa)$ and the $T$ dependence of the fluctuation parameter $\kappa$

\[
A' = -\frac{1}{J} \left. \frac{d \ln f(\kappa)}{d \ln T} \right|_{T=T_3D} = \frac{1}{T} \left[ \frac{d \ln |a|}{d \ln T} - \frac{d \ln f(\kappa)}{d \ln \kappa} \right] \left|_{T=T_3D} \right.
\]

Assuming that the coefficients $a$, $b$, and $c$ are temperature independent ([57]) reduces to

\[
A' = -\frac{2}{J} \left. \frac{d \ln f(\kappa)}{d \ln \kappa} \right|_{T=T_3D}
\]

The specific heat jump, coherence lengths, and critical region width can now be calculated. It turns out that they can each be written in a dimensionless form that only depends on the value of the fluctuation parameter $\kappa$ at the three-dimensional transition. The specific heat jump per chain given by ([3], [13] and [57]) is

\[
\Delta C = \frac{\sqrt{8 \kappa}^{3/2}}{\xi_0} g(\kappa) \left( \frac{d f(\kappa)}{d \kappa} \right)^2
\]

where $\xi_0$ is the single chain coherence length given by ([13]). Hence the specific heat jump only depends on two quantities, $\xi_0$ and $\kappa$ (or equivalently the interchain coupling) (see Figure 3). Note that as the coherence length decreases the specific heat jump increases. For moderate interchain coupling ($J > 0.05|a|$) the specific heat jump becomes independent of the interchain coupling. The origin of this independence is not clear.

The longitudinal coherence length is

\[
\frac{\xi_{0z}}{\xi_0} = \frac{2}{\lambda_{0,1}(\kappa) - \lambda_{0,0}(\kappa)} \left( -\frac{d \ln f(\kappa)}{d \kappa} \right)^{-1/2}
\]

The dependence of the longitudinal coherence length on the interchain coupling is shown in Figure 2.

Quantitative comparison of these expressions for the specific heat jump and longitudinal coherence length with experimental data is not possible without accurate values of $\xi_0$ from microscopic theory. However, for all interchain coupling strengths the product of the specific heat jump and the longitudinal coherence length, $\Delta C\xi_{0z}$, depends only roughly on the interchain coupling (see the dashed curve in Figure 3). Since this quantity is dimensionless it can be compared with experiment. If $\Delta C_{3D}$ is the specific heat jump per unit volume then

\[
\frac{\Delta C_{3D} x a_0 y \xi_{0z}}{k_B} \approx 1.2 - 2.6.
\]

For the blue bronze $K_{0.3}$MoO$_3$ experiment [3] gives $\Delta C_{3D}/k_B = (2.6 \pm 0.3) \times 10^{-3} \cdot A^{-3}$, $\xi_{0z} = 15 \pm 3 \cdot A$ [2], and $a_x a_y = 16 \cdot A^2$ which gives $\Delta C_{3D} a_x a_y \xi_{0z}/k_B = 0.6 \pm 0.2$.

The transverse coherence length is

\[
\frac{\xi_{0x}}{a_x} = \left( \frac{J_x}{J} \right)^{1/2} \left( -\frac{d \ln f(\kappa)}{d \ln \kappa} \right)^{-1/2}
\]

The dependence of the right hand side on $\kappa$ is fairly weak. Consequently the transverse coherence length depends only weakly on the interchain coupling (Figure 3). This result is somewhat counterintuitive: it might be expected that as the interchain coupling increases the transverse coherence length increases. However, $\xi_{0x}$ is not just determined by the coefficient $C_z$ but also by the coefficient $A'$ ($\xi_{0x} = (C_z/A')^{1/2}$). It turns out that both these quantities have roughly the same dependence on $J$.

A crossover temperature, $T_x$, can be defined at which correlations between chains become weak, by $\xi_x(T_x) = a_x$. Hence,

\[
\Delta t_x = \frac{T_x}{T_{3D}} - 1 = \left( \frac{\xi_{0x}}{a_x} \right)^2
\]
and it can be seen from Figure 3 that for a tetragonal crystal $\Delta t_{3D} \approx 0.1$ virtually independent of any parameters. This value is comparable to the value obtained for by Schulz [4] for a slightly different model involving only fluctuations in the phase of the order parameter. This narrow crossover region is consistent with estimates for $K_{0.3}\text{MoO}_3$ based on X-ray scattering [4]. It may be possible to argue that this narrow crossover region, which is comparable to the width of the critical region estimated below, is consistent with the neglect of interchain fluctuations in the derivation in Section III.

The width of the critical region given by the Ginzburg criterion (8) is

$$\Delta t_{3D} = \frac{1}{16\pi^2 J_x J_y} \frac{g(\kappa)^2 (\lambda_{0,1}(\kappa) - \lambda_{0,0}(\kappa))^2}{-\kappa f(\kappa)^3 \frac{\partial f(\kappa)}{\partial \kappa}}$$

(64)

Note that for a tetragonal crystal ($J_x = J_y = J$) this depends solely on the fluctuation parameter $\kappa$. Figure 3 shows the resulting dependence of $\Delta t_{3D}$ on the interchain coupling. It is striking that the width of the critical region is independent of any parameters, $\Delta t_{3D} \sim 0.05 - 0.08$. As for the transverse coherence length this result is somewhat surprising since intuitively it might be expected that as the the interchain coupling increases the system becomes less one dimensional and fluctuations decrease. However, this independence is result of the transverse coherence lengths being only weakly dependent on the interchain coupling. The values obtained for $\Delta t_{3D}$ are comparable to the value obtained for by Schulz [4] for a slightly different model. It is interesting that even if the width of the one-dimensional critical region is large, say of order $T_0$ (i.e., $\Delta T_{1D} \sim T_0$), the actual observable critical region will be much smaller ($\Delta T_{3D} \ll T_{3D} \ll T_0$). This small width of the critical region is important because it shows that a mean-field treatment of the three-dimensional Ginzburg-Landau functional [3] is justified except in a narrow temperature region close to $T_{3D}$. Note that this result is based on the assumption that the temperature dependence of the single chain parameters $a$, $b$, and $c$ can be neglected.

The value of $\Delta t_{3D} \sim 0.05 - 0.08$ can be compared to experimental results. The analysis in Reference 3 and the data of Reference 4 suggest that $\Delta t_{3D} \sim 0.01$ for the CDW transition in $K_{0.3}\text{MoO}_3$. The data of Reference 4 suggests that $\Delta t_{3D} \sim 0.01$ for the SDW transition in (TMTSF)$_2PF_6$. It should be stressed that these are very rough estimates based on the Ginzburg criterion [3].

**Rough estimate of $\kappa$ in several CDW materials.** Since $\kappa$ is such an important parameter it is worthwhile making a very rough estimate of its value in various materials. It turns out that most materials lie outside the regime of validity of the lowest-level approximation, discussed in the Appendix.

The longitudinal coherence length given by (A15) can be used to estimate $\kappa$. Equation (23) and the lowest-level approximation, (A7), can be used to provide a rough estimate of $\xi_1$,

$$\xi_1 \approx \xi_0 \left(\frac{8 \lambda}{\kappa}\right)^{1/2}$$

(65)

where $\xi_0$ is the single chain coherence length given by (15). Hence, $\kappa$ is roughly given by

$$\kappa \sim \frac{4 \xi_0^2}{\xi_{z0}}$$

(66)

$\xi_{z0}$ can be estimated from X-ray and neutron scattering experiments (Table I). Deriving an accurate value of $\xi_{z0}$ from microscopic theory is a subtle matter which will not be discussed here. For purposes of this paper it is sufficient to use the results of the simplest microscopic theory [3]. In that case

$$\xi_0 \approx \frac{0.23h v_F}{\Delta(0)}$$

(67)

where $v_F$ is the Fermi velocity and $\Delta(0)$ is the zero-temperature energy gap. Table I lists estimates of $\xi_{z0}$, $v_F$, and $\Delta(0)$ for several materials that undergo a three-dimensional CDW ordering transition. These values are used in equation (67) to give an order of magnitude estimate for $\kappa$ in each material. In all the materials $\kappa > 10^{-2}$ suggesting that the lowest-level approximation will give poor results. Given the experimental uncertainty in the parameters discussed above it is hoped that this discussion will generate more precise studies of this question.

V. CONCLUSIONS

The main points of this paper are the following. (1) To derive a reliable Ginzburg-Landau functional to describe three-dimensional ordering transitions in quasi-one-dimensional materials one must give a careful treatment of the
large intrachain order-parameter fluctuations. (2) Most physical properties are determined by a single dimensionless parameter $\kappa$, defined in equation (4), which is a measure of the size of the intrachain fluctuations. (3) Commonly studied charge-density-wave materials lie outside the regime of the lowest-level approximation and so their accurate description requires an exact treatment of the intrachain fluctuations. (4) If the single chain Ginzburg-Landau coefficients are assumed to be temperature independent then the width of the three-dimensional critical region, estimated by the Ginzburg criterion, is virtually independent of any parameters, $\Delta t_{3D} \sim 0.05 - 0.08$.

This paper leaves a number of open questions and opportunities for future work. (a) It needs to be established whether the temperature dependence of the single chain Ginzburg-Landau coefficients $a$, $b$, and $c$ is important in realistic microscopic models. If so how are the results of Figures 1, 2, and 3 modified? (b) Quantitative comparison of the results here with measurable quantities such as the specific heat jump and longitudinal coherence length requires realistic microscopic models. If so how are the results of Figures 1, 2, and 3 modified? (c) For moderate interchain coupling the specific heat jump is given by $\Delta C \xi \sim 0.7$, independent of the strength of the interchain coupling. Is there a simple physical argument that can justify this simple result? (d) This paper treats the intrachain fluctuations exactly and the interchain interactions in the mean-field approximation. This neglect of the interchain fluctuations is presumably reasonable if the system is sufficiently anisotropic. It is desirable to have a quantitative criterion that defines the validity of this treatment. Furthermore, presumably when the interchain interactions become sufficiently strong the system is better described by an anisotropic XY model in which the fluctuations in all three directions are treated on an equal footing. It would be nice to have a description of the crossover from a transition at $T_{3D} \ll T_0$ (ensured by the criterion (55)) to the case $T_{3D} \sim T_0$ for strong interchain coupling. It is not clear how to attack this problem within any particular approximation scheme. It may be necessary to use a numerically intensive technique such as series expansions or a Monte Carlo simulation. Hopefully this paper will stimulate such a study.

ACKNOWLEDGMENTS

I have benefited from numerous discussions with J. W. Wilkins. This work was stimulated by discussions with J. W. Brill. I am grateful to him for showing me his group’s data prior to publication. I thank J. W. Brill, G. Mozurkewich and J. W. Wilkins for helpful comments on the manuscript. Some computational assistance was provided by M. C. B. Ashley. Some of this work was performed at The Ohio State University where it was supported by the U.S. Department of Energy, Basic Energy Sciences, Division of Materials Science and the OSU Center for Materials Research. Work at UNSW was supported by a Queen Elizabeth II Fellowship from the Australian Research Council.

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The longitudinal coherence length is normalized to the single chain coherence length on the interchain coupling. The width of the critical region, $\Delta T$, is defined by the temperature at which the fluctuation contribution to the specific heat below the transition temperature, calculated in the Gaussian approximation, equals the mean-field specific heat jump $\Delta C$. It should be stressed that this gives only a very rough estimate of the importance of fluctuations and that there are several alternative definitions of the width of the critical region (see for example Reference 22). Consequently, care should be taken when comparing estimates from different references. This is particularly true since definitions in different references often differ by numerical factors such as $32\pi^2$!

For a tetragonal crystal the vertical scale is changed by a factor depending on the anisotropy (see equations (62) and (64)).

If $a$ is given by (1) then $a = 2t^2(\Delta t_{1d}/(1 - t))^3$ where $\Delta t_{1d}$ is given by the one-dimensional Ginzburg criterion (2). Scalapino, Sears and Ferrell assumed that $T \sim T_0$ and in their notation $\Delta T = 2\Delta t_{1d}$. Hence $(1 - t)/\Delta t$ in their paper corresponds to $(1/4\kappa)^{1/3}$.

The code used was an adapted version of Example 3 in S. E. Koonin and D. C. Meredith, *Computational Physics*, Fortran Version, (Addison Wesley, Redwood City, 1990), p. 67ff.

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FIG. 1. Dependence of the three-dimensional transition temperature $T_{3d}$ and the fluctuation parameter $\kappa$ on the interchain coupling $J$. It has been assumed that the single chain Ginzburg-Landau parameters $a$, $b$, and $c$ are independent of temperature. The reduction of $T_{3d}$ below the mean-field transition temperature $T_0$ for a single chain also depends on the width of the one-dimensional fluctuation region $\Delta t_{1d}$.

FIG. 2. Dependence of the specific jump per chain $\Delta C$ and the longitudinal coherence length $\xi_0$ on the interchain coupling $J$. It has been assumed that the single chain Ginzburg-Landau parameters $a$, $b$, and $c$ are independent of temperature. The longitudinal coherence length is normalized to the single chain coherence length $\xi_0$ defined by (15). Note that for moderate interchain coupling ($J > 0.05|a|$) the specific heat jump is determined solely by the single chain coherence length $\xi_0$.

FIG. 3. Very weak dependence of the width of the critical region for the three dimensional transition and the transverse coherence length on the interchain coupling. The width of the critical region $\Delta t_{3d}$ is calculated from the Ginzburg criterion. The transverse coherence length $\xi_{0z}$ is normalized to the lattice constant $a_z$. The results shown are for a tetragonal crystal. For an orthorhombic crystal the vertical scale is changed by a factor depending on the anisotropy (see equations (62) and (64)). This figure establishes the striking result that the width of the critical region is virtually parameter independent.

FIG. 4. Failure of different approximation schemes for treating the effects of fluctuations in a single chain. The dependence of the order parameter susceptibility function $f(\kappa)$ (defined in equation (22)) on the fluctuation parameter $\kappa$ (defined in equation (23)) is shown. The solid curve is the exact result obtained by numerically solving the eigenvalue equation (25). The dashed curve is the result, $f(\kappa) = 1/\kappa$, of the lowest-level approximation (LLA) which has been used in previous treatments of quasi-one-dimensional phase transitions. The dashed curves are the results of the Hartree-Fock approximations.
FIG. 5. Deviation of the lowest-level approximation from the exact results. The linear susceptibility \( f(\kappa) \), the third-order susceptibility \( g(\kappa) \) (defined in equation (35)), and the derivative \( \frac{d \ln f}{d \ln \kappa} \) (which determines the coefficient \( A' \) (see equation (58)), all normalized to their values in the lowest-level approximation, are shown as a function of the fluctuation parameter \( \kappa \). Note that the horizontal scale is logarithmic. Clearly the lowest-level approximation is only quantitatively reliable for \( \kappa < 10^{-3} \). In Table II it is estimated that typical materials have \( 10^{-2} < \kappa < 1 \). In this range the lowest-level approximation will predict a specific heat jump up to an order of magnitude smaller than the exact results.

### TABLE I. Summary of symbols for the important quantities for a single chain and a three-dimensional (3D) system of weakly coupled chains. The items in parentheses refer to relevant equations and figures.

| Quantity                        | Single chain | 3D               |
|---------------------------------|--------------|------------------|
| Order parameter                | \( \phi(z) \) | \( \Phi(x, y, z) \) \((42)\) |
| Ginzburg-Landau free energy    |               | (1) (3)          |
| Mean-field transition temperature | \( T_0 \)   | \( T_{3D} \ll T_0 \) \([Fig. 1]\) |
| Ginzburg-Landau coefficients   | \( a, b, c \) | \( A, B, C_x, C_y, C_z \) \((48-51)\) |
| Specific heat jump             | \( \Delta C_{1D} \) \((14)\) | \( \Delta C \) \((59), \text{Fig. 2}\) |
| Intrachain coherence length    | \( \xi_0 \) \((13)\) | \( \xi_{0z} \) \((2)\), \text{Fig. 2}\) |
| Fluctuation region width       | \( \Delta t_{1D} \) \((10)\) | \( \Delta t_{3D} \) \((64), \text{Fig. 3}\) |

### TABLE II. Order of magnitude estimate of the fluctuation parameter \( \kappa \) in several materials that undergo a three-dimensional charge-density-wave transition. The intrachain coherence length \( \xi_{0z} \), measured by X-ray or neutron scattering, and the single-chain coherence length \( \xi_0 \) are used to estimate the value of the fluctuation parameter \( \kappa \) at the three-dimensional ordering transition (see equation (66)). \( \xi_0 \) is estimated from the Fermi velocity \( v_F \) and the zero-temperature energy gap \( \Delta(0) \), using equation (67), based on the simplest microscopic theory. The estimates of \( \xi_{0z}, v_F, \) and \( \xi_0 \) are probably only accurate to within a factor of two. Consequently, the estimate of \( \kappa \) is only accurate within an order of magnitude. Nevertheless, clearly all these materials lie outside the regime of validity \( (\kappa < 10^{-3}) \), see Figure 5 of the lowest-level approximation (see Section A2) and so an exact treatment of the intrachain fluctuations of the order parameter is necessary. Also note that these values of \( \kappa \) can be used to estimate the values of \( J/|a| \) and they are in roughly the same regime as considered in Figures 3-5.

| Material                | \( \xi_{0z} \) \(\AA\) | \( 10^6 v_F \) m/sec | \( \Delta(0) \) meV | \( \xi_0 \) \(\AA\) | \( \kappa \) |
|-------------------------|--------------------------|----------------------|---------------------|---------------------|-------------|
| \( K_2\text{MgO}_3 \)  | 15\(^a\)                  | 2.0\(^a\)            | 100\(^a\)           | 3                   | 0.2         |
| \( (\text{TaSe}_4)_2\text{I} \) | 60\(^d\)                 | 14\(^e\)            | 200\(^j\)           | 10                  | 0.1         |
| \( K_2\text{Pt(CN)}_4\text{Br}_3 \) | 100\(^h\)             | 10\(^h\)            | 100\(^i\)           | 15                  | 0.1         |
| \( \text{TSeF-TCNQ} \) | 30\(^i\)                  | 0.15\(^j\)          | 10\(^k\)            | 2                   | 0.02        |

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APPENDIX: PREVIOUS APPROXIMATE TREATMENTS OF FLUCTUATIONS

1. Hartree and Hartree-Fock treatment

For completeness these approximations which have been considered in the literature are discussed here. The replacement $|\phi(z)|^4 \rightarrow 2q <|\phi|^2>|\phi(z)|^2$ is made in the free energy functional (1) in the partition function (17). The cases $q = 1$ and $q = 2$ correspond to the Hartree and Hartree-Fock approximations, respectively. The functional integral is then over a Gaussian field and can be performed analytically. In effect one makes the Gaussian approximation with

$$a \rightarrow a + \Sigma \equiv a + 2qb <|\phi|^2>.$$  \hspace{1cm} (A1)

The expectation value $<|\phi|^2>$ is calculated self consistently

$$\frac{\Sigma}{2qb} = \frac{1}{2\pi} \int dk \frac{T}{a + \Sigma + ck^2} = \frac{T}{2\sqrt{c(a + \Sigma)}}.$$  \hspace{1cm} (A2)

Consequently, the dimensionless self energy $\tilde{\Sigma} \equiv \Sigma/|a|$ satisfies the self-consistent equation

$$\tilde{\Sigma} = \left( \frac{q^2\kappa}{2(\Sigma - 1)} \right)^{1/2}.$$  \hspace{1cm} (A3)

Since the linear susceptibility is

$$\chi_1(0) = \frac{1}{a + \Sigma}$$  \hspace{1cm} (A4)

the function $f(\kappa)$ in the susceptibility is given by

$$f(\kappa) = \frac{1}{4(\Sigma - 1)}.$$  \hspace{1cm} (A5)

The results of the Hartree and Hartree-Fock approximations are shown as dashed curves in Figure 4; they are in qualitative but not quantitative agreement with the exact results. As $\kappa \rightarrow 0$, $\tilde{\Sigma} \rightarrow 1$, and so (A3) implies $\tilde{\Sigma} \rightarrow 1 + q^2 \kappa/2$. Hence, this approximation gives

$$f(\kappa) \rightarrow \frac{1}{2q^2 \kappa} \quad \text{as} \quad \kappa \rightarrow 0.$$  \hspace{1cm} (A6)

2. The lowest-level approximation

Close to the three-dimensional ordering transition $\kappa \ll 1$. This limit corresponds to the semi-classical limit of the Schrödinger-type equation (28). Previously a Gaussian wavefunction, sharply peaked at $\rho = 1$, has been used as a variational ground state wave function for (28). The results are

$$\lambda_{0,\ell} - \lambda_{0,0} = \kappa \ell^2.$$  \hspace{1cm} (A7)

In this approximation the correlation length (given by (1), (23) and (A7)) is

$$\xi_1(T) = \frac{2|\rho|c}{bT}.$$  \hspace{1cm} (A8)

This result was given previously in Reference and. In this limit it is to be expected that $\rho^2$ has an expectation value of 1 in the ground state. If it is further assumed that the $n = 0$ states form a complete set (the lowest-level approximation) then

$$1 = <u_{0,0}|\rho^2|u_{0,0}> = <u_{0,0}|\rho e^{-i\varphi} \left( \sum_{\ell} |u_{0,\ell}><u_{0,\ell}| \right) \rho e^{i\varphi}|u_{0,0}> = |<u_{0,1}|\rho|u_{0,0}>|^2.$$  \hspace{1cm} (A9)
The expression (31) then reduces to

\[ f(\kappa) = \frac{1}{\kappa}. \]  \hspace{1cm} (A10)

Note that in the lowest-level approximation the sum on the left hand side of (32) is only 1/2.

In the lowest-level approximation the dimensionless function \( g(\kappa) \) in the third-order susceptibility is given by

\[ g(\kappa) = 4\frac{|<u_{0,1}\rho|u_{0,0}>|^2}{(\lambda_{0,1} - \lambda_{0,0})^3} - 2\frac{|<u_{0,1}\rho|u_{0,0}>|^2|<u_{0,2}\rho|u_{1,0}>|^2}{(\lambda_{0,1} - \lambda_{0,0})(\lambda_{0,2} - \lambda_{0,1})} = \frac{7}{2\kappa^3}. \]  \hspace{1cm} (A11)

Figure 5 shows how the results of (A10) and (A11) deviate significantly from the exact results for \( \kappa > 10^{-3} \). Previously Bishop and Krumhansl pointed out the shortcomings of the lowest-level approximation for the case of a real order parameter.

The three-dimensional transition. Scalapino, Imry and Pincus, Manneville, and Dieterich studied the three-dimensional transition using the lowest-level approximation (defined in Section A.2), i.e., they assumed that only the lowest eigenstate (for \( n = 0 \)) for each of the angular momentum values \( \ell = 0, \pm 1, \) and \( \pm 2 \), is important. As mentioned earlier they also assumed that the single chain coefficients \( a, b, \) and \( c \) are independent of temperature. The zero-wavevector linear susceptibility is given by

\[ \chi_1(0) = \frac{4}{\kappa} \frac{|a|}{b^2 T^2}. \]  \hspace{1cm} (A12)

Solving (53) for the transition temperature gives

\[ T_{3D} = \sqrt{2Jc} \frac{|a|}{b}. \]  \hspace{1cm} (A13)

Equation (59) for the specific heat jump reduces to

\[ \Delta C = \frac{16}{7\xi_1}. \]  \hspace{1cm} (A14)

The coherence length parallel to the chains is

\[ \xi_{z0} = \frac{\xi_1}{\sqrt{2}}. \]  \hspace{1cm} (A15)

The transverse coherence lengths (for \( J_x = J_y \)) are

\[ \xi_{x0} = \frac{a_x}{\sqrt{8}}, \quad \xi_{y0} = \frac{a_y}{\sqrt{8}}. \]  \hspace{1cm} (A16)

The above expressions (A13, A16) were previously obtained by Manneville and Dieterich.

In the lowest-level approximation the expression (64) for the width of the critical region (for \( J_x = J_y \)) reduces to

\[ \Delta t_{3D} = \left( \frac{7}{8\pi} \right)^2 \simeq 0.08. \]  \hspace{1cm} (A17)
\[ \frac{\text{d} \ln f}{\text{d} \ln \kappa} \]

\[ \kappa f(\kappa) \]

\[ \frac{2}{7} \kappa^3 g(\kappa) \]

\[ \log \kappa \]
$T_{3D} \Delta t_{1D}^{3/2} / T_0$

$k(T_{3D})$
