Peierls instability of a one-dimensional quantum liquid

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Whether Peierls distortion occurs for a system of one-dimensional spinless fermions is determined by the exponent g that characterizes the decay of correlations among the electrons in the undistorted state. Noninteracting electrons ($g=1$) is the marginal case, for which the Peierls effect just barely occurs. For repulsive interactions between the electrons ($g<1$) the instability is enhanced and the leading dependence of the ground-state energy E on the lattice distortion δ is $E\propto-\delta^{2/(2-g)}$. For attractive interactions ($g>1$) a continuous phase transition between a normal metal and a Peierls insulator takes place for sufficiently strong electron-ion interaction. [S0163-1829(96)09919-5]

Forty years ago Peierls suggested that a one-dimensional metal at zero temperature is subject to a spontaneous distortion of the lattice that converts the metal into an insulator.[1] This does indeed happen for noninteracting electrons;[2] however, electron-electron interactions are expected to have a drastic effect on the Peierls instability, just as they completely destroy the Fermi-liquid picture in one dimension.[3]

In this paper we present a phenomenological theory of the Peierls effect in a one-dimensional spinless quantum liquid of interacting fermions or repulsive bosons. Invoking the large ratio of ion and electron masses, M and m, correspondingly, we will assume that the ionic subsystem can be treated classically.

There have been several attempts to study this problem. Luther and Peschel,[4] contributed the important qualitative conclusion that the lattice is stable in the presence of attractive electron-electron interactions. Krivnov and Ovchinnikov[5] treated a weakly interacting half-filled band electronic system perturbatively, while Kivelson, Thacker, and Wu[6] and Voit and Schulz[7] analyzed a model that could be related to the exactly solvable massive Thirring model.[8] However, a phenomenological picture of the effect of electronic correlations on the Peierls instability has not been developed.

Here we will show that the fate of the Peierls effect is determined entirely by the same combination g of the interaction parameters that governs the macroscopic properties of an undistorted electronic liquid; in this context g can be regarded as a parameter that tells us at once how ''far'' a given system is from the case of free fermions. The macroscopic character of our findings goes beyond perturbation theory, and is more general than what can be concluded from a specific model.

Our starting point is a macroscopic bosonized action describing a one-dimensional quantum liquid of electrons and classical system of ions coupled by a weak short-range interaction of an amplitude $V=\int_{-\infty}^{\infty}V_{\text{electron-ion}}(x)dx$:

$$A=\frac{1}{2}\int dx\, dt(K_1\dot{u}^2+K_2u'^2+C_2v'^2+2\rho nVu'v') +2\rho nV\int dx\, dt\, \cos 2\pi[(n-\rho)x-nu+\rho v]. \quad (1)$$

Here x and t stand for the spatial and imaginary time coordinates, and primes and dots denote spatial and time derivatives, respectively. The displacement field $u(x,t)$ describes the quantum fluctuations of electrons away from their average spacing n^{-1}, and $v(x)$ is a static displacement of the ions from their average spacing ρ^{-1} (n and ρ are the electron and ion densities). In writing (1) we dropped the ion kinetic-energy term of the form $C_1\,\dot{v}^2$, and therefore neglected the quantum fluctuations of ions in view of the large mass ratio M/m. The parameters entering the harmonic part of action (1) are the effective mass density $K_1=mn$ of the electronic subsystem, and the compliances (K_2 and C_2). To lowest order in the electron-ion interaction V, the compliances can be expressed entirely in terms of the ground-state properties of the uncoupled electron and ion populations. For example, if the dependence of the electronic chemical potential μ on electron density n (and interaction) is known, then one has $K_2=n^2\partial\mu/\partial n$. The electronic system is characterized by the dimensionless parameter

$$g=\frac{\pi\hbar n^2}{\sqrt{K_1K_2}} \quad (2)$$

that determines all of the correlation exponents of the interacting electronic subsystem uncoupled from the ions.[9] The parameter g in (2) is unity for the free fermions (Fermi-liquid picture); for repulsive interactions one has $g<1$, while for attractive interactions the inverse inequality $g>1$ holds.[10] In writing (1) we neglected all irrelevant (in renormalization-group sense) terms.

The nonharmonic terms of the action (1) represent the moiré pattern of the electron and ion periodicities. The long-wavelength ($|u'|$, $|v'| \ll 1$) Action (1) is valid on scales exceeding both the interelectron (n^{-1}) and interion (ρ^{-1}) average spacings. A detailed derivation of (1) will be given elsewhere;[11] however, the functional form (1) (with some undetermined phenomenological parameters) can be understood as follows. Assuming the long-wavelength spectrum of the electronic liquid uncoupled from the ions to be of acoustic type with sound velocity $(K_2/K_1)^{1/2}$ determines the K part of the action; C_2 is the elastic constant for the ions. Introducing a short-range interaction between the subsystems gives rise to two interaction effects. First, regarding the two systems as continuous media, there will be a gradient coupling between u and v; the term $2\rho nV\, u'v'$ in (1) is the lowest-order term of this type [the prefactor comes from a perturbative expansion and is valid for $(\rho nV)^2 \ll K_2C_2$]. Moreover, each subsystem consists of discrete particles with some average spacing; each creates an effective periodic potential for the other population, and the effect is described by the sum in (1).

Our ultimate goal is to understand the ground state of the electron-ion system in the presence of the weak electron-ion interaction V (we will assume $n^2|V|/K_2 \ll 1$). Peierls[1] realized that a distortion of the ion positions creating a Fourier component of the electron-ion potential commensurate with the electrons could lead to a band gap at the Fermi surface, lowering the energy.

We will show how this effect arises from action (1). With $v=0$ (and $n \neq \rho$) the last term would be irrelevant under renormalization of the field u; but a static modulation $v=v_0(x)=\delta \sin 2\pi(n-\rho)x$ (with a small amplitude δ to be determined) gives a potential with a $k=0$ Fourier component, and thus acts like a commensurate potential.

The distortion of the ion subsystem will cause the electronic liquid to distort as well, due to the gradient terms. The equilibrium positions of the electrons are shifted, requiring the introduction of an electronic displacement field $w=u+\rho nVv_0(x)/K_2$; this eliminates the term linear in u'; so that the part of the integrand of (1) dependent on spatial derivatives takes the form $(K_2/2)w'^2+(C_2/2)[1-(\rho nV)^2/K_2C_2]v_0'^2$, from which the V^2 correction can be dropped. At the same time the integrand of the last term of (1) transforms into $\cos 2\pi((n-\rho)x-nw+\rho v_0[1+(n^2V/K_2)])$, which for small δ and V reduces to $\pi\rho^2 n\delta|V|\cos 2\pi nw+$ irrelevant terms. Thus (1) reduces to the form

$$A=\frac{1}{2}\int dx\, dt(K_1\dot{w}^2+K_2w'^2) -2\pi\rho^2 n|V|\delta\int dx\, dt \cos 2\pi nw+\int dx\, dtE_{\mathrm{el}}(\delta), \tag{3}$$

where

$$E_{\mathrm{el}}(\delta)=\frac{C_2[2\pi(n-\rho)]^2}{4}\delta^2 \tag{4}$$

is the increase in the elastic energy due to the distortion.

The prefactor of the cosine term in (3) can be taken to be positive, since the sign of this term can be reversed by a homogeneous shift of the field w. Thus, regardless of the sign of the electron-ion interaction, the commensuration of electron and ion populations lowers the system energy; this lowering can compensate for the increase of the elastic energy. The resulting decrease in the energy will now be calculated, regarding δ to be a fixed parameter. This gives an energy expression similar to the Landau free-energy[12] expansion, with δ being the order parameter. Then we will discuss the conditions under which the minimum energy occurs for nonzero δ.

The part of action (3) dependent on the field w is a standard sine-Gordon theory, and the evolution of its parameters under a renormalization-group transformation is described by the Kosterlitz equations[13]

$$\frac{d\nu}{\nu}=(2-g)\frac{da}{a}, \tag{5a}$$

$$dg=-g^3\nu^2\frac{da}{a}, \tag{5b}$$

$$dE=-\frac{\hbar^2 n}{m}\nu^2\frac{da}{a^3}. \tag{5c}$$

Nonuniversal numerical factors of order unity dependent on the cutoff procedure have been dropped from (5b) and (5c). Here a is the current length scale, and the parameter ν is the dimensionless amplitude of the cosine term in Eq. (3): $\nu=(2\pi\rho^2 n|V|\delta a^2/\hbar)(K_1/K_2)^{1/2}=(2\rho^2a^2mg/\hbar^2)|V|\delta$; it is conveniently regarded as a measure of the distortion δ, but we will later need to notice that it is also linear in $|V|$. Equations (5) are valid for $\nu(a) \ll 1$. The macroscopic behavior of the system is determined by the solution of Eqs. (5) in the limit $a\to\infty$, where the "initial" scale a_0 is set by the interelectron distance n^{-1}. Equation (5c) describes the contribution to the ground-state energy of the short-wavelength degrees of freedom that have been integrated out.

According to Eq. (5a), the induced potential ν is relevant whenever the parameter g is less than 2; then there is a gap in the excitation spectrum of action (3). The energy gap will suppress the quantum fluctuations on scales exceeding the correlation length ξ, which we will take to be the scale a at which $\nu(a)=1$. For scales less than ξ, $\nu(a) \ll 1$, and (for $g<2$) we can ignore the renormalization of g described by Eq. (5b). Then the solution to (5a) has the form $\nu(a)=\nu_0(a/a_0)^{2-g}$, where ν_0 is the "initial" value of ν, evaluated with microscopic parameters (in particular $a_0=n^{-1}$): $\nu_0=(2\rho^2mg/\hbar^2n^2)|V|\delta$. This determines $\xi n \cong \nu_0^{-1/(2-g)} \cong (\rho^2mg/\hbar^2n^2)^{-1/(2-g)}(|V|\delta)^{-1/(2-g)}$.

The elementary excitations of action (3) for $g<2$ are soliton-antisoliton pairs of the sine-Gordon theory, so that the energy gap Δ is twice the soliton energy. The latter can be estimated as $K_2\int dx\, w_0'^2$, where $w_0(x)$ is a profile corresponding to the presence of a single soliton. Using the fact that $w_0(x)$ is a constant almost everywhere excepting the region of width ξ over which it varies by $1/2\pi n$, we find

$$\Delta \cong K_2\xi(n\xi)^{-2} \cong (\hbar^2n^2/mg^2)(\rho^2mg/\hbar^2n^2)^{1/(2-g)} \times(|V|\delta)^{1/(2-g)} \tag{6}$$

in agreement with Refs. 3.

Integrating Eq. (5c) with $\nu(a)=\nu_0(a/a_0)^{2-g}$ from $a_0=n^{-1}$ to $\xi\cong n^{-1}v_0^{-1/(2-g)}\cong n^{-1}(\rho^2 mg|V|\delta/\hbar^2 n^2)^{-1/(2-g)}$, and omitting an overall undetermined factor of order unity, for the energy change arising from the commensuration of electron and ion populations we find

$$E_{\rm com}(\delta\propto\nu_0)\cong-\frac{\hbar^2 n^3}{m(1-g)}\,[\nu_0^{2/(2-g)}-\nu_0^2]. \qquad (7)$$

For the marginal free-fermion case $g=1$, this reduces to $E_{\rm com}\cong(\hbar^2 n^3/m)\nu_0^2\ln\nu_0\propto\delta^2\ln\delta$; combining this with the elastic energy (4) reproduces the standard conclusions on the Peierls effect for free fermions:[1,2] for a range of small δ, $E_{\rm com}$ lowers the energy more than $E_{e1}\propto\delta^2$ raises it, so that the minimum energy occurs for nonzero distortion δ. Voit and Schulz[7] extracted an expression analogous to (7) from the exact solution of the massive Thirring model.[8]

For general $g\neq1$ the combination of (4) and (7) leads to our main result

$$E(\delta)=\mathscr{A}\delta^2+\mathscr{B}\,\frac{V^2\delta^2}{1-g}-\mathscr{C}\,\frac{(|V|\delta)^{2/(2-g)}}{1-g}, \qquad (8)$$

where $\mathscr{A}\cong C_2(n-\rho)^2$, $\mathscr{B}\cong(\hbar^2 n^3/m)\ (\rho^2 mg/\hbar^2 n^2)^2$, and $\mathscr{C}\cong(\hbar^2 n^3/m)\ (\rho^2 mg/\hbar^2 n^2)^{2/(2-g)}$ are positive constants.

For repulsive electron-electron interactions ($g<1$), the minimum $E(\delta)$ is given by a distortion

$$\delta_{\rm eq}\cong\left(\frac{\mathscr{C}}{\mathscr{A}(1-g)(2-g)}\right)^{(2-g)/2(1-g)}|V|^{1/(1-g)} \qquad (9)$$

in the limit $|V|\to0$. Combining (6) and (9) we find that the energy gap Δ is proportional to the equilibrium distortion: $\Delta\propto\delta_{\rm eq}\propto|V|^{1(1-g)}$. We conclude that repulsive electron-electron interactions ($g<1$) in general enhance the Peierls effect, as has been previously proposed.[5–7]

For attractive electron-electron interactions ($g>1$) the second term of (8) is the leading contribution coming from the commensuration effects, and is negative, while the last term is positive. For very small $|V|$ the minimum of (8) occurs at $\delta_{\rm eq}=0$, and the Peierls instability is suppressed in accordance with previous results.[4–6] However, another possibility arises for finite $|V|$: the sign of the term quadratic in δ will change for sufficiently large $|V|$, giving a second-order phase transition from a normal metal to a Peierls insulator stabilized by the last term. For g, close to unity (weak electron-electron attraction) the sign change occurs for $|V_c|\propto\sqrt{g-1}\ll1$, and thus lies within the range of validity of our theory. Minimizing (8) for $V^2\geqslant V_c^2$, we find the critical dependence of the equilibrium distortion

$$\delta_{\rm eq}\propto(V^2-V_c^2)^{(2-g)/2(g-1)}. \qquad (10)$$

Combined with Eq. (6), this gives the critical behavior of the energy gap $\Delta\propto\delta_{\rm eq}^{1/(2-g)}\propto(V^2-V_c^2)^{1/2(g-1)}$.

In conclusion, we have constructed a phenomenological theory of the Peierls effect in one-dimensional quantum fluids that treats the electron-electron interaction nonperturbatively. The only microscopic parameter entering our formulas is the amplitude of the electron-ion interaction. The most important effect of the electron-electron interactions is accumulated in the parameter g (2) that determines the majority of the physics and all the exponents we found here, just as it governs the behavior of all correlation functions of a one-dimensional electronic liquid in the undistorted state. Therefore any one-dimensional many-body system (including repulsive bosonic models) that can be described macroscopically as a harmonic liquid (i.e., having its own g) is covered by this theory. For example, the perturbative results of Krivnov and Ovchinnikov[5] can be recovered by expanding the expression (8) near $g=1$ to lowest order in $1-g$, and then expressing $1-g$ in terms of the amplitude of electron-electron interaction. We also note that the ideas presented here can be readily generalized to the case of spin-$\frac{1}{2}$ quantum liquid.[11]

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