# Electron-phonon interaction and phonon dynamics in one-dimensional conductors: Spinless fermions

J. Voit* and H. J. Schulz
*Laboratoire de Physique des Solides, Universite Paris-Sud, 91405 Orsay, France*
(Received 3 March 1987)

We consider electron-electron and electron-phonon interactions, in particular backward scattering by phonons, in one-dimensional metals. Particular emphasis is laid on the effects of finite phonon frequency. We calculate effective interaction constants and the effective mass enhancement due to the electron-phonon coupling. We find a significant enhancement of charge-density-wave fluctuations and of the electronic specific heat. A new theoretical approach allows us to discuss electron-electron and electron-phonon interactions on an equal footing; it is based on the limits of weak electron-phonon coupling, high phonon frequency, and strong coupling, low frequency, and gives good agreement in intermediate cases.

## I. INTRODUCTION

This paper presents a new theoretical approach to the description of electron-phonon interactions in one-dimensional fermion systems. The motivation for this study stems largely from many interesting results and unsolved questions in the field of organic conductors and superconductors.[1] Typical materials we have in mind are, e.g., tetrathiafulvalene-tetracyanogunodimethene (TTF-TCNQ) or the Bechgaard salts $(TMTSF)_2X$, where TMTSF denotes tetramethyl tetraselenafulvalene. They may or may not be commensurate, but for the sake of simplicity, we shall limit ourselves in the present paper to incommensurate systems. This restriction will be released in a subsequent publication. Many of the results obtained here are also relevant to conducting polymers such as doped polyacetylene,[2] but caution should be taken in applying them literally because of the commensurability of these materials.

Experimentally, there are strong indications for the importance of both electron-electron and electron-phonon interactions in real quasi-one-dimensional (1D) solids. Concerning the low-temperature instabilities of 1D fermion systems, the simplest theories based solely on Coulomb interactions predict only a spin-density-wave (SDW) instability at low temperature provided the interaction decreases monotonically with distance. For example, in the familiar model introduced in Ref. 3, we would have $g_2 > g_1 > 0$ and the dominant divergence would therefore be in the SDW correlation function. In real materials, SDW instabilities are however a small minority. In particular, before the synthesis of the $(TMTSF)_2X$ compounds, most of the low-temperature phases were of the charge-density-wave (CDW) type.[1(b)] It became rapidly evident, however, that at least in some materials, the simple Peierls model,[4] predicting a modulation of the charge density with wave vector $2k_F$, was not adequate for the description of the CDW state. In TTF-TCNQ, a $4k_F$-modulated CDW was observed in addition to the $2k_F$ one.[5] In *N*-methylphenazinium TCNQ, both CDW's are also found in coexistence.[6] The theoretical explanation of the $4k_F$ CDW suggested the presence of fairly strong repulsive interactions.[7,8]

Turning to superconducting instabilities, BCS theory is based on the attractive electron-phonon interaction. Nuclear magnetic resonance experiments on $(TMTSF)_2ClO_4$, however, clearly show strong antiferromagnetic fluctuations immediately before the transition into the superconducting state,[9] suggesting again the importance of repulsive interactions. (Let us mention only in passing that this observation has led to several proposals for non-phonon-based mechanisms for organic superconductivity.[10])

Thermodynamic and transport properties, too, give indications of the importance of both electron-electron and electron-phonon interactions. In many compounds, e.g., the Pauli susceptibility is enhanced over its free-electron value by a factor of 2 to 5, which can only be understood by assuming relatively strong electronic correlations.[11]

On the other hand, optical measurements[12] demonstrate that in addition to the usual acoustic and optical phonons, there is a broad spectrum of intramolecular vibration modes, ranging from about 50 to 3000 $cm^{-1}$, i.e., up to values comparable to typical bandwidths ($\sim 1$ eV). Moreover, it was shown[13] that high-frequency intramolecular vibrations couple quite well to the electrons. Another theory[14] demonstrates that in a system of electrons coupling to several phonon modes of different frequencies, the stability of the CDW state is mainly determined by the high-frequency intramolecular modes which are relatively strongly coupled to the electrons, whereas the low-frequency intermolecular phonons make up the major contribution to the CDW's effective mass.

The theoretical effort to date has focused mainly on incorporating the effects of the *attractive interaction* mediated by the phonons into the current models. However, most of the work has been limited either to the region of very high phonon frequencies (of the order of the Fermi energy or so) or to very low frequencies, treating the phonons in the mean-field approximation. As an example for

 

the first category, one can mention attempts to justify the possibility of negative coupling constants, e.g., in the picture of Ref. 3 or in the Hubbard model invoking the attractive nature of the phonon-mediated effective electron-electron interaction.[15] Although this is probably a good starting point for very-high-frequency phonons ($\omega \lesssim E_F$) it surely fails for intermediate- or low-frequency modes.

The classical mean-field theory of Peierls[4] was extended to the simultaneous presence of electron-electron and electron-phonon interaction by Baeriswyl and Forney[16] and Horowitz *et al.*,[17] yielding however incompatible low-temperature phase diagrams. More recently, Horovitz and Sólyom[18] have produced a refined treatment of the electron-electron coupling using renormalization-group methods, but the phonons are again treated in the mean-field approximation. Mean-field theory neglects any fluctuations of the phonon degrees of freedom and should therefore be reliable only for extremely low frequencies ($\omega \to 0$). Although there is actually a quite good understanding of the very high and very low phonon frequency range, the physically relevant case of intermediate frequencies has only rarely been investigated.

An extension over mean-field results in the low-frequency region has been given by Fukuyama[19] who pointed out the importance of phase fluctuations in CDW systems. In fact, in an incommensurate CDW, the order parameter is complex. Whereas there is a finite restoring force against fluctuations of its amplitude, long-wavelength phase excitations exist at arbitrarily small energy ($\omega_\chi \sim v_\chi \mid q \mid$) and destroy long-range order even at zero temperature. This approach has been limited to systems without electronic correlations. This very same limitation also applies to a more recent work treating a much wider range of phonon frequencies[20] through the use of Grassmann variables. Electron-electron interactions have been included in an approach based on two-cutoff renormalization.[21] In this method, one makes the hypothesis that electronic fluctuations with energies higher than the Debye frequency are unaffected by the phonons, whereas below this scale, the phonons are treated as effectively nonretarded and included in effective coupling constants. Although not explicitly stated, this method is also limited to relatively high phonon frequencies.

Finally, numerical (Monte Carlo) simulations on finite systems have provided considerable insight into systems with both electron-electron and electron-phonon interaction.[22] Being nonperturbative, one can avoid many problems related to the necessity of having small parameters for perturbation expansions in analytic work. However, these simulations are limited to systems of finite temperature; ground-state properties have to be obtained by extrapolation. Moreover, it seems difficult to obtain reliable information on weakly coupled systems from such simulations.

More generally, the crossover between retarded and unretarded behavior of the phonon system as well as the interplay between the repulsive Coulomb correlations and the attractive electron-phonon interaction have not been studied in a systematic and unified manner to date. In particular, it is unclear which parameters eventually control this interplay.

For these reasons, it is highly desirable to have a formalism treating Coulomb and electron-phonon interaction with phonons of arbitrary frequency on an equal footing. It is the purpose of this paper to present a new approach for the theoretical description of 1D metals with retarded and nonretarded interactions. Its focus is on the physically relevant case of large-momentum-transfer ($q \sim 2k_F$) scattering of electrons by phonons and on the effects of the quantum dynamics of the phonon system. Small-momentum-transfer ($q \sim 0$) scattering by phonons has previously been treated exactly by direct diagonalization of the Hamiltonian[23,24] and will be ignored in the present paper. The calculation of correlation functions provides the basis for a unified description of both the low-temperature instabilities and of the thermodynamic and transport properties of the 1D electron-phonon system.

The solution procedure for the problem of backscattering of spin-$\frac{1}{2}$ electrons by phonons is quite involved due to a coupling of charge- and spin-density degrees of freedom in the interaction Hamiltonian on the one hand and finite retardation on the other. Limitation to spinless fermions allows considerable simplification and is therefore better suited to discuss the effects introduced by the finite retardation of the phonons. Note, however, that this seemingly pathological model is not without physical relevance. Via a Jordan-Wigner transformation, spin-Peierls systems[25] are related to spinless fermions coupled to phonons. The magnetic field in the spin-Peierls problem is related to the chemical potential of the spinless-fermion model. The zero-magnetic-field situation corresponds to a half-filled band in the fermion model; on applying a finite magnetic field the equivalent fermion system becomes incommensurate, and the present theory can give important information on the behavior of the spin-Peierls system.

This is the first in a series of papers presenting the results of a comprehensive study of one-dimensional electron-phonon systems. The focus of the study is on the combined effects of electron-electron and electron-phonon interaction in one-dimensional systems, and on the effects of the finite retardation of the phonons, both on the low-temperature instabilities and on the thermodynamic and transport properties of one-dimensional materials.

This paper is organized as follows: Sec. II presents the model Hamiltonian. Fundamental technical aspects, related to the bosonization method used in the major part of this paper, are also discussed. In order to obtain a description for arbitrary electron-phonon coupling and, more importantly, arbitrary phonon frequency, two complementary approaches have to be used. Section III presents the weak-coupling–weak-retardation case, whereas Sec. IV contains the strong-coupling–strong-retardation results. The influence of the coupling of the electrons to the phonons on low-temperature instabilities and thermodynamic properties is determined in Sec. V. A more general discussion is given in Sec. VI, while some technical details are relegated to the Appendix.

## II. THE MODEL

In this paper we discuss a Tomonaga-Luttinger model (TLM) extended to include electron backscattering

through emission or absorption of a phonon with wave vector $|q| \sim 2k_F$. Its Hamiltonian is given by

$$H = H_{\text{el}}^{(0)} + H_{\text{el-el}} + H_{\text{ph}}^{(0)} + H_{\text{el-ph}} \ . \tag{2.1}$$

The free-electron part is

$$H_{\text{el}}^{(0)} = \sum_{k,r} v_F(rk - k_F) a_{r,k}^{\dagger} a_{r,k} \tag{2.2a}$$

$$= \frac{\pi v_F}{L} \sum_{p(\neq 0)} [\rho_+(p)\rho_+(-p) + \rho_-(-p)\rho_-(p)] \ , \tag{2.2b}$$

and the electron-electron interaction is

$$H_{\text{el-el}} = \frac{g_1}{L} \sum_{k_1,k_2,p} :a_{-,k_2}^{\dagger} a_{+,k_1}^{\dagger} a_{+,k_2+2k_F+p} a_{-,k_1-2k_F-p}: + \frac{g_2}{L} \sum_{k_1,k_2,p} :a_{+,k_1}^{\dagger} a_{-,k_2}^{\dagger} a_{-,k_2-p} a_{+,k_1+p}: \tag{2.3a}$$

$$= \frac{g_2 - g_1}{L} \sum_p \rho_+(p)\rho_-(-p) \ . \tag{2.3b}$$

The free-phonon and electron-phonon parts are

$$H_{\text{ph}}^{(0)} = \tfrac{1}{2} \int dx \left[ \frac{1}{\rho_I} \tilde{\Pi}_{2k_F}^2(x) + \frac{K}{a} \tilde{\varphi}_{2k_F}^2(x) \right] \tag{2.4a}$$

$$= \tfrac{1}{2} \int dx \left[ \Pi_{2k_F}^2(x) + \omega_{2k_F}^2 \varphi_{2k_F}^2(x) \right] \ , \tag{2.4b}$$

$$H_{\text{el-ph}} = \gamma_1 \int dx \, \psi_+^{\dagger}(x)\psi_-(x)\varphi_{2k_F}(x) e^{2ik_F} + \text{H.c.} \tag{2.5a}$$

$$= \frac{\gamma_1}{2\pi\alpha} \int dx \, e^{2i\Phi(x)} \varphi_{2k_F}(x) + \text{H.c.} \tag{2.5b}$$

$a_{r,k}^{\dagger}$ creates an electron with momentum $k$ on the branch $r = +, -$ of the linear dispersion relation $E(k) = v_F(rk - k_F)$, and $\Psi_r^{\dagger}(x)$ is the corresponding operator in real space. : : denotes normal ordering of the Fermi operators with respect to the ground state of (2.2). $v_F$ is the Fermi velocity, and $g_1$ and $g_2$ are the coupling constants for electron-electron backward and forward scattering, respectively, (Fig. 1). We take these couplings independent of $p$; in order to obtain well-defined results, we introduce a momentum transfer cutoff into the TLM; the bandwidth of the model is not cut off.

The complex phonon field $\tilde{\varphi}_{2k_F}(x)$ is the slowly varying part of the $2k_F$ component of the displacement field

$$u_{2k_F}(x) = \text{Re}[e^{2ik_F x} \tilde{\varphi}_{2k_F}(x)]$$

describing phonons with frequency $\omega_{2k_F}^2 = K/(a\rho_I)$, where $K$ is the spring constant, $a$ the spacing of the lattice, and $\rho_I$ the ionic mass density. $\tilde{\Pi}_{2k_F}$ is the canonically conjugate momentum to $\tilde{\varphi}_{2k_F}$, and $\varphi_{2k_F} = (\rho_I)^{1/2} \tilde{\varphi}_{2k_F}$, $\Pi_{2k_F} = \tilde{\Pi}_{2k_F}/(\rho_I)^{1/2}$ have been introduced for practical purposes. $\gamma_1$ is the electron-phonon coupling constant. If we think about a tight-binding model for the electrons, characterized by a transfer integral $t$ and a highest occupied molecular energy level $E$, the coupling constant is

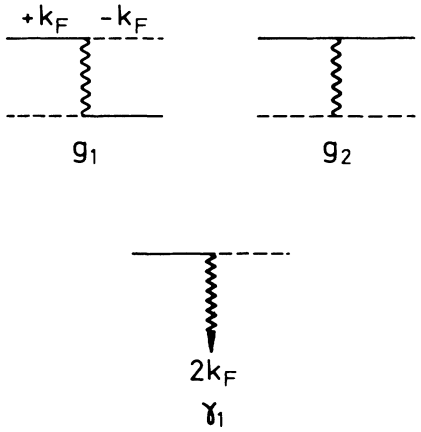


FIG. 1. Schematic representation of the interaction processes $g_1$, $g_2$, and $\gamma_1$. Solid (broken) lines denote electrons with momentum close to $k_F$ ($-k_F$).

given by

$$\gamma_1 = \frac{4ig_{\text{ac}}}{(\rho_I)^{1/2}} \sin(k_F a) \tag{2.6a}$$

for acoustic phonons, and by

$$\gamma_1 = \frac{g_{\text{mol}}}{(\rho_I)^{1/2}} \tag{2.6b}$$

for intramolecular vibrations. Here, $g_{\text{ac}}$ ($g_{\text{mol}}$) is the first derivative of the electronic transfer integral (the molecular energy level) with respect to the intermolecular distance $u$ (an intramolecular coordinate). In the following we always suppose optical phonons; the coupling constant for acoustic phonons being purely imaginary, the results in this case can be obtained by replacing $\gamma_1^2 \to |\gamma_1|^2$ everywhere. As we consider an incommensurate system, electron-electron and electron-phonon umklapp scattering are irrelevant.

Let us now discuss some of the approximations involved to this point: we have used a continuum model with a linear dispersion relation (without bandwidth cutoff) for the electrons. This should be a good approximation to the low-energy properties of the model in the asymptotic regime $|x|, |t| \to \infty$, where only states very near the Fermi surface are relevant. We are therefore restricted to low temperatures ($T \ll E_F$) and to weak coupling strength ($g_i/2\pi v_F \ll 1$); while the condition $T \ll E_F$ is easily fulfilled in all physically relevant situations, the limitation to weak electron-electron coupling is more serious. This restriction can or cannot apply to real materials.[26] The restriction to backward scattering by dispersionless phonons is a good approximation for acoustic phonons which usually have very little dispersion at $q \sim 2k_F$. This is the only relevant term for interaction of electrons with acoustic phonons since an exact solution of the forward-scattering part[23] has shown that its contribution is reduced by a factor $(C_s/v_F)^2$ where $C_s$ is the speed of sound, which is of the order $10^{-4}$–$10^{-6}$ in real materials and can safely be neglected. For optical phonons and intramolecular vibrations (which will not be distinguished

in what follows) one should take account of the forward-scattering part; previously, it has been shown,[23] how this interaction can be incorporated into the correlation function exponents $\exp(2\xi)$ arising from the diagonalization of the Tomonaga-Luttinger model [cf. Eq. (2.10)].

The fermion representation of the Hamiltonian has been given in Eqs. (2.2a), (2.3a), and (2.5a); in Eqs. (2.2b), (2.3b), and (2.5b) we have represented the same Hamiltonian in terms of density operators

$$\rho_r(p)=\sum_k a^\dagger_{r,k+p}a_{r,k} \ , \tag{2.7}$$

which obey Bose commutation relations

$$[\rho_r(p),\rho_{r'}(-p')]=-\delta_{r,r'}\delta_{p,p'}\frac{rpL}{2\pi} \ , \tag{2.8}$$

and the boson phase field

$$\Phi(x)=-\frac{i\pi}{L}\sum_{p(\neq 0)}\frac{1}{p}e^{-\alpha|p|/2-ipx}[\rho_+(p)+\rho_-(p)] +(N_++N_-)\frac{\pi x}{L} \ . \tag{2.9}$$

The Tomonaga-Luttinger model with electron-electron interaction only can be diagonalized exactly[27,28] by a Bogoliubov transformation. Its essential effect is to introduce a renormalized coupling constant

$$\exp(4\xi)=\frac{2\pi v_F-g_2+g_1}{2\pi v_F+g_2-g_1} \ , \tag{2.10}$$

which is relevant for the transformation of the $\Phi$ field [$\Phi(x)\rightarrow\tilde{\Phi}(x)=e^{\xi}\Phi(x)$], and a renormalized velocity of the collective excitations

$$v_\rho=\left[v_F^2-\left[\frac{g_2-g_1}{\pi}\right]^2\right]^{1/2} \ . \tag{2.11}$$

The following calculations will mostly use correlation functions

$$R_i(xt,x't')=-i\langle TO_i(xt)O_i^\dagger(x't')\rangle \tag{2.12}$$

for the fluctuations of charge-density-wave ($i=$CDW) or superconducting ($i=$SC) type; $T$ denotes the time-ordering operator. The respective operators are given by

$$O_{\rm CDW}(xt)=\Psi_-^\dagger(xt)\Psi_+(xt) \tag{2.13a}$$

$$=\frac{e^{2ik_Fx}}{2\pi\alpha}e^{2i\Phi(xt)} \ , \tag{2.13b}$$

$$O_{\rm SC}(xt)=\Psi_-(xt)\Psi_+(xt) \tag{2.14a}$$

$$=(2\pi\alpha)^{-1}e^{2i\Theta(xt)} \ , \tag{2.14b}$$

where the phase field $\Theta(x)$ is related to the momentum $\Pi(x)$ conjugate to $\Phi(x)$ by $\nabla\Theta(x)=\pi\Pi(x)$. The asymptotic behavior of the correlation functions for $|t|\rightarrow\infty$, $|x|\rightarrow\infty$ is given by

$$R_{\rm CDW}\sim|t|^{-2+\alpha_{\rm CDW}}, \ e^{2ik_Fx}|x|^{-2+\alpha_{\rm CDW}} \ , \tag{2.15}$$

$$R_{\rm SC}\sim|t|^{-2+\alpha_{\rm SC}}, \ |x|^{-2+\alpha_{\rm SC}} \ , \tag{2.16}$$

where

$$\alpha_{\rm CDW}=2-2\exp(2\xi) \ , \tag{2.17}$$

$$\alpha_{\rm SC}=2-2\exp(-2\xi) \tag{2.18}$$

measure the deviations of the correlations function exponents from their noninteracting value ($\alpha_i=0$).

Note that, the exponent $\exp(2\xi)$ governing the decay of the correlation functions is universal only to first order in the coupling constants $g_i$ (compare, e.g., Ref. 3). However, the low-energy properties of any interacting one-dimensional spinless fermion system are correctly described by (2.17) and (2.18) if the system is incommensurate.[29] In particular, relations between the exponents are believed to be universal. Furthermore, $\exp(2\xi)$ and the renormalized velocity of the collective excitations $v_\rho$ are sufficient for a complete description of the physics of the model.

In the following two sections we shall discuss the model described above with two different methods for the case of high phonon frequencies and/or weak electron-phonon coupling and for low phonon frequencies and/or strong electron-phonon coupling. All physically relevant parameters can be computed in both approaches, and therefore it is possible to describe the whole range of frequencies and coupling constants if the results obtained with the two approaches match. This will be shown explicitly to be the case.

## III. SOLUTION FOR HIGH PHONON FREQUENCIES AND/OR WEAK COUPLING

In this limit, our strategy will be to eliminate the phonon degrees of freedom from the problem, and to discuss the effective, phonon-mediated electron-electron interaction. Starting from the boson representation of the Hamiltonian [Eqs. (2.2b), (2.3b), and (2.5b)], we first diagonalize the purely electronic part of the Hamiltonian. We are now left with a "free" Hamiltonian ($\tilde{H}_{\rm el}$), describing independent bosons, and a Hamiltonian ($\tilde{H}_{\text{el-ph}}$) for the interaction of these bosons with the phonons, both containing renormalized parameters, which can be obtained technically by the replacements $\Phi(x)\rightarrow(\exp\xi)\Phi(x)$ in (2.5b) and (2.11) in (2.2b), respectively.

We now go to the Matsubara formalism of imaginary times $\tau=it$. Writing $y=v_F\tau$ allows one to map our system onto a 2D one with position vector $\mathbf{r}=(x,y)$. The free Hamiltonian now describes Gaussian fluctuations of the (classical) field $\Phi(\mathbf{r})$ in two dimensions.

Specifically, we consider the partition function $Z$ at temperature $T=\beta^{-1}$

$$Z=\mathrm{Tr}_{\Phi,\varphi}\left[\exp\left[-\int_0^\beta d\tau H(\tau)\right]\right] =\mathrm{Tr}_{\Phi,\varphi}\left[\exp\left[-\int_0^{v_F\beta}\frac{dy}{v_F}\tilde{H}_{\rm el}[\Phi(\mathbf{r})]-\int_0^{v_F\beta}\frac{dy}{v_F}H^{(0)}_{\rm ph}[\varphi(\mathbf{r})]-\int_0^{v_F\beta}\frac{dy}{v_F}\tilde{H}_{\text{el-ph}}[\Phi(\mathbf{r}),\varphi(\mathbf{r})]\right]\right] \ , \tag{3.1}$$

where the symbol $\mathrm{Tr}_{\Phi,\varphi}$ denote the trace with respect to the phase and phonon fields. In what follows we are mostly interested in the limit $T\to 0$; then we shall drop the integration limits. The Hamiltonian being bilinear in the phonon field $\varphi(\mathbf{r})$, $\mathrm{Tr}_{\varphi}$ can be performed exactly; we obtain a functional $U[\Phi(\mathbf{r})]$ for effective phonon-induced electron-electron interaction

$$Z=\mathrm{Tr}_{\Phi}\left[\exp\left[-\int\frac{dy}{v_F}\tilde{H}_{\mathrm{el}}[\Phi(\mathbf{r})]\right]\times T_{\tau}\exp\{-U[\Phi(\mathbf{r})]\}\right], \tag{3.2}$$

$$U[\Phi(\mathbf{r})]=-\left[\frac{\gamma_1}{2\pi\alpha v_F}\right]^2\int d^2r\int d^2r' D_0(\mathbf{r}-\mathbf{r}')\times\cos\{2e^{\xi}[\Phi(\mathbf{r})-\Phi(\mathbf{r}')]\}\ . \tag{3.3}$$

Here,

$$D_0(\mathbf{r})=(2\omega_{2k_F})^{-1}\delta(x)\exp(-|y|/\xi_{\mathrm{ph}})\ , \tag{3.4}$$

$$\xi_{\mathrm{ph}}=v_F/\omega_{2k_F} \tag{3.5}$$

is the bare propagator for dispersionless phonons. Note that the integral in (3.3) is convergent for any nonzero phonon frequency; its consequences will be discussed below.

It is difficult to discuss in more detail the physical behavior of the system with the functional (3.3). We therefore perform a perturbation expansion of $\exp(-U)$ in the partition function (3.2)

$$Z=Z_0\Delta Z\ , \tag{3.6}$$

where $Z_0$ includes the diagonalized parts of the Hamiltonian and

$$\Delta Z=\left\langle T_{\tau}\exp\left[-\int d\tau H_{\text{el-ph}}(\tau)\right]\right\rangle=\left\langle T_{\tau}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\left[\frac{\gamma_1}{2\pi\alpha v_F}\right]^{2n}\prod_{k=1}^{2n}\int d^2r_k\prod_{l\ \mathrm{odd}}^{2n-1}\cos\{2e^{\xi}[\Phi(\mathbf{r}_l)-\Phi(\mathbf{r}_{l+1})]\}D_0(\mathbf{r}_l-\mathbf{r}_{l+1})\right\rangle, \tag{3.7}$$

and the average is defined as

$$\langle\cdots\rangle\equiv Z_0^{-1}\mathrm{Tr}_{\Phi}\exp\left[-\int d\tau\tilde{H}_{\mathrm{el}}(\tau)\right]\cdots\ . \tag{3.8}$$

Evaluating $\langle\cdots\rangle$, we obtain

$$\Delta Z=\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\left[\frac{\gamma_1}{2\pi\alpha v_F}\right]^2\prod_{k=1}^{2n}\int d^2r_k\prod_{l\ \mathrm{odd}}^{2n-1}\{\exp[-2e^{2\xi}V(\mathbf{r}_l-\mathbf{r}_{l+1})]D_0(\mathbf{r}_l-\mathbf{r}_{l+1})\} \tag{3.9}$$

where the "potential"

$$V(\mathbf{r})=\tfrac{1}{2}\ln[(r^2+\alpha^2)/\alpha^2] \tag{3.10}$$

satisfies the two-dimensional Poisson equation

$$\nabla^2V(\mathbf{r})=2\pi\delta(\mathbf{r})\ . \tag{3.11}$$

In the absence of the phonon propagator, $\Delta Z$ can be interpreted as the grand-canonical partition function of a 2D classical globally neutral plasma of oppositely charged particles ("Coulomb gas"). The mapping is achieved through the relations

$$\beta_{\mathrm{CG}}q^2=2\exp(2\xi)\ , \tag{3.12}$$

$$Y_{\mathrm{ph}}^2=\frac{\gamma_1^2}{2\pi v_F\omega_{2k_F}^2}\ , \tag{3.13}$$

where $\beta_{\mathrm{CG}}$, $q$, and $Y_{\mathrm{ph}}$ are the inverse temperature, charge, and fugacity of the Coulomb gas, respectively. (The index on $Y_{\mathrm{ph}}$ has been introduced to point out the analogy to a similar construction that will appear in the problem including spin.) Note that the relation between $Y_{\mathrm{ph}}$ and the frequently used effective electron-phonon coupling constant $\lambda$ [Refs. 1(b) and 4] is $Y_{\mathrm{ph}}^2=\lambda/4$. The equivalence of a similar 1D fermion system to a classical 2D Coulomb gas has been pointed out long ago by Chui and Lee.[30]

Kosterlitz and Thouless[31] have shown that there is a continuous phase transition in the 2D Coulomb gas from a low-temperature phase in which opposite charges form bound dipoles to a high-temperature phase where the charges are free. Again in the absence of the phonon propagator in (3.9), the low-temperature Coulomb gas phase would correspond to the metallic phase of the 1D fermion system, whereas the high-temperature Coulomb-gas phase would correspond to the Peierls phase of the 1D system with a gap in the charge-density-wave excitation spectrum.

What is the effect of the electron-phonon interaction and of the finite phonon frequency on the electronic properties? From Eqs. (3.4) and (3.9) it is clear that the phonon propagator introduces a linear ("confinement") potential ($\propto|y|/\xi_{\mathrm{ph}}$) between two Coulomb-gas charges in addition to the logarithmic potential (3.10). This linear potential prevents the Kosterlitz-Thouless dipole-unbinding transition, and therefore a Peierls transition in our 1D electron-phonon system for any $\omega_{2k_F}>0$ ($\xi_{\mathrm{ph}}<\infty$). On a sufficiently large length scale ( and we are only interested in asymptotic properties in this paper) the system will see the charges always bound to dipoles. This statement is equivalent to the one made above,

namely that the integral in Eq. (3.3) is convergent for any $\omega_{2k_F} > 0$. We cannot have a gap in the CDW excitation spectrum at finite phonon frequency; translated into the soliton language, this means that amplitude solitons are unstable against the phonon quantum fluctuations.

Although all integrals in our problem are convergent for finite $\omega_{2k_F}$ ($\xi_{\rm ph}$) due to the presence of the phonon propagator, we derive scaling equations because we are mainly interested in the crossover from behavior with finite retardation to quasistatic behavior of the phonons, where the integrals do not converge any longer. Technical details are relegated to the Appendix. The scaling equations read

$$\frac{d\exp(2\xi)}{d\ell} = -\exp(4\xi) Y_{\rm ph}^2 (\alpha_0/\xi_{\rm ph}) \exp(-\alpha/\xi_{\rm ph}) , \tag{3.14a}$$

$$\frac{dY_{\rm ph}}{d\ell} = Y_{\rm ph}[\tfrac{3}{2} - \exp(2\xi)] , \tag{3.14b}$$

$$\frac{dv_F}{d\ell} = -v_F \exp(2\xi) Y_{\rm ph}^2 (\alpha_0/\xi_{\rm ph}) \exp(-\alpha/\xi_{\rm ph}) , \tag{3.14c}$$

where $\ell = \ln(\alpha/\alpha_0)$, $\alpha$ being the renormalized cutoff. Equations (3.14a) and (3.14b) describe the mutual renormalization of the electron-electron and electron-phonon coupling constants. Equation (3.14c) is not present in the common 2D Coulomb gas. It arises because the phonon propagator (3.4) is a very anisotropic object in the $x$-$y$ plane: at each renormalization step, we add an anisotropic contribution to the initially isotropic partition or correlation function which thereby becomes more and more anisotropic. This can be accounted for by a renormalization of the velocity of the collective modes in our system (which plays the role of the Fermi velocity in a single-particle picture). Its physical significance will be discussed below.

Figure 2 shows typical scaling trajectories (solid lines). Due to the exponential factors introduced by the phonon propagators into Eqs. (3.14a) and (3.14c) scaling of the electronic parameters will stop at $\ell = \ell^*$, i.e., when $\alpha^* \sim \xi_{\rm ph}$, or $E_F(\ell^*) \sim \omega_{2k_F}$ (denoted by asterisk in Fig. 2). At this length scale the system can no longer distinguish the phonon propagator from a $\delta$ function; all electronic fluctuations with energies higher than $\omega_{2k_F}$ have been integrated out, and the electron-phonon system behaves as effectively nonretarded. We then can expand the argument of the cosine in Eq. (3.3) for small arguments

$$\cos\{2e^{\xi}[\Phi(\mathbf{r}) - \Phi(\mathbf{r}')]\} \cong 2e^{2\xi} \exp[-2e^{2\xi} V(\mathbf{r}-\mathbf{r}')][(\mathbf{r}-\mathbf{r}')\cdot\nabla\Phi]^2 . \tag{3.15}$$

Note the exponential term in this expansion; as has been pointed out by Knops and den Ouden,[32] powers of $\Phi(\mathbf{r}) - \Phi(\mathbf{r}')$ larger than two in the expansion of the cosine are not simply irrelevant, but consist of a linear combination of an irrelevant operator and a term $[\Phi(\mathbf{r}) - \Phi(\mathbf{r}')]^2$, and therefore contribute to any order in the expansion. Their contribution can, however, be summed and yields the exponential term in (3.15). We can now perform the $\mathbf{r} - \mathbf{r}'$ integral in (3.3) using (3.15), and then obtain exactly the functional form of a Tomonaga-Luttinger Hamiltonian with nonretarded interactions only, with the replacement

$$\exp(2\xi) \to z \exp(2\xi) , \tag{3.16}$$

$$z^{-2} = 1 + \left[1 - \frac{g_2 - g_1}{2\pi v_F}\right] \left[\frac{\gamma_1^2}{\pi v_F \omega_{2k_F}^2}\right] \Gamma(3 - 2e^{2\xi}, 1) , \tag{3.17}$$

where all parameters have to be taken from the solution of the scaling equations at $\ell = \ell^*$. $\Gamma(x,y)$ is the incomplete $\Gamma$ function.[33]

Obviously the success of the present approach depends crucially on the possibility of performing a perturbation expansion of $\exp(-U)$, cf. Eq. (3.8), and therefore necessitates the presence of a small parameter, namely the effective electron-phonon interaction constant $Y_{\rm ph}$. In order to have a consistent description of our system, we must require that $Y_{\rm ph}(\ell)$ remains small for all $\ell < \ell^*$. In Fig. 2, *initial* values *above* the dash-dotted line scale *outside* the range of validity of the perturbation expansion ($Y_{\rm ph} \lesssim 1$) and therefore cannot be described consistently by the present approach. Initial values below the dash-dotted line (such as those shown in Fig. 2) are consistently described. Note that the dash-dotted line in Fig. 2 shifts

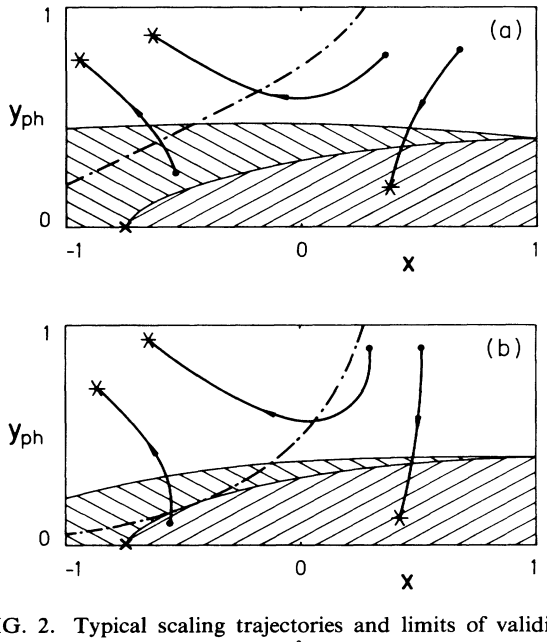


FIG. 2. Typical scaling trajectories and limits of validity of scaling and MTM approach. $X \simeq \frac{3}{2} - \exp(2\xi)$. $\omega_{2k_F}/E_F = 0.1$ (a) and 0.01 (b). Scaling (solid lines) stops at $\ell^* = \ln(\omega_{2k_F}/E_F)$ (denoted by asterisk). Initial values above the dash-dotted lines scale outside the range of validity of the scaling equations. Lower right hatched area: MTM has only zero-order parameter solution; upper hatched area: important amplitude fluctuations preclude MTM approach. $\times$ on the $X$ axis indicated locus of the noninteracting system.

downward with decreasing phonon frequency: the Coulomb gas approach is typically a high frequency and/or weak coupling approach and not suited for the description of the low phonon frequency region. A complementary approach will be described in the next section.

## IV. SOLUTION FOR LOW PHONON FREQUENCIES AND/OR STRONG COUPLING

In the weak coupling approach of the preceding section we integrated over the phonon degrees of freedom to discuss an effective electronic problem. For very low phonon frequencies or strong electron-phonon coupling we shall follow the inverse strategy: we shall first eliminate the electronic degrees of freedom and solve an effective phonon Hamiltonian. The results of this solution can then be used to obtain information on the properties of the electron system which we are mostly interested in.

The important observation is that the phonon field $\varphi_{2k_F}(x)$ entering the electron-phonon Hamiltonian (2.5), is a very slowly varying function of time at low phonon frequencies. As a first approximation, we can neglect completely the fluctuations of the phonon field

$$\varphi_{2k_F}(\mathbf{r}) \cong \text{const} \equiv \varphi_0 \ . \tag{4.1}$$

*A priori* we cannot make this restriction for the spatial variations. We take it as a hypothesis, and it will show up to be consistent at the end. Then our Hamiltonian [(2.1)–(2.5)] can be written as

$$H = H_{\text{ph}}^{(0)} + H_{\text{MTM}} \ , \tag{4.2}$$

where $H_{\text{MTM}}$ is the Hamiltonian of the massive Thirring model[34] (MTM). Its electron-electron interaction term is usually written (in fermion language) as

$$H_g = 2g \int dx \Psi_+^\dagger(x)\Psi_-^\dagger(x)\Psi_-(x)\Psi_+(x) \ , \tag{4.3a}$$

and its mass term

$$H_m = m_0 \int dx [\Psi_+^\dagger(x)\Psi_-(x) + \Psi_-^\dagger(x)\Psi_+(x)] \ . \tag{4.3b}$$

is related to the electron-phonon interaction of our problem by

$$m_0 = \gamma_1 \varphi_0 / v_F \ . \tag{4.4}$$

$\gamma_1\varphi_0$ plays the role of an order parameter (or, more precisely, its amplitude). Due to the different cutoff procedures of the TLM and MTM, the relation between the electronic coupling constants is

$$\frac{2}{\pi}\text{arccot}\left[\frac{-g}{2}\right] = 1 + \alpha_{\text{CDW}}/2 \ , \tag{4.5}$$

giving in lowest order $g = (g_2 - g_1)/2v_F$, in agreement with what has been said in Sec. II about universality. This identification can be obtained, e.g., from parameters which can be computed in both models such as the dependence of the gap in the electronic spectrum on the bare mass.[34,35]

The massive Thirring model has been solved exactly by Bethe ansatz.[34] Its ground-state energy is given by

$$E_{\text{gr}}[\varphi_0] = -L\frac{v_F}{4}\left\{\frac{\alpha_{\text{CDW}}}{4+\alpha_{\text{CDW}}}\frac{\cot(\pi\alpha_{\text{CDW}}/4)}{2\alpha^2} - \left[\frac{\alpha\gamma_1\varphi_0}{v_F}\right]^2 \frac{1}{\sin(\pi\alpha_{\text{CDW}}/2)}\left[\left[\frac{\alpha\gamma_1\varphi_0}{v_F\cos(\pi\alpha_{\text{CDW}}/4)}\right]^{4/2+\alpha_{\text{CDW}}} - 1\right]\right\}. \tag{4.6}$$

Minimization of the total ground-state energy $E_{\text{gr}}[\varphi_0] + H_{\text{ph}}^{(0)}[\varphi_0]$ with respect to $\varphi_0$ allows one to determine the amplitude of the order parameter

$$\gamma_1\varphi_0 = \frac{v_F}{\alpha}\cos\left[\frac{\pi\alpha_{\text{CDW}}}{4}\right]\left[\left[1+\frac{\alpha_{\text{CDW}}}{2}\right]\left[1+\frac{\sin(\pi\alpha_{\text{CDW}}/2)}{2\pi Y_{\text{ph}}^2}\right]\right]^{-(2+\alpha_{\text{CDW}})/2\alpha_{\text{CDW}}} . \tag{4.7}$$

The somewhat complex structure of this equation is due to the exact inclusion of the electronic correlations; in the limit $g \to 0$ (i.e., $\alpha_{\text{CDW}} \to 0$), it reduces to the exponential familiar from the classical Peierls theory.

$$\gamma_1\varphi_0 = \frac{v_F}{\alpha}\exp-\left[\frac{1}{4Y_{\text{ph}}^2}+\frac{1}{2}\right] \quad (\alpha_{\text{CDW}} \equiv 0) \ ,$$

$$\cong \frac{v_F}{\alpha}\exp-\left[\frac{1}{4Y_{\text{ph}}^2}\right] \quad (Y_{\text{ph}} \ll 1) \ .$$

Note that for

$$2\pi Y_{\text{ph}}^2 < -\sin(\pi\alpha_{\text{CDW}}/2) \ , \tag{4.8}$$

we only obtain the solution $\gamma_1\varphi_0 = 0$.

The nonvanishing order parameter amplitude (4.7) in a wide parameter range suggests long-range order in our system. This is due to the initial neglect of fluctuations in the phonon field, as we shall show now. We decompose the phonon field

$$\varphi_{2k_F}(\mathbf{r}) = \varphi_0[1+\delta\varphi(\mathbf{r})]\exp[i\chi(\mathbf{r})] \tag{4.9}$$

into amplitude $[\delta\varphi(\mathbf{r})]$ and phase fluctuations $[\chi(\mathbf{r})]$. There is a finite restoring force acting against amplitude fluctuations, and at $T=0$ they are completely frozen out (at least for what concerns the long-range properties of our system). Phase fluctuations, however, do not have a restoring force and will be important even at $T=0$. We describe the phase fluctuations by a Hamiltonian similar to that given previously by Fukuyama[18,36]

$$H_\chi = \int dx \left[\frac{\rho}{2}(\partial_t\chi)^2 + \frac{c}{2}(\nabla\chi)^2\right] , \tag{4.10}$$

where

$$\rho=(1+2\pi v_F\varphi_0^2)/4\pi v_J, \quad v_J=v_\rho\exp(2\xi) , \tag{4.11}$$

$$c=v_N/4\pi, \quad v_N=v_\rho\exp(-2\xi) , \tag{4.12}$$

where $\exp(2\xi)$ and $v_\rho$ are given by Eqs. (2.10) and (2.11). $\rho$ is the effective mass density of the CDW condensate, and $c$ is its unrenormalized phase velocity; $v_N$ and $v_J$ are the velocities for charge and current excitations in the TLM introduced by Haldane.[28] $v_J$ is the relevant velocity describing the $2k_F$ excitation of particles in the TLM, thereby giving a finite current; it is produced, for example, by coupling to $2k_F$ phonons. In the interacting TLM, it is renormalized from $v_F$ by electron-electron interactions. $v_N$ sets the energy scale for adding charge to the TLM without creating a current excitation. In our electron-phonon system this is done by a local compression of the CDW, described by the $\nabla\chi$ term in the Fukuyama Hamiltonian. Again, this velocity is renormalized by electron-electron interaction. The renormalized velocity of the collective excitations is then given by

$$v_\chi=v_\rho(1+2\pi v_F\varphi_0^2)^{-1/2}\ll v_\rho . \tag{4.13}$$

The effective renormalized phonon propagator becomes

$$-D(\mathbf{r}-\mathbf{r}')=\langle T_\tau[\varphi_{2k_F}(\mathbf{r})\varphi^\dagger_{2k_F}(\mathbf{r}')]\rangle$$
$$=\varphi_0^2\exp[R_\chi(\mathbf{r}-\mathbf{r}')]=\sim|\mathbf{r}-\mathbf{r}'|^{-\eta} \tag{4.14}$$

in terms of the phase fluctuation propagator

$$-R_\chi(\mathbf{r}-\mathbf{r}')=\langle T_\tau[\chi(\mathbf{r})-\chi(\mathbf{r}')]^2\rangle . \tag{4.15}$$

Now, $\mathbf{r}=(x,v_\chi\tau)$ and the exponent $\eta$ is

$$\eta=2\exp(2\xi)(1+2\pi v_F\varphi_0^2)^{-1/2}\ll 1 . \tag{4.16}$$

Via Dyson's equation, it can be seen that this same exponent $\eta$ also governs the decay of the CDW correlations

$$R_{\rm CDW}\sim|\mathbf{r}-\mathbf{r}'|^{-2+\alpha_{\rm CDW}}, \quad \alpha_{\rm CDW}=2-\eta . \tag{4.17}$$

Again, we obtain nonuniversal power laws for the correlation functions and therefore conclude that the phase fluctuations of the coupled electron-phonon system suppress the long-range order suggested by the solution of the massive Thirring model. The fact that $\eta\ll 1$ and $v_\chi\ll v_F$ shows that these phase modes determine the long-distance (time) behavior of the correlation functions.

It is not possible to compute directly the decay of the superconducting correlation function $R_{\rm SC}(\mathbf{r})$, because the MTM-Hamiltonian does not describe harmonic fluctuations of the electronic degrees of freedom. As the logarithmic behavior of the correlation functions is only determined by the first cumulant, it is justified to replace $\Phi(\mathbf{r})$ [cf. Eq. (2.13b)] by $\chi(\mathbf{r})$; then one can conclude that $R_{\rm SC}$ behaves as

$$R_{\rm SC}(\mathbf{r})\sim r^{-2+\alpha_{\rm SC}}, \quad \alpha_{\rm SC}=2-4/\eta . \tag{4.18}$$

Note that when long-range CDW order is stabilized ($\eta\to 0$) $4/\eta\to\infty$ which has to be interpreted as exponential decay of fluctuations.

Let us finally give a limit of validity of the present strong coupling approach. We had already noted that for $2\pi Y_{\rm ph}^2<-\sin(\pi\alpha_{\rm CDW}/2)$, only the solution $\gamma_1\varphi_0=0$ minimizes $E_{\rm gr}[\varphi_0]+H^{(0)}_{\rm ph}[\varphi_0]$. This is the lower hatched area in Fig. 2. Furthermore we have to require for a consistent description of our system, that the zero-point amplitude fluctuations of the order parameter (neglected in the present description) must be smaller than the order parameter amplitude itself

$$\langle[\delta\varphi(\mathbf{r})]^2\rangle\ll\varphi_0^2 . \tag{4.19}$$

We can have a rough idea about the importance of amplitude fluctuations by assuming that the coefficients of the kinetic energy and of the gradient term in the amplitude fluctuation Hamiltonian are the same as in the Fukuyama phase Hamiltonian. The requirement (4.19) then prohibits the application of the MTM approach also in the upper hatched area in Fig. 2. This area shrinks with *decreasing* phonon frequency.

## V. INSTABILITIES AND THERMODYNAMIC PROPERTIES

We argued in Sec. II that two parameters only, the exponents $\alpha_i$ characterizing the decay of correlations, and the renormalized velocity $v_\rho$ of the collective excitations, are sufficient to describe completely the physics of our model. In this section we give some examples.

Although a strictly one-dimensional system cannot have a phase transition at finite temperature to a long-range ordered CDW or SC state, the importance of the respective fluctuations, which may lead to a phase transition in the presence of a suitable three-dimensional coupling mechanism, can be assessed through the exponents $\alpha_i$. The boundary between domains of diverging CDW and SC correlations ($\alpha_i=0$) is given by $g_2-g_1=0$ in the absence of electron-phonon coupling. Inspection of Eqs. (3.14a) and (4.17) shows that electron-phonon backscattering favors charge density waves over superconductivity because $d\exp(2\xi)/d\ell<0$ and $\eta\ll 1$. Figure 3 shows the CDW versus SC boundary determined for different phonon frequencies from Eq. (3.14a). We have also indicated

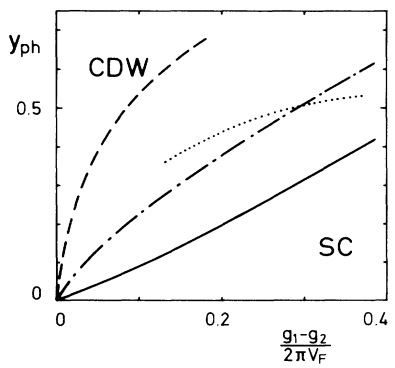


FIG. 3. Microscopic phase diagram including electron-phonon backscattering as obtained from TLM approach. $\omega_{2k_F}/E_F=0.5$, dashed; 0.1, dash-dotted; and 0.01, solid lines. Dotted lines indicates boundary as obtained from MTM for $\omega_{2k_F}/E_F=0.1$ (however see text).

the boundary for $\omega_{2k_F}/E_F=0.1$ as obtained from the MTM approach. Despite the reasonable agreement, the latter should be taken with caution, for the following reason. The boundary line between domains of diverging CDW and SC fluctuations is determined by the cancellation of the effects of electron-electron and electron-phonon interaction. For what concerns the *electron-electron* interaction, the MTM is a *weak-coupling* model. Bergknoff and Thacker[34] have pointed out that for $\alpha_{\rm CDW}<-\frac{2}{3}$ $[(g_1-g_2)/2\pi v_F>0.35]$, the simple cutoff structure of the model (which has also been used in the present study) is altered. As a consequence, for the determination of the separation line between CDW and SC, we can use the MTM only in the weak electron-phonon coupling regime; there, however, its results are doubtful because of the neglect of fluctuations of the amplitude of the CDW order parameter which then are important.

Figure 4 shows the renormalization of the velocity of the collective modes $v_\rho(\ell^*)$, $v_\chi$ as obtained from (3.14c) and (4.13) as a function of $Y_{\rm ph}^2$ for different phonon frequencies. Comparing (3.14a), (3.14c), (4.13), and (4.16), we see that similar curves also describe the renormalization of $\exp[2\xi(\ell^*)]$ and $\eta$, and thereby of the exponents $\alpha_{\rm CDW}$ and $\alpha_{\rm SC}$ of the correlation functions. The decrease as a function of $Y_{\rm ph}$ and $\omega_{2k_F}/E_F$ in the curves in Fig. 4 is then a direct measure of the depression of the superconducting fluctuations.

The electronic specific heat is

$$c_{\rm el}=(\pi^2/3)k_B^2TN(0)\ , \tag{5.1}$$

independent of the dimension of the system.[37] In a quasiparticle picture, $N(0)$ is the density of states at the Fermi level; in the present 1D system which has no quasiparticle excitations, $N(0)=1/2\pi v_\rho$ is the density of states of the collective modes. The inverse of the curves in Fig. 4 then gives the increase of the electronic specific heat, or what would be in a quasiparticle picture the electronic effective mass. Note that in the TLM region the increase is linear in the effective electron-phonon coupling constant $\lambda\sim Y_{\rm ph}^2$, whereas for stronger coupling or lower phonon frequency, $c_{\rm el}$ increases more slowly.

The homogeneous electronic compressibility is defined as

$$\kappa_{\rm el}=\lim_{q\to 0}\lim_{\omega\to 0}\chi_{\rho\rho}(q,\omega) \tag{5.2}$$

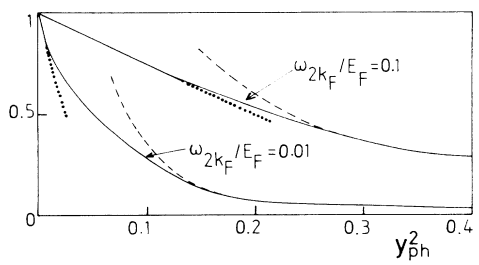


FIG. 4. Renormalized velocity of collective charge density excitations as obtained from TLM, dotted lines, and MTM, dashed lines, approach for $g_2-g_1=0$. The same curves describe the renormalization of $\exp[2\xi(\ell^*)]$ and $\eta$, and therefore of the correlation function exponents $\alpha_{\rm CDW,SC}$.

in terms of the density-density correlation function, and can be evaluated as

$$\kappa_{\rm el}=\frac{2}{\pi}\frac{e^{2\xi}}{v_\rho}\ . \tag{5.3}$$

$\kappa_{\rm el}$ is *not* renormalized by electron-phonon backscattering, as can be seen easily by computing $d\kappa_{\rm el}/d\ell$ using (3.14) in TLM or the fact that $\eta/v_\chi$ is independent of the phonons in MTM. This perhaps somewhat unexpected result is, however, compatible with the tendency towards a Peierls instability induced by electron-phonon backscattering, as it only implies a softening of the lattice at $q=2k_F$.

## VI. DISCUSSION

In the preceding sections, we have discussed a one-dimensional electron-phonon system in two limiting cases of weak coupling and/or high phonon frequency and strong coupling and/or low phonon frequency. We have been able to extract the same physical quantities from both descriptions, namely correlation functions for CDW or SC fluctuations together with the exponents that characterize their algebraic decay, and the renormalized velocity of the collective excitations of the system. All quantities have been obtained as a function of electron-electron, electron-phonon coupling, and the phonon frequency. We have argued that, despite their nonuniversality, both coefficients together are sufficient for a complete description of the low-energy physics of our system.

We have been able to give limits of validity for the different approaches from consistency requirements. They show both approaches to be complementary: when we decrease the phonon frequency, the range of applicability of TLM becomes more and more restricted (because the scaling trajectories become longer) whereas the one of MTM increases (because the fluctuations of the amplitude of the order parameter are suppressed). Moreover, the explicit computation of a physical quantity ($v_\rho^R$) showed that results from both approaches match together very satisfactorily. Note in this context that deviations of the TLM and MTM lines from the extrapolated line in Fig. 4 become significant at about the same point where the consistency criteria forbid the application of the respective approach.

Finally we can examine in which temperature range we can expect the effects discussed above. In the TLM, it is possible to calculate at finite temperature. The central point of the present treatment, the equivalence of the 1D electron-phonon system to a generalized 2D classical Coulomb gas, can also be maintained. Due to the finite temperature, the Coulomb gas is now on a cylinder with a perimeter $\beta=1/T$. The "potential" $V(\mathbf{r}-\mathbf{r}')$ is no longer a simple logarithm but, again, is the solution of the 2D Poisson equation in the new geometry.[38] Scaling stops again at $\alpha\sim\xi$, but now $\xi^{-1}=\xi_{\rm ph}^{-1}+\xi_T^{-1}$, where $\xi_T=v_F/2\pi T$. In lowest order, only the bigger of the quantities $\omega_{2k_F}$ and $2\pi T$ is important. This is the phonon frequency if $2\pi T<\omega_{2k_F}$, and then the effects discussed above for $T=0$ should be observable.

In the strong coupling limit, the thermal amplitude

fluctuations of the order parameter must be sufficiently small so that the phase fluctuations still determine the asymptotic long-range behavior of our system. We therefore have to consider the condition (4.19) as a function of temperature. Unfortunately, it is not possible to solve the MTM at finite temperature directly, so that we limit ourselves to the Peierls model without electron-electron interactions. Due to the relatively weak dependence of the solution of (4.19) on the electron-electron interaction, as evidenced by the hatched area in Fig. 2, we argue that the noninteracting limit gives a qualitatively good insight also into the more general model.

To describe the Peierls model in the vicinity of the mean-field critical temperature $T_c$, we use a Ginzburg-Landau functional together with a Hartree-Fock approximation on the fourth-order term.[39–41] Then, we find that amplitude fluctuations can be considered frozen out below a temperature $T_x \sim 0.6T_c$. [This is not inconsistent with the result $T_x \sim 0.25T_c$ of Lee, Rice, and Anderson[39] who reduced the treatment of the Ginzburg-Landau functional to the (numerical) solution of the Schrödinger equation of an anharmonic oscillator.] In lowest order, we can compare this temperature to the phonon frequencies obtained from an evaluation of the condition (4.19) at $T=0$ as a function of phonon frequency; we then obtain that for $T < T_x$ and $3\pi T < \omega_{2k_F}$, thermal and quantum amplitude fluctuations of the order parameter are unimportant and phase fluctuations dominate the physical behavior of our system, in agreement with the conditions derived from the TLM approach.

The results obtained in this paper have probably important applications to the description of spin-Peierls systems, where the nonadiabaticity of the phonons is important. The present discussion applies to the situation under magnetic field, whereas in the zero-field limit, the spin-Peierls systems are equivalent to a commensurate spinless electron-phonon system. Then, umklapp processes are relevant; therefore, we defer an extensive discussion of the applications of the present theory to a forthcoming paper, where the effect of umklapp scattering will be determined.

## APPENDIX

In this appendix we want to give a derivation of the scaling equations (3.14). Rather than using the partition sum (3.2), it is more convenient to consider a (2D) correlation function

$$-R_\Phi(\mathbf{r}-\mathbf{r}') \equiv \langle T_\tau[\Phi(\mathbf{r})-\Phi(\mathbf{r}')]^2 \rangle \tag{A1}$$

with

$$\langle \cdots \rangle = Z^{-1}\mathrm{Tr}_\Phi \cdots \exp\left[-\int \frac{dy}{v_F}\tilde{H}_{\mathrm{el}}[\Phi(\mathbf{r})]-U[\Phi(\mathbf{r})]\right] \tag{A2}$$

and $Z$ is defined in (3.2). $U[\Phi]$ is given in Eq. (3.3). The CDW correlation function (2.21) is then given in terms of $R_\Phi$ by

$$-R_{\mathrm{CDW}}(\mathbf{r}-\mathbf{r}') = \frac{e^{2ik_F(x-x')}}{2\pi\alpha}\exp[-R_\Phi(\mathbf{r}-\mathbf{r}')] \, . \tag{A3}$$

We now expand $\exp(-U[\Phi])$, and keep only the first-order term in $U$ to obtain

$$-R_\Phi(\mathbf{r}-\mathbf{r}') = \frac{Z}{Z_0}\left\langle T_\tau[\Phi(\mathbf{r})-\Phi(\mathbf{r}')]^2\left[1+\left[\frac{\gamma_1}{2\pi\alpha v_F}\right]^2\int d^2r\int d^2r' D(\mathbf{r}-\mathbf{r}')\cos\{2e^{\xi}[\Phi(\mathbf{r})-\Phi(\mathbf{r}')]\}\right]\right\rangle_0 . \tag{A4}$$

Evaluating the average yields

$$-R_\Phi(\mathbf{r}-\mathbf{r}') = V(\mathbf{r}-\mathbf{r}') - e^{2\xi}\left[\frac{\gamma_1}{2\pi\alpha v_F}\right]^2\int d^2r_1\int d^2r_2 D(\mathbf{r}-\mathbf{r}')\exp[-2e^{2\xi}V(\mathbf{r}_1-\mathbf{r}_2)][V(\mathbf{r}-\mathbf{r}_1)-V(\mathbf{r}'-\mathbf{r}_1) - V(\mathbf{r}-\mathbf{r}_2)+V(\mathbf{r}'-\mathbf{r}_2)]^2 \, . \tag{A5}$$

$V(\mathbf{r})$ is defined in Eq. (3.10).

The standard real space method to obtain renormalization group equations from (A5) is well documented in the literature.[42] Its disadvantages are (i) the difficulty to generalize it to more complicated problems involving more than two $\mathbf{r}$ integrals, and (ii) its limitation to isotropic systems. From Eq. (3.4) it is clear that the phonon propagator $D(\mathbf{r})$ is an extremely anisotropic object; its anisotropy must be treated correctly if we want to describe the effects of the phonon dynamics.

Both limitations can be bypassed by Fourier transformation. In the isotropic case, the Fourier transform of (3.10) is

$$V(\mathbf{q}) = -2\pi/q^2 \, . \tag{A6}$$

An anisotropic potential

$$\tilde{V}(\mathbf{r}) = (\tfrac{1}{2})\ln(x^2+y^2/A^2) \tag{A7}$$

is Fourier transformed to

$$\tilde{V}(\mathbf{q}) = -2\pi(q_x^2+A^2q_y^2)^{-1} \, , \tag{A8}$$

and for $|A-1| \ll 1$

$$\tilde{V}(\mathbf{q}) \cong -2\pi\left[\frac{2}{(1+A^2)q^2} - 2\frac{1-A^2}{(1+A^2)^2}\frac{\cos(2\Theta)}{q^2}\right] , \tag{A9}$$

where

$$\cos(2\Theta) = \frac{q_x^2-q_y^2}{q_x^2+q_y^2} \, . \tag{A10}$$

Let us now Fourier-transform Eq. (A5) and expand for

$|\mathbf{q}| \ll |\mathbf{q}_1|$

$$-R_\Phi(\mathbf{q}) = V(\mathbf{q}) + e^{2\xi}\left[\frac{\gamma_1}{2\pi v_F}\right]^2 \int \frac{d^2q_1}{(2\pi)^2} V^2(\mathbf{q}) D(\mathbf{q}_1) \times (\mathbf{q}_1\cdot\nabla_q)^2 f(-\mathbf{q}_1) , \tag{A11}$$

where

$$f(\mathbf{q}) = \int d^2r \exp(-i\mathbf{q}\cdot\mathbf{r}) \exp[-2e^{2\xi}V(\mathbf{r})] . \tag{A12}$$

Taking account of the local nature of the phonon propagator in $x$ direction, we obtain

$$-R_\Phi(\mathbf{q}) = V(\mathbf{q})\left[1 - 2\pi e^{2\xi}\left[\frac{\gamma_1}{2\pi v_F}\right]^2 I[1-\cos(2\Theta)]\right] \tag{A13}$$

with

$$I = \int \frac{d^2q_1}{(2\pi)^2} D(\mathbf{q}_1) \frac{\partial^2}{\partial q_{1,y}^2} f(-\mathbf{q}_1) . \tag{A14}$$

Note that in (A11)–(A14) we have always used the isotropic form (A6) for $V(\mathbf{q})$. Comparison of (A13) with (A9) shows that, due to the anisotropy of the phonon propagator, we always obtain an anisotropic contribution to an initially isotropic correlation function. (A13) can now be Fourier-transformed back to $\mathbf{r}$ space, where one can apply the familiar Kosterlitz-Thouless ideas. The scaling equations (3.14a) and (3.14b) for the coupling constants are obtained immediately. In the same way, one can also treat the integral involving the $\cos 2\Theta$ (i.e., anisotropy) term. Remembering that $y = v_F\tau$, one sees from (A7) that a change in $A$ can be translated into a renormalization of the Fermi velocity, thereby leading to (3.14c).

*Present address: Theoretische Physik 1, Universität Bayreuth, D-8580 Bayreuth, Federal Republic of Germany.

[1](a) For a review of recent progress: Proceedings of ICSM 1984, Abano-Terme [Mol. Cryst. Liq. Cryst. **117-121** (1985)]; (b) D. Jérome and H. J. Schulz, Adv. Phys. **31**, 299 (1982).

[2]For review on $(CH)_x$: S. Etemad, A. J. Heeger, and A. J. MacDiarmid, Annu. Rev. Phys. Chem. **33**, 443 (1982); D. Baeriswyl, G. Harbeke, H. Kiess, and W. Mayer, in *Electronic Properties of Polymers,* edited by J. Mort and G. Pfister (Wiley, New York, 1982).

[3]J. Sólyom, Adv. Phys. **28**, 201 (1979).

[4]R. E. Peierls, *Quantum Theory of Solids* (Oxford University Press, Oxford, 1955).

[5]J. P. Pouget, S. Khanna, F. Denoyer, R. Comès, A. F. Garito, and A. J. Heeger, Phys. Rev. Lett. **37**, 437 (1976); S. Kagoshima, T. Ishiguro, and H. Anzai, J. Phys. Soc. Jpn. **41**, 2061 (1976).

[6]J. P. Pouget, R. Comès, A. J. Epstein, and J. S. Miller, Mol. Cryst. Liq. Cryst. **85**, 203 (1982).

[7]P. A. Lee, T. M. Rice, and R. A. Klemm, Phys. Rev. B **15**, 2984 (1977).

[8]V. J. Emery, Phys. Rev. Lett. **37**, 107 (1976).

[9]C. Bourbonnais, F. Creuzet, D. Jérome, K. Bechgaard, and A. Moradpour, J. Phys. Lett. (Paris) **45**, L755 (1984).

[10]V. J. Emery, Synth. Met. **13**, 21 (1986); K. A. Muttalib and V. J. Emery, Phys. Rev. Lett. **57**, 1370 (1986); C. Bourbonnais and L. G. Caron (unpublished).

[11]J. C. Scott, A. F. Garito, and A. J. Heeger, Phys. Rev. B **10**, 3131 (1975); Y. Tomkiewicz, B. A. Scott, L. J. Tao, and R. S. Title, Phys. Rev. Lett. **32**, 1363 (1974).

[12]H. K. Ng, T. Timusk, and K. Bechgaard, Mol. Cryst. Liq. Cryst. **119**, 191 (1985); Phys. Rev. B **30**, 5842 (1984); C. S. Jacobsen, D. B. Tanner, and K. Bechgaard, *ibid.* **28**, 7019 (1983); M. Krauzman, H. Poulet, and R. M. Pick, *ibid.* **33**, 99 (1986); M. Meneghetti, R. Bozio, I. Zanon, C. Pecile, C. Ricotta, and M. Zanetti, J. Chem. Phys. **80**, 6210 (1984); J. E. Eldridge, C. C. Homes, F. E. Bates, and G. S. Bates, Phys. Rev. B **32**, 5156 (1985).

[13]M. J. Rice, L. Pietronero and P. Bruesch, Solid State Commun. **21**, 757 (1977).

[14]M. J. Rice, C. B. Duke, and N. O. Lipari, Solid State Commun. **17**, 1089 (1975).

[15]V. J. Emery, Phys. Rev. B **14**, 2989 (1976); M. Fowler, *ibid.* **17**, 2989 (1978).

[16]D. Baeriswyl and J. J. Forney, J. Phys. C **13**, 3203 (1980).

[17]B. Horowitz, H. Gutfreund, and M. Weger, Solid State Commun. **39**, 541 (1981).

[18]B. Horovitz and J. Sólyom, Phys. Rev. B **32**, 2681 (1985).

[19]H. Fukuyama, J. Phys. Soc. Jpn. **41**, 513 (1976); H. Fukuyama and H. Takayama, in *Electronic Properties of Inorganic Quasi-One-dimensional Solids,* edited by P. Monceau (Reidel, Dordrecht, 1985).

[20]D. Schmeltzer, R. Zeyher, and W. Hanke, Phys. Rev. B **33**, 5141 (1986).

[21]L. G. Caron and C. Bourbonnais, Phys. Rev. B **29**, 4230 (1984); G. S. Grest, E. Abrahams, S.-T. Chui, P. A. Lee, and A. Zawadowski, *ibid.* **14**, 1225 (1976).

[22]E. Fradkin and J. E. Hirsch, Phys. Rev. B **27**, 1680 (1983); J. E. Hirsch and E. Fradkin, *ibid.* **27**, 4302 (1983); J. E. Hirsch, *ibid.* **31**, 6022 (1985).

[23]J. Voit and H. J. Schulz, Mol. Cryst. Liq. Cryst. **119**, 449 (1985).

[24]S. Engelsberg and B. B. Varga, Phys. Rev. **136**, A1583 (1964).

[25]M. C. Cross and D. S. Fisher, Phys. Rev. B **19**, 402 (1979).

[26]J. B. Torrance, in *Chemistry and Physics of Low Dimensional Metals,* edited by H. J. Keller (Plenum, New York, 1977); J. Phys. (Paris) Colloq. **44**, C3-799 (1983).

[27]D. C. Mattis and E. H. Lieb, J. Math. Phys. **6**, 304 (1965).

[28]F. D. M. Haldane, J. Phys. C **12**, 4791 (1979); **14**, 2585 (1981); see also R. Heidenreich, R. Seiler, and D. A. Uhlenbrock, J. Status Phys. **22**, 27 (1980), and for earlier work on bosonization see A. Luther and I. Peschel, Phys. Rev. B **9**, 2911 (1974); and D. C. Mattis, J. Math. Phys. **15**, 315 (1974).

[29]F. D. M. Haldane, Phys. Rev. Lett. **45**, 1358 (1980); **47**, 1840 (1981).

[30]S.-T. Chui and P. A. Lee, Phys. Rev. Lett. **35**, 315 (1975).

[31]J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973); J. M. Kosterlitz *ibid.* **7**, 1046 (1974).

[32]H. J. F. Knops and L. W. J. den Ouden, Physica **103A**, 597 (1980).
[33]I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic, New York, 1980).
[34]N. Bergknoff and H. B. Thacker, Phys. Rev. D **19**, 6111 (1979).
[35]M. P. M. den Nijs, Phys. Rev. B **23**, 6111 (1981).
[36]K. Takano, Prog. Theor. Phys. **68**, 1 (1982).
[37]N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Holt, Rinehard, and Winston, New York, 1976).
[38]H. Schulz, Z. Phys. B **26**, 377 (1977).
[39]P. A. Lee, T. M. Rice, and P. W. Anderson, Phys. Rev. Lett. **31**, 462 (1973).
[40]D. Jérome and H. J. Schulz, in *Extended Linear Chain Compounds,* edited by J. S. Miller (Plenum, New York, 1982), Vol. 2.
[41]A. A. Maradudin and A. E. Fein, Phys. Rev. **128**, 2589 (1962).
[42]D. R. Nelson, Phys. Rev. B **18**, 2318 (1978).