Incipient quantum melting of the one-dimensional Wigner lattice

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Abstract

A one-dimensional tight-binding model of electrons with long-range Coulomb interactions is studied in the limit where double site occupancy is forbidden and the Coulomb coupling strength \( V \) is large with respect to the hopping amplitude \( t \). The quantum problem of a kink–antikink pair generated in the Wigner lattice (the classical ground state for \( t = 0 \)) is solved for fillings \( n = 1/s \), where \( s \) is an integer larger than 1. The pair energy becomes negative for a relatively high value of \( V \), \( V_c/t \approx s^3 \). This signals the initial stage of the quantum melting of the Wigner lattice.

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1. Introduction

Three decades ago, Rice et al. have introduced nonlinear phase excitations of a charge-density wave condensate as a new type of charged states and referred to them as \( \eta \)-particles [1]. Their arguments were based on the peierls instability of a one-dimensional coupled electron–phonon system, in the limit where the charge-density wave amplitude is much smaller than the average electronic charge-density. Shortly after, Hubbard discussed qualitatively the role of dimer pairs (domain boundaries) in a nearly quarter-filled band with dominant long-range Coulomb interactions [2]. As we will argue, the two types of charged states are closely related.

We consider a one-dimensional system of spinless fermions described by the Hamiltonian

\[
H = -t \sum_{i} (c_{i}^{\dagger} c_{i+1} + c_{i+1}^{\dagger} c_{i}) + \sum_{\ell \geq 1} V \delta_{\ell} n_{\ell} n_{\ell+1},
\]

where \( c_{i}^{\dagger} \) and \( c_{i} \) are fermionic creation and annihilation operators, respectively, \( n_{i} = c_{i}^{\dagger} c_{i} \), \( \ell \) is the occupation number of site \( i \) and \( V \) = \( V/l \) represents the long-range Coulomb potential. Such a model may describe molecular compounds where the interaction between two (valence) electrons on the same molecule is so large that double occupancy can safely be discarded. The spin quantum number is then redundant because the exchange of two electrons is dynamically forbidden.

We have in mind systems where the average site occupancy is a rational number between 0 and 1, \( n = r/s \). Depending on the band filling the fermions then represent either electrons or holes. The classical ground state (\( t = 0 \)) is charge-ordered and forms a “generalized Wigner lattice” [2]. In the special case \( n = 1/s \), the unit cell contains \( s \) sites, one of which is occupied. A generalized Wigner lattice is clearly insulating and therefore the long-range Coulomb interactions remain unscreened. Insulating charge-ordered phases have been reported for organic chain compounds. For a collection of recent results see [3] and in several cases the nature of charge ordering is more likely that of a (small-amplitude) charge-density wave.

We have recently used a variational wave function for describing the modifications of the classical ground state (the generalized Wigner lattice) induced by a small but finite hopping term (\( t \ll V \)) [4]. Here we consider the same regime, but follow a different route by introducing the notion of charge defects, as was done in [5] in the case of...
electron-phonon interactions. Such defects occur in pairs (kinks–antikinks) and can be viewed as fractionally charged particles, in close analogy to the $\mathbb{Q}$-particles of Michael Rice.

2. Kink–antikink pair for $n = 1/2$

We start our discussion for a density $n = 1/2$. In order to guarantee overall charge neutrality we introduce a rigid compensating background ($n = 1/2$ charge of opposite sign at each site). The classical ground state in this case corresponds to alternating filled and empty sites (Fig. 1a). Note that this configuration, already at the classical level, is doubly degenerate, since exchanging the empty and occupied sites does not change the overall energy. The most simple antikink separated by a distance $2d$ sites.

The classical energy of a kink–antikink pair is readily evaluated. Introducing a pair of size $2d$, i.e. a kink and an antikink separated by a distance $2d$ (see Fig. 1), costs an energy

$$\Delta(d) = \sum_{p=0}^{\infty} \sum_{m=0}^{\infty} [V_{2m+1} + V_{2m-1} - 2V_{2m}].$$

This sum can be transformed into a power series in $1/2d$ with leading terms

$$\Delta(d) = \frac{V}{2} - \frac{V}{4}d^2 + \frac{V}{8}d^3.$$

Here the first term represents the creation energy of two well separated defects. The second term is the Coulomb attraction between kink and antikink with a coupling reduced by a factor of four as compared to the original Hamiltonian (1). Therefore, the defects carry effective charges $\pm 1/2$ (measured in units of the electronic charge). This result agrees with what one obtains by adding or subtracting an electron to the classical ground state configuration [2]. In fact, adding an electron at an empty site results in a high-energy configuration with a three-electron cluster. The energy is lowered by moving away one of these electrons, thus creating a pair of defects (two kinks in our language). Since the overall added charge is $-1$, each kink carries a charge $-1/2$. Similarly, removing an electron produces two antikinks, each of which carries a charge $+1/2$. The third term in Eq. (3) can be interpreted as the interaction of two dipole moments pointing in opposite directions parallel to the chain axis. The size of the dipoles is equal to the fractional charge times half a lattice constant, in our units $1/4$. We conclude that kinks and antikinks behave like fractionally charged particles with electric dipole moments. The dominant interaction is the Coulomb attraction, even at the shortest possible distance $2d = 2$.

We now turn to the quantum problem of a defect pair, i.e. we diagonalize the Hamiltonian within the subspace of states $[m,d]$, corresponding to a kink at site $m - d$ and an antikink at site $m + d$ (on thus indicates the center-of-mass of the pair). In general the effect of a hopping event on the state $[m,d]$ is either to move an existing defect by two lattice sites, which modifies both the size $(2d \rightarrow 2d \pm 2)$ and the center $(m \rightarrow m \pm 1)$ of the pair (see Fig. 1), or to create (annihilate) an additional pair. Restricting ourselves to the subspace of single-pair states, creation, and annihilation processes are forbidden and the quantum problem reduces to the eigenvalue equation

$$[H - \Delta(d)]\langle m,d \rangle + \langle m-1,d+1 \rangle + \langle m+1,d-1 \rangle = 0.$$  

The center-of-mass and relative motions can be separated by introducing the Bloch superposition

$$\langle \psi \rangle = \sum_{m,d \geq 1} e^{iKm} \langle \psi \rangle [m,d].$$

Introducing this Ansatz into Eq. (4) leads to the following eigenvalue equation for the wave function $\langle \psi \rangle (d)$,

$$E \langle \psi \rangle (d) = \Delta(d) \langle \psi \rangle (d) - 2\cos K \langle \psi \rangle (d + 1) + \langle \psi \rangle (d - 1),$$

$$d \geq 1.$$  

Seeking the lowest-energy excited state we restrict ourselves to the pair at rest ($K = 0$). The classical ground state (no defect pairs) is excluded by imposing the boundary condition $\langle \psi \rangle (0) = 0$. This eigenvalue problem can be treated to arbitrary accuracy numerically, but more insight is gained by solving it in the continuum limit, $\langle \psi (d) \rightarrow \phi (x), \langle \psi (d) \rightarrow \psi (x), \langle \psi (d+1) \rightarrow \psi (x+1), \langle \psi (d-1) \rightarrow \psi (x-1), \rangle \rangle$.

Neglecting the dipolar interaction in Eq. (3) we obtain the eigenvalue equation

$$\epsilon \langle \psi \rangle (x) = -\frac{d^2}{dx^2} \langle \psi \rangle (x) - \frac{V}{4|x|}\langle \psi \rangle (x),$$

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We seek an excited state which is orthogonal to the classical ground state. This is the natural procedure for estimating at which point in parameter space a trial ground state becomes the “wrong vacuum.”
ψ(channel, and the boundary conditions are also the same, eigenvalue equation of the hydrogen problem in the s-wave lowest-energy wave function of a pair, period as for the Wigner lattice[6]. Therefore the critical ble with respect to a charge-density wave with the same strength $V$, indicates a crossover between a Wigner lattice and a simple picture is available. Mean-field theory applied to the Hamiltonian (1) yields a ground state with a modulated charge-density $\langle \delta n_l \rangle = a \cos (ql + q_l)$, (11)

where $Q = 2k_l = 2\pi n$ for the case of spinless fermions, and $a < n$ for $V < t$. The phase $q_l$ is an arbitrary constant for an incommensurate situation (a irrational), but locked to one of $s$ possible values in the commensurate case, where $n = r/s$ with integer $r$ and $s$ [7]. Adding an electron to an incommensurate charge-density wave results in a slight shift of the wave vector $Q', Q' = \{l + (1/L)l\}Q$, where $L$ is the chain length. In view of Eq. (11), this effect can also be attributed to a phase shift $q_l' = 2\pi l/L$. For a commensurate case the phase achieves the change of $2\pi$ from $l = 0$ to $L$ through $s$ steps, i.e. there are $s$ $\delta$-particles, each of which carries a fractional charge $-1/s$.

Let us now return to the large $V$ limit and restrict ourselves to simple ratios $n = 1/s, s \geq 3$. In this case the classical ground state is $s$-fold degenerate and there are several types of domain walls separating the different configurations. It turns out that the low-energy domain walls are those which connect nearly ground state configurations, i.e. Wigner lattices where the locations of electrons differ by one lattice constant (see Fig. 2). These “kink” and “antikink” defects again occur in pairs. Repeating the arguments of the steps of the previous section, we evaluate the classical energy of a kink-antikink pair of size $sd$,

$$\Delta (d) = \sum_{p, l = 1, p} (V_{m+1} + V_{m-1} - 2V_m).$$ (12)

The summation can again be performed for large sizes, and we find up to first order in $1/sd$

$$\Delta (d) = \frac{V}{s} \left[ 1 - \frac{\pi}{s} \cot \left( \frac{\pi}{s} \right) \right] - \frac{V}{s} \frac{1}{sd}$$ (13)

The first term, the pair creation energy $\Delta_{\infty}$ at infinite separation, agrees with the corresponding quantity in Eq. (3) for $s = 2$. The second term corresponds to the Coulomb attraction for two particles with fractional charges $\pm 1/sd$ at a distance $sd$, in agreement with the counting argument presented above for the $\delta$-particles.
We can again use the continuum limit for calculating the lowest-energy quantum pair state for general \( s \). The wave function is again given by Eq. (8), but with a Bohr radius

\[
a_0 = \frac{4s^4}{\sqrt{V}}.
\]

Thus the pair size increases strongly with decreasing density \( n = 1/s \). Correspondingly, the binding energy decreases, as seen in the pair energy

\[
E_0 = -4t + \Delta_\infty - \frac{4s^2}{3V},
\]

where the first two terms dominate for large \( s \). In fact, for \( s \gg 1 \) we can safely use the asymptotic value

\[
E_0 \approx -4t + \frac{\pi^2}{3sV}
\]

(16)

to locate the crossover region, where this energy becomes negative. The result,

\[
V_c = \frac{12}{\pi^2 n^2}
\]

agrees well with our previous variational estimate [4]. This is not surprising because the creation of a pair can be achieved through a hopping event that moves a particle out of the ground state configuration. The probability of such a hopping event was evaluated in [4], and was used to determine a criterion for the instability of the generalized Wigner lattice.

In contrast to the case \( n = 1/2 \), for lower density this criterion does not signal a crossover to a small-amplitude charge-density wave, it rather indicates that part of the electronic charge is spilled over to neighboring sites of the classical Wigner lattice.

4. Discussion

In this paper we have determined the lowest-energy quantum state of a kink–antikink pair in a one-dimensional generalized Wigner lattice. We have calculated the critical value \( V_c \) of the interaction strength below which the pair energy is negative, and charge defects will be generated spontaneously. Kinks (or antikinks) are the strong-coupling analogs of the \( \phi \)-particles studied a long time ago by Rice et al. [1].

The true quantum ground state of electrons interacting through long-range Coulomb forces contains kink–antikink pairs due to quantum fluctuations, even above \( V_c \). It would be interesting to proceed from the single-pair solution to that of an arbitrary number of pairs. This step is highly non-trivial, although at first sight it looks similar to that from the Cooper problem to the BCS wave function. One of the difficulties arises from the mutual interactions between pairs, another from their non-local character.

If the density of pairs in the ground state is large enough, they lose their identity, and kinks and antikinks may move rather independently. In this case one can imagine a dc charge transport due to moving defects. Whether such a mechanism is responsible for the observed Drude peak in the Bechgaard salts [8] is an interesting open question.

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References