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Influence of long-range Coulomb interaction on the metal-insulator transition in one-dimensional strongly correlated electron systems

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We study the influence of long-range Coulomb interactions on the properties of one-dimensional (1D) strongly correlated electron systems in the vicinity of the metal-insulator Mott-Hubbard phase transition. It is shown that, in the metallic phase, the standard square-root singularity of the compressibility at the transition point changes to a logarithmic one, due to the formation of a 1D Wigner crystal of solitons (holons). On increasing the soliton density in a finite-size chain, the behavior of the compressibility reflects a sequence of crossovers between classical, low-density regimes of perfectly or nearly ordered Wigner-crystal states, and quantum regimes of a nearly free Fermi gas of solitons, followed (in the high-density limit) by a liquid phase of strongly correlated solitons. In a mesoscopic situation, where the screening length in a 1D chain is controlled by a massive electrode (gate) placed near the chain, there is a narrow region near the transition point where quantum fluctuations melt the Wigner crystal and recover the universal square-root singularity of the compressibility. Strong Coulomb interaction affects the formation of the charge excitations in the insulating phase, transforming the sine-Gordon solitons into quasiclassical Coulomb solitons. Multiplicative logarithmic renormalizations of the characteristic soliton size and rest energy are found.

I. INTRODUCTION

The metal-insulator transition induced by strong correlations in an electron system is a problem of continuing theoretical interest. In recent years, this problem has become particularly important in connection with the discovery of high-temperature superconductivity and subsequent attempts to develop a consistent theory of this phenomenon.[1]

It is well known that the one-dimensional repulsive Hubbard model

$$H = - t \sum_{i,\sigma} (c_{i\sigma}^{\dagger} c_{i+1,\sigma} + \text{H.c.}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \qquad (1)$$

is a prototypical model in which analytical description of the dynamics of the Mott-Hubbard transition is available on the basis of its exact solution and well developed nonperturbative methods. At exactly half filling (one electron per site), the model (1) describes a Mott insulator with a charge gap in the excitation spectrum. At weak interaction, $U \ll t$, when the bare single-particle spectrum can be linearized about two Fermi points and the bosonization method is applicable,[2,3] the low-energy part of the charge sector can be mapped onto a quantum sine-Gordon (SG) field theory given by the Hamiltonian[4] (see also Refs. 5 and 6),

$$H_{\rm SG} = \int_0^L dx \left[\frac{c_s}{2} [\Pi^2 + (\partial_x \varphi)^2] + \frac{\omega_0^2}{\beta^2 c_s} \, (1 - \cos\beta\varphi) \right] . \qquad (2)$$

Here, c_s is the velocity of the charge excitations, $\Pi(x)$ is the momentum density conjugate to the scalar field $\varphi(x)$, and the coupling constant $\beta^2 = 8\pi$.[7] The cosine term in Eq. (2) originates from the Umklapp scattering of electrons with momentum transfer $4k_F = 2\pi/a_0$, where a_0 is the lattice constant. The massive charge excitations, or "holons," are then identified as topological solitons of model (2), the local holon density thus being defined as

$$\rho_s(x) = (\beta/2\pi) \partial_x \varphi(x). \qquad (3)$$

The metallic phase of the Hubbard model, realized at finite deviations from half filling, is described by the SG model in the sector with a finite density n_s of the topological charge.[8] When the chemical potential term $-\mu L n_s$ is added to $H_{\rm SG}$, the transition to the metallic phase occurs at the threshold value of μ equal to the charge gap $\Delta = m_s c_s^2$, m_s being the soliton rest mass.

At low holon densities, $n_s\xi_0 \ll 1$, where $\xi_0 = \hbar c_s/\Delta$ is the characteristic quantum soliton length, interaction between the solitons is weak.[8,6] Therefore, the properties of the system near the transition are completely determined by Fermi statistics of massive quantum solitons. In particular, the compressibility of the system has a universal square-root singularity $\kappa \sim (\mu - \Delta)^{-1/2}$, typical for quantum commensurate-incommensurate transitions in one space dimension.[9–11]

Notice that, within a classical description, a soliton system with a finite density would form a lattice at zero temperature.[12] However, quantum fluctuations representing the Goldstone mode of the soliton lattice destroy the periodic structure. Therefore, in one-dimensional (1D) electron systems, irrespective of the strength of the interaction, the transition to the Mott phase always occurs from a disordered phase, provided the interaction between the electrons is short ranged.

In this paper, we shall be interested in qualitative changes in the above described conventional picture of the metal-insulator transition in a 1D correlated electron system, caused by long-range Coulomb interaction. The effects of long-range Coulomb forces need to be taken into account for an isolated electron chain, where the Coulomb interaction remains unscreened,[13] or in a "mesoscopic" situation, where the screening length in a 1D chain is controlled by its distance $D < L$ from a massive electrode (gate) and can be made very large (see, e.g., Ref. 14).

In Sec. II, we shall consider the case of a weak Coulomb interaction, characterized by small dimensionless coupling constant $\alpha = e^2/\hbar c_s = \xi_0/a_B$, where $a_B = \hbar^2/e^2 m_s$ is the Bohr radius. We shall, therefore, assume that the Coulomb interaction does not affect significantly the insulating Mott phase of the system and focus on the influence of the long-range forces on the soliton dynamics in the metallic phase by adding to $H_{\rm SG}$ the Coulomb energy of interacting solitons:[13]

$$H_C = \frac{e^2\beta^2}{8\pi^2}\int dx \int dy \frac{\partial_x\varphi(x)\partial_y\varphi(y)}{\sqrt{(x-y)^2+\lambda^2}}. \quad (4)$$

Here, λ is a transverse dimension of the system.

The basic effect of the unscreened repulsive Coulomb forces in the metallic phase is the formation of a Wigner crystal (WC) of solitons.[13] Strictly speaking, in a 1D infinite chain of charges, the $1/r$ interaction does not fall off fast enough to remove the infrared divergence in the density-density correlation function. However, as shown in Ref. 11, the $4k_F$ part of the correlator, describing the density oscillations with a period equal to the average spacing between the solitons, decays slower than any power law, thus making it reasonable to speak of a nearly ordered state. At low densities $n_s a_B \ll 1$, the Wigner lattice with period $a \equiv n_s^{-1}$ is not destroyed at exponentially large distances $L \le L_m$, where

$$L_m \sim a \exp(\text{const}/n_s a_B). \quad (5)$$

Therefore, one can expect that in finite-size (mesoscopic) samples the "holons" form a WC with true long-range order, so that the transition to the insulating phase takes place from the Wigner-crystal phase.

Note that, in the absence of impurities producing pinning of the WC, the soliton lattice can freely slide along the one-dimensional channel. Therefore, in the ideal system, the response of the soliton WC to a low-frequency electric field is identical to that of a Fermi gas of solitons. On the other hand, it is clear that thermodynamic properties of the two systems should be different. We show that upon crystallization of solitons in an isolated chain, taking place near the transition to the insulating phase, the square-root singularity of the compressibility at the transition point is changed by a logarithmic one, $\kappa \sim 1/\ln[L(\mu-\Delta)/e^2]$. Using simple arguments based on the comparison of relative contributions of the classical Coulomb energy of the 1D WC and quantum effects, we show that, on increasing the density of solitons ("holons"), the behavior of the compressibility reflects a sequence of crossovers between classical, low-density regimes of perfectly ($L < L_m$) and nearly ($L > L_m$) ordered WC states, and a quantum regime of a nearly free Fermi gas of solitons, which in the high-density limit $n_s\xi_0 \gg 1$ is followed by the liquid phase of strongly correlated solitons.

The presence of a large electrode near the chain does not lead to qualitative changes in the weak screening limit $n_s D \ge 1$. However, in the strong screening case, $n_s D \ll 1$, the above logarithmic behavior of the compressibility is replaced by a power law, $\kappa \sim (\mu - \Delta^*)^{-2/3}$, Δ^* being a renormalized gap. We also show that there exists a vicinity of the transition point where quantum fluctuations melt the Wigner lattice and recover the universal square-root singularity of κ.

In Sec. III, we turn to the case of strong Coulomb interaction, $(\xi_0/\lambda)\alpha \gg 1$, affecting the formation of the topological excitations and magnitude of the gap in the insulating phase. In this case, the charge excitations may be called Coulomb solitons: they become heavier ($\Delta_C \gg \Delta$) due to the strong electrostatic energy, and extended ($\xi_C \gg \xi_0$) due to the unscreened Coulomb repulsion of charges "inside" the soliton. The behavior of the Coulomb solitons in the conduction band at $\mu > \Delta_C$ differs from that described above. Namely, at low densities, $n_s\xi_C \ll 1$, the Coulomb solitons still condense into a Wigner crystal and display the logarithmic threshold singularity of the compressibility. However, at densities $n_s\xi_C \ge 1$, but still much lower than a_B^{-1}, the Wigner lattice is transformed to a sine-Gordon soliton lattice. The compressibility saturates at values $\kappa \sim (\Delta_C\xi_C)^{-1}$, characteristic for a charge-density wave. In the Appendix, we prove that the soliton system with strong Coulomb interaction can be treated quasiclassically at *arbitrary* values of β, thus justifying the applicability of results obtained in Sec. III, to the Hubbard model ($\beta^2 = 8\pi$).

II. WEAK LONG-RANGE COULOMB INTERACTION IN THE METALLIC PHASE

In this section, we consider the influence of a weak ($\alpha \ll 1$) long-range Coulomb forces on the properties of the metallic phase near the transition to the insulating state. In what follows, we shall assume that the transition is of the Mott-Hubbard type, although our conclusions remain valid for any one-dimensional charged system near the commensurate-incommensurate transition. For example, one can imagine a 1D system of spinless interacting particles moving in a periodic potential and consider the case when the period is close to the mean interparticle distance (see, e.g., Ref. 15).

Assuming that the transverse width of the chain $\lambda \gg \xi_0$, we expect that weak Coulomb interaction does not affect intrinsic characteristics of the solitons, but changes the character of interaction between them at distances $|x| \gg \lambda$. Treating then the solitons as pointlike objects, forming at low densities a Wigner lattice,

$$\rho_s(x) \simeq \sum_{i=1}^{N_s} \delta(x - ia), \tag{6}$$

we shall take into account the long-range repulsive forces by adding the Coulomb interaction energy (4) to the total energy of the system.

Here, it is worth stressing that by doing this, one assumes tacitly the violation of the charge neutrality of the chain. Such a situation occurs usually in mesoscopic semiconductor devices (quantum wires and dots), where electrons and the positive background charge are spatially separated [see, e.g., review (Ref. 14)]. In what follows, we will assume this kind of experimental setup.

The noncompensated (in the range accessible for electrons) charge may be associated, for instance, only with electrons above commensurate filling (this very case is considered below). However, from the general point of view the commensurate (dielectric) state can be assumed charged as well. It should be noted that the total electrostatic energy plays a different role in the two cases considered. In the metallic phase, it is the energy that determines the minimal energy charge distribution (which is a perfect Wigner crystal at low densities). On the contrary, in the commensurate phase, charge distribution is fixed by underlying lattice (or by periodic external potential). Then, the total electrostatic energy enters the free energy of finite-size charged dielectric system as a nonvarying quantity and can be omitted when studying the intrinsic properties (such as gap for the charged excitations) of the commensurate phase. Nevertheless the long-range forces between particles can lead to (finite) gap renormalization. It is the case of strong Coulomb interaction that will be studied in the next section.

We first recall the standard picture of the Mott-Hubbard transition in an isolated chain in the absence of long-range interactions. Near the transition point, $(\mu - \Delta)/\Delta \ll 1$, the limit of low soliton density is realized, $n_s\xi_0 \ll 1$, and the properties of the system approach those of a free spinless Fermi gas. The ground state energy (per unit length) is given by the expansion

$$\mathcal{E}_0(n_s) = \Delta n_s \left[1 + \frac{\pi^2}{6}(n_s\xi_0)^2 + 0(n_s\xi_0)^3\right] - \mu n_s, \tag{7}$$

leading immediately to the square-root singularities in the equilibrium density of holons and compressibility near the phase transition to the insulating phase:[9,10]

$$n_s(\mu) = \frac{\sqrt{2\Delta}}{\pi\hbar c_s}\sqrt{\mu - \Delta}, \qquad \kappa = \frac{\sqrt{\Delta/2}}{\pi\hbar c_s}\frac{1}{\sqrt{\mu - \Delta}}. \tag{8}$$

Let us now take into account the long-range Coulomb interaction. Using Eqs. (3), (4), and (6), one estimates the electrostatic energy of a finite-size WC of solitons as

$$\mathcal{E}_{\rm Coul}(n_s) \simeq e^2 n_s^2 \ln(n_s L). \tag{9}$$

Comparing this with the kinetic energy of the solitons, given by the second term in the right-hand side of Eq. (7), we find that the Coulomb effects are dominant, if $n_s \ll a_B^{-1}\ln(L/a_B)$. (The same criterium could have been obtained by estimating quantum corrections to the energy of the WC caused by zero-point fluctuations.) At these densities, instead of (7), for the total energy we get

$$\mathcal{E}_{\rm WC} = (\Delta - \mu)n_s + e^2 n_s^2 \ln(n_s L). \tag{10}$$

In the region $n_s a_B < \ln^{-1}(L/a_B)$, where the condition $L < L_m$ is satisfied, with the length L_m given by Eq. (5), the soliton system forms a long-ranged ordered WC. Thus, the transition to the insulating Mott phase occurs from the ordered WC phase, the latter being characterized by a logarithmic singularity of the compressibility,

$$n_s = \frac{\mu - \Delta}{2e^2}\frac{1}{\ln[L(\mu - \Delta)/e^2]}, \qquad \kappa = \frac{1}{2e^2}\frac{1}{\ln[L(\mu - \Delta)/e^2]}. \tag{11}$$

It is assumed in Eqs. (12) that the deviation $\mu - \Delta$ exceeds the Coulomb energy e^2/L.

The results (12), reflecting the dominant role of the Coulomb effects, are valid for a much wider interval of the densities, $n_s a_B \ll \ln(L/a_B)$, although at $n_s \sim a_B^{-1}$, true crystalline long-range order is already lost, and the soliton system occurs in a quasiordered, "Wigner-liquid"-like state, in which the density-density correlations fall out slower than any power law:[13] $\langle\rho(x)\rho(0)\rangle \sim \cos(2\pi n_s a)\exp[-C\sqrt{n_s a_B \ln(n_s|x|)}]$. At higher densities, quantum effects become dominant. If the Coulomb interaction is so weak that the condition $\alpha\ln(L/a_B) \ll 1$ is satisfied, further increase of the density brings it first to the interval $a_B^{-1}\ln(L/a_B) \ll n_s \ll \xi_0^{-1}$, where the thermodynamic properties of the soliton system are close to those of a free Fermi gas of low density. In this region, the compressibility follows the square-root behavior, Eqs. (8). On further increasing the density, the high soliton-density limit is eventually reached, $n_s\xi_0 \gg 1$, where the short-range interaction between the solitons becomes significant. The system occurs in a strongly incommensurate liquid phase.[8] If, on the other hand, $\alpha\ln(L/a_B) \geq 1$, the low-density regime of nearly free quantum solitons cannot be realized.

Now we consider a more interesting situation typical for "mesoscopic" experiments, when a massive metallic electrode (gate) is placed at the distance D ($\lambda \ll D \ll L$) from the chain. The electrode provides screening of the Coulomb interaction, which becomes strong at $n_s D \ll 1$, leading to recovery of the quantum behavior of the soliton system near the transition.

The classical electrostatic energy of the lattice, with the electrode screening effect taken into account, equals[16]

$$\mathcal{E}_{\text{Coul}} = \frac{e^2 n^2}{2}\left[\sum_{i\neq 0}\frac{1}{|i|} - \sum_{i=-\infty}^{\infty}\frac{1}{\sqrt{i^2+(2D/a)^2}}\right] = e^2 n^2\left[\ln(nD) + C - 2\sum_{k=1}^{\infty}K_0(4\pi k n D)\right], \quad (12)$$

where C is the Euler constant, and $K_0(x)$ is the Macdonald function.

In the weak screening limit, $n_s D \gg 1$, from (12) one finds

$$\mathcal{E}_{\text{Coul}} \simeq e^2 n_s^2 \ln(n_s D). \quad (13)$$

This expression differs from Eq. (9) only in the replacement $L \to D$. Therefore, as long as the soliton density satisfies the condition $n_s \gg D^{-1}$, all the above described results concerning the sequence of crossovers between different regimes in an isolated chain, together with the corresponding changes in the behavior of the compressibility, remain valid in this case as well.

In the strong screening limit, $n_s D \ll 1$, the density dependence of the Coulomb energy (12) is changed by

$$\mathcal{E}_{\text{Coul}} \simeq n_s\left(-\frac{e^2}{4D}\right) + 2\zeta(3)(eD)^2 n_s^4. \quad (14)$$

As a result, the logarithmic behavior of the compressibility, Eq. (12), is changed by a power law:

$$n_s = \left[\frac{\mu-\Delta^*}{8\zeta(3)(eD)^2}\right]^{1/3}, \quad \kappa^{-1} = 3(8\zeta(3))^{1/3}\left[(eD)^2(\mu-\Delta^*)\right]^{2/3}, \quad (15)$$

where $\Delta^* = \Delta - e^2/4D$. The last formula describes an additive renormalization of the charge gap caused by the image forces (see, e.g., Ref. 17) which is small for a weak Coulomb coupling.

The range of applicability of Eqs. (15) is easily estimated as $a_B D^{-2} \ll n \ll a_B^{-1}$; in this interval, quantum corrections to (14) are small. However, at lower densities, $n_s \leq a_B D^{-2}$, the Wigner lattice is destroyed locally by quantum fluctuations. Therefore, there is a region near the threshold, $\mu - \Delta^* < (e^2/D)(a_B/D)^3$, where the universal square-root singularity of the susceptibility, characterizing the quantum commensurate-incommensurate transition, is recovered.

III. STRONG COULOMB INTERACTION

For strong Coulomb coupling, $\alpha \geq 1$, the characteristic (Bohr) radius a_B turns out to be shorter than the correlation length ξ_0, indicating the possibility of strong renormalization of the characteristics of single solitons by Coulomb interaction. From physical considerations one expects that, in this limit, solitons become heavier and extended, i.e., the effective correlation length ξ_C, being the size of the "Coulomb" soliton, may substantially exceed ξ_0. We shall study this situation assuming that $\lambda \leq \xi_0$.

A consistent solution of this problem suggests introducing the long-range Coulomb interaction at the level of the Hubbard model (1) and calculating the resulting spectrum of the charge excitations in such a system. However, for a half-filled system, repulsive Coulomb effects can only increase the charge gap. For this reason, reduction of the problem to the sine-Gordon model still remains reasonable. First, we shall study the effect of Coulomb forces on topological solitons of the quasiclassical sine-Gordon model. Then, we shall present arguments explaining the applicability of the obtained results to the holon dynamics in the Hubbard model (see also Appendix).

We shall be interested in topological solitons of the sine-Gordon model (2) extended to include long-range Coulomb interaction (4):

$$H = H_{\text{SG}} + H_C. \quad (16)$$

At $\beta^2 \ll 1$ the model is quasiclassical, and the excitations we are interested in can be found by using trial functions. A trial function, describing a static topological soliton $\Delta\varphi \equiv \varphi(x=+\infty) - \varphi(x=-\infty) = 2\pi/\beta$, will be chosen in the form corresponding to the sine-Gordon model:

$$\varphi_C(x) = \frac{4}{\beta}\arctan\left[\exp\left(\frac{x-x_0}{d^*}\right)\right]. \quad (17)$$

Here, x_0 is the center of the soliton, and d^* is a variational parameter that determines the soliton size. Its value is found by minimizing the soliton rest energy:

$$E(d^*) = \frac{\hbar}{c_s}\int_{-\infty}^{\infty}dx\left[\frac{c_s^2}{2}(\partial_x\varphi_C)^2 + \frac{\omega_0^2}{\beta^2}(1-\cos\beta\varphi_C)\right] + \frac{e^2\beta^2}{8\pi^2}\int\int dx\, dy\,\frac{\partial_x\varphi_C(x)\partial_y\varphi_C(y)}{\sqrt{(x-y)^2+\lambda^2}}. \quad (18)$$

Substituting (17) into (18) and doing the integrals, we easily find that, for a weak coupling $\alpha \ll 1$, the parameter d^* coincides with the size of an unperturbed kink, $d^* = d_0 = c_s/\omega_0$, $E(d^*) = E_s = 8\hbar\omega_0/\beta^2$. For strong coupling, $\alpha \geq 1$, the unscreened Coulomb interaction leads to multiplicative renormalizations of the size and energy of the soliton:

$$d^* = d_0\left(\alpha\frac{\beta^2}{2\pi^2}\right)^{1/2}\ln^{1/2}\left[\frac{d_0}{\lambda}\sqrt{\alpha\frac{\beta^2}{2\pi^2}}\right] \gg d_0, \quad (19)$$

$$E_C = \frac{8\hbar\omega_0}{\beta^2}\left(\alpha\frac{\beta^2}{2\pi^2}\right)^{1/2}\ln^{1/2}\left[\frac{d_0}{\lambda}\sqrt{\alpha\frac{\beta^2}{2\pi^2}}\right] \gg E_0. \quad (20)$$

Let us show that expression (20) can be obtained within a consistent scheme, using solutions of the sine-Gordon equations. For a linearized problem, the Coulomb interaction can be taken into account exactly, leading to a modification of the spectrum of small perturbations ("optical phonons") of the field φ (see, e.g., Ref. 13),

$$\omega^2(k) = \omega_0^2 + k^2 c_s^2 \left[1 + \alpha \frac{\beta^2}{2\pi^2} K_0(k\lambda)\right]. \tag{21}$$

Since at $x \geq 1$ $K_0(x)$ is exponentially small, the Coulomb interaction mostly affects the long-wavelength dynamics, where the spectrum (21) takes the form

$$\omega^2(k) = \omega_0^2 + k^2 c_s^2(k), \tag{22}$$

with

$$c_s(k) = \left(\frac{\alpha}{2\pi^2}\right)^{1/2} \beta \ln^{1/2} \frac{1}{|k|\lambda}, \quad k\lambda \ll 1. \tag{23}$$

Expression (22), differs from the "phonon" spectrum of the unperturbed sine-Gordon equation in that the constant velocity c_s has been replaced by a momentum dependent effective "velocity" (23). Analyzing the structure of the last term in Eq. (18), one concludes that, when studying the influence of weakly screened ($\lambda \ll d_0$) Coulomb interaction on the topological soliton of the sine-Gordon model, it is sufficient to change the exact Hamiltonian, Eqs. (16), (2), and (4), by an approximate one in which the effects of Coulomb interaction are incorporated in a coordinate dependent velocity,

$$c_s^2 \to c^2(x - x_0) = c_s^2 \frac{\alpha\beta^2}{2\pi^2} \ln \frac{|x - x_0|}{\lambda}. \tag{24}$$

In Eq. (24), it is assumed that $|x - x_0| \gg \lambda$. For this reason, it is possible to neglect in all calculations terms containing derivatives of the "velocity," $|c'(x)/c(x)| \ll 1$. In the framework of such an "adiabatic" perturbation theory, the topological soliton has the standard form:

$$\varphi_C(x) = \pm \frac{4}{\beta} \arctan \left[\exp\left(\frac{x - x_0}{d(x)}\right)\right], \tag{25}$$

where the soliton size, d_0, is replaced by a coordinate dependent, smooth function $d(x) \equiv c(x)/\omega_0$. One can easily check that the energy of the Coulomb soliton (25) exactly coincides with Eq. (20).

Using the solution (25), the standard scheme of quasiclassical quantization can be easily developed (see, e.g., Ref. 18). It can be shown that the one-loop quantum correction to the classical energy of the Coulomb soliton has the same form as in the usual sine-Gordon model, $\Delta E_s = -\hbar\omega_0/\pi$. Within the traditional scheme of quasiclassical quantization of solitons of the SG model, the relative smallness of quantum corrections is provided by the small value of the coupling constant $\beta^2 \ll 1$. In our case, the solitons can be treated classically already, due to the large Coulomb energy. Therefore, it seems natural to expect that formula (20) remains valid for arbitrary values of β, including the "extreme quantum case" $\beta^2 \sim 8\pi$ (from the point of view of the usual SG model). This conjecture is confirmed in the Appendix where we show that, in the presence of long-range Coulomb forces, the small parameter controlling the onset of quasiclassical regime, is in fact $\beta/\sqrt{\alpha}$, and not β itself, as is the case for the "pure" SG model. This enables one to conclude that, in the strong-coupling case $e^2/\hbar c_s \gg 1$, the long-range Coulomb interaction leads to a multiplicative renormalization of the Mott-Hubbard gap,

$$\Delta \to \Delta_C = \Delta \sqrt{\frac{e^2}{\hbar c_s}} \ln^{1/2} \left(\frac{\xi_0}{\lambda} \sqrt{\frac{e^2}{\hbar c_s}}\right). \tag{26}$$

The appearance of fractional powers of a large logarithm is typical for various quantum problems that explicitly incorporate long-range Coulomb forces.[16,13,19]

Now we consider Coulomb solitons in the conduction band at $\mu > \Delta_C$. At low densities $n\xi_C \ll 1$, where

$$\xi_C \simeq \xi_0 \alpha^{1/2} \ln^{1/2} \left(\frac{\xi_0}{\lambda}\sqrt{\alpha}\right) \tag{27}$$

is the characteristic size of the Coulomb soliton, the charges in the conduction band can be considered as pointlike. The unscreened, long-range Coulomb interaction leads to the formation of a Wigner crystal, with the energy density and compressibility still given by formulas (9) and (12), respectively. On increasing the density $n \geq \xi_C^{-1} \ll a_B^{-1}$, the solitons start to overlap, thus gradually diminishing the role of long-range forces. The WC state crosses over to a classical SG lattice.

The energy density of such a classical lattice can be readily estimated, using well-known periodic solutions of the sine-Gordon model,

$$\varphi_p(x) = \frac{1}{\beta}\left\{\pi + 2am\left[\frac{x}{d^*}\frac{1}{k(n_s)}\right]\right\}. \tag{28}$$

Here, $am(z)$ is the elliptic amplitude, and $k(n)$ is the elliptic modulus fixed by the soliton density,

$$2kK(k) = (n_s d^*)^{-1}, \tag{29}$$

where $K(k)$ is the complete elliptic integral of the I order, and d^* is defined in Eq. (19). The energy density of the soliton lattice equals (see also Ref. 20)

$$E_p(n) = E_C \frac{n_s}{k} \left\{E(k) - \tfrac{1}{2}(1 - k^2)K(k)\right\} \tag{30}$$

[$E(k)$ is the complete elliptic integral of the II order].

Strictly speaking, expressions (28)–(30) are valid quantitatively in the high-density limit $n_s d^* \gg 1$ ($k \to 0$), where the lattice of strongly overlapping solitons smoothly transforms into a charge-density wave. The energy is then given by

$$E_p(n) \simeq \frac{\pi^2}{4}(\Delta_s d^*) n_s^2, \tag{31}$$

and the compressibility of the system is no longer dependent on the density: $\kappa^{-1} \sim \Delta_c d^* = \text{const}$.

IV. CONCLUSIONS

In conclusion, we have shown that long-range Coulomb forces drastically modify the properties of 1D electron systems in the vicinity of the metal-insulator phase transition. In the metallic phase, the long-range Coulomb interaction leads to the formation of a Wigner crystal of charged quasiparticles and, therefore, changes qualitatively the critical behavior of the system at the transition point. The properties of the insulating phase are also changed, if the Coulomb interaction is strong. In this case, the Mott-Hubbard gap is strongly renormalized, and the charged excitations in the Mott phase can be described as quasiclassical Coulomb solitons.

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APPENDIX

Let us rewrite our model, given by Eqs. (2) and (4), in the Langrangian formalism. Being interested in distances along the chain, much larger than its transverse dimension λ, we introduce the "Minkowsky" action in 1 + 1 dimensions:

$$S = \int d^2x \left\{ \frac{1}{2}(\partial_\mu \varphi)^2 + \frac{\omega_0^2}{\beta^2 c_s^2} \cos\beta\varphi \right\} -\alpha_C \beta^2 \int dx_0 \int dx_1 \int dx_1' \frac{\partial_{x_1}\varphi \, \partial_{x_1'}\varphi}{|x_1 - x_{1'}|}, \quad \text{(A1)}$$

where $x_\mu = (c_s t, x)$, $(\mu = 0,1)$, $\partial_\mu = \partial/\partial x_\mu$, and α_C is the dimensionless Coulomb coupling constant that differs from that introduced in the Introduction by a numerical coefficient. It will be proven in this appendix that strong Coulomb interaction ($\alpha_C \gg 1$) brings the model (A1) to a quasiclassical regime at arbitrary β. We shall first consider two simple cases.

(1) Case $\alpha_C = 0$. This case corresponds to the "pure" SG model. Following Ref. 21, we rescale the field,

$$\varphi = \frac{1}{\beta}\phi, \quad \text{(A2)}$$

to obtain

$$S_{\rm SG} = \frac{1}{2\beta^2} \int d^2x \left\{ (\partial_\mu \phi)^2 + \frac{\omega_0^2}{c_s^2} \cos\phi \right\}. \quad \text{(A3)}$$

Since in the Feynmann formulation of quantum mechanics, the action enters the path integral as $\exp(iS/\hbar)$, one immediately observes that the SG coupling constant β leads to an effective renormalization of $\hbar$: $\hbar \to \hbar\beta^2$. The quasiclassical limit, therefore, corresponds to the region of small β ($\beta^2 \ll 8\pi$)—the well-known fact in the theory of quantum SG model.[21]

(2) Case $\omega_0^2 = 0$. This model describes Coulomb effects in a Luttinger liquid, or equivalently, small quantum fluctuations in a 1D Wigner crystal.[13] Notice that in this case β has lost its SG meaning; it simply redefines the Coulomb coupling constant. Since at $\omega_0^2 = 0$ both terms of the action are bilinear in ϕ, rescaling of the field would be of no use. Therefore, we are left with possible (temporal and/or space) coordinate transformations:

$$x_\mu \to \lambda_\mu x_\mu \quad (\mu = 0,1). \quad \text{(A4)}$$

Then the action transforms to

$$S = \frac{1}{2}\int d^2x \left[\left(\frac{\lambda_1}{\lambda_0}\right)(\partial_0\varphi)^2 - \left(\frac{\lambda_0}{\lambda_1}\right)(\partial_1\varphi)^2 \right] -\alpha_C\beta^2 \left(\frac{\lambda_0}{\lambda_1}\right) \int dx_0 \int dx_1 \int dx_{1'} \frac{\partial_1\varphi\partial_{1'}\varphi}{|x_1 - x_{1'}|}.$$

(We see that there is actually one rescaling parameter, the ratio λ_0/λ_1. So in this case, it was sufficient to rescale either space or time.)

Let us choose

$$\frac{\lambda_1}{\lambda_0} = \sqrt{\alpha_C}\beta. \quad \text{(A5)}$$

Then

$$S = \sqrt{\alpha_C}\beta \left\{ \frac{1}{2}\int d^2x \left[(\partial_0\varphi)^2 - \frac{1}{\alpha_C\beta^2}(\partial_1\varphi)^2 \right] + \int dx_0 \int dx_1 \int dx_{1'} \frac{\partial_1\varphi \, \partial_{1'}\varphi}{|x_1 - x_{1'}|} \right\}. \quad \text{(A6)}$$

This representation has a very simple meaning. The overall prefactor is proportional to $\sqrt{\alpha_C}$. Therefore, large α_C have a tendency to drive the system to a quasiclassical regime. At the same time, we observe that the local gradient term $\sim (\partial_x\varphi)^2$ becomes of minor importance compared to the Coulomb one. This means that the spectrum of renormalized plasmons is entirely determined by the long-range Coulomb effects. In our paper, this is clearly seen in formula (21) (without ω_0^2 term), where one is allowed to drop 1 in the square brackets to obtain (22) (also without ω_0^2 term). The spectrum is simply given by[13]

$$\omega^2(k) \sim \alpha_C\beta^2k^2 \ln(1/|k|). \quad \text{(A7)}$$

(3) General case: $\alpha_C, \omega_0^2 \neq 0$. We now turn to the action (A1) and rescale the field and coordinates according to (A2) and (A4), respectively. We obtain

$$S = \frac{1}{\beta^2}\int d^2x \left\{ \frac{1}{2}\left(\frac{\lambda_1}{\lambda_0}\right)(\partial_0\phi)^2 - \frac{1}{2}\left(\frac{\lambda_0}{\lambda_1}\right)(\partial_1\phi)^2 + \lambda_0\lambda_1\frac{\omega_0^2}{c^2}\cos\phi \right\} - \alpha_C\left(\frac{\lambda_0}{\lambda_1}\right)\int dx_0 \int dx_1 \int dx_{1'} \frac{\partial_1\phi\,\partial_{1'}\phi}{|x_1 - x_{1'}|}. \quad \text{(A8)}$$

First, we define the ration λ_1/λ_0, requiring that

$$\frac{1}{\beta^2}\left(\frac{\lambda_1}{\lambda_0}\right) = \alpha_C\left(\frac{\lambda_0}{\lambda_1}\right). \quad \text{(A9)}$$

Then, we set $\lambda_0 = 1/\beta^2$ and arrive at the following expression for the action:

$$S = \frac{\sqrt{\alpha_C}}{\beta}\left\{ \int d^2x \left[\frac{1}{2}(\partial_0\phi)^2 - \frac{1}{2\alpha_C\beta^2}(\partial_1\phi)^2 + \frac{\omega_0^2}{c^2}\cos\phi\right] - \int dx_0 \int dx_1 \int dx_{1'} \frac{\partial_1\phi\,\partial_{1'}\phi}{|x_1 - x_{1'}|}\right\}. \quad \text{(A10)}$$

As expected, formula (A10) explicitely shows that the quasiclassical regime is controlled not by β, but by the ratio $\sqrt{\alpha_C}/\beta$. This means that we are able to approach the quasiclassical limit either in the standard, "sine-Gordon" way, i.e., by *decreasing* β, or in the "Coulomb" way, by *increasing* α_C. This is a direct confirmation of our guess (see Sec. III) that the soliton system with strong long-range Coulomb interaction behaves quasiclassically at *arbitrary* values of β. Second, the topological, cosine term has a standard amplitude, so that there is no special reason to neglect it even in the presence of strong Coulomb interaction. Its role becomes less important in the limit of large total topològical charge, i.e., high soliton-density limit; but this is the standard situation even for the "pure" SG model. And finally, the charge-density space correlations, including those between the solitons, as well as those responsible for the transformation of SG individual solitons into Coulomb ones, are mostly controlled by the Coulomb, triple-integral term, provided that $\alpha_C\beta^2 \gg 1$.

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