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QUANTUM MELTING ON A LATTICE AND A DELOCALIZATION TRANSITION

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ABSTRACT

We consider 1D and 2D gas of spinless fermions with the Coulomb and the short range interactions on a square lattice at $T = 0$. Using exact diagonalization technique we study finite clusters with up to 16 and in some cases up to 20 particles at filling factors $\nu = 1/2$ and $1/6$. By increasing the hopping amplitude we obtain the low-energy spectrum of the system in a wide range from the classical Wigner crystal to almost free gas of fermions. The most efforts are made to study the mechanism of the structural and insulator-metal transitions. We show that both transitions are determined by the energy band of the defect with the lowest energy in the Wigner crystal.

INTRODUCTION

The insulator-metal (IM) transition and the role of electron-electron interaction in this transition is a problem of permanent interest, both theoretical and experimental. It has been shown[1, 2, 3] that in the systems with strong disorder the interaction is in favor of delocalization because electrons may help each other to overcome the random potential. In clean systems the role of the interaction is opposite. It may create the so-called correlated insulator in a system which would be metallic otherwise. The Wigner crystal (WC) is a good example of such insulator.

WC in continuum is not an insulator itself, since it can move as the whole and carry current. However, due to shear modulus it can be pinned by a small disorder. The ground-state energy of the continuum WC and its zero-temperature melting was widely studied in the recent years both with and without magnetic field.[4]

In contrast to the continuum case, the WC on a lattice can be an insulator without any disorder due to the Umklapp processes in a host lattice. The WC on a lattice does not have any sound or soft plasma modes and its excitation spectrum has a gap.

Here we report on the study of the structural and IM transitions for spinless fermions at $\nu = 1/2$ and $1/6$. To detect these transitions we use the ground-state

splitting and the flux sensitivity[5, 6] respectively. The purpose of the work is to take advantage of the exact diagonalization technique and to study the modification of the low-energy part of the spectrum in a wide interval of the hopping amplitude J all the way from the classical WC to the free fermion limit.

GENERAL REMARKS

We consider spinless fermions at $T = 0$ on the 2D square lattice described by the following model Hamiltonian

$$H = J \sum_{\mathbf{r},\mathbf{s}} a^{\dagger}_{\mathbf{r}+\mathbf{s}} a_{\mathbf{r}} \exp(i\phi\mathbf{s}) + \frac{1}{2} \sum_{\mathbf{r}\neq\mathbf{r}'} n_{\mathbf{r}} n_{\mathbf{r}'} V(|\mathbf{r}-\mathbf{r}'|). \quad (1)$$

Here $n_{\mathbf{r}} = a^{\dagger}_{\mathbf{r}} a_{\mathbf{r}}$, the summation is performed over the lattice sites $\mathbf{r}$, $\mathbf{r}'$ and over the vectors of translations $\mathbf{s}$ to the nearest-neighbor sites. We consider long-range (LR) Coulomb potential $V(r) = 1/r$ and short-range (SR) strongly screened Coulomb potential $V(r) = \exp(-r/r_s)/r$ with $r_s = 0.25$ in the units of lattice constant. We study rectangular clusters $L_x \times L_y$ with the periodic boundary conditions. The dimensionless vector potential $\phi = (\phi_x, \phi_y)$ in the Hamiltonian is equivalent to the twist of the boundary conditions by the flux $\Phi_i = L_i\phi_i$, $i = x, y$. The energy spectrum is periodic in Φ_x and Φ_y with the period 2π.

As a basis for computations we use many-electron wave functions at $J = 0$ in the coordinate representation: $\Psi_\alpha = \prod_{i=1}^{N} a^{\dagger}_{\mathbf{r}_i} |\mathrm{VAC}>$. They can be visualized as pictures, which we call *icons*. The total number of icons is C^N_M, where $M = L_x \times L_y$ is the area of a system, and N is the number of particles. The icon with the lowest energy is a fragment of the crystal. The icons with higher energies represent different types of defects in WC.

The Hamiltonian Eq. (1) is translationally invariant. For each icon α there are m_α different icons that can be obtained from it by various translations. These icons are combined to get the wave function with total quasimomentum $\mathbf{P}$:

$$\Psi_{\alpha\mathbf{P}} = \frac{1}{\sqrt{m_\alpha}} \sum_{\mathbf{r}} \exp(i\mathbf{P}\mathbf{r}) T_{\mathbf{r}} \Psi_\alpha. \quad (2)$$

The summation is performed over m_α translations $T_{\mathbf{r}}$.

For the icons with periodic structures the number m_α of different functions $\Psi_{\alpha\mathbf{P}}$ is smaller than M. For example, the icon Ψ_0 of the WC with one electron per primitive cell generates $m_0 = 1/\nu$ different values of $\mathbf{P}$. Note that the total number of allowed values of $\mathbf{P}$ for the WC is the property of the WC and remains finite at infinite cluster size. Contrary, an icon representing a point defect in a WC generates all vectors $\mathbf{P}$. Their total number is equal to the volume M of the first Brillouin zone of the background lattice.

In the macroscopic system all the states generated by the WC icon form the ground state degenerate at small J. This degeneracy appears because the effective matrix elements which connect translated WC's are zero in the macroscopic limit. The total energy as a function of quasimomentum $\mathbf{P}$ has identical minima at all $\mathbf{P}$ generated by the WC icons. The spectra of excitations in the vicinity of these minima are also identical. The lifting of the ground state degeneracy at some critical value J_c indicates a structural phase transition and restoration of the host lattice symmetry.

The flux sensitivity of a macroscopic system is zero at small J. It becomes non-zero at some finite value of J which might be different from J_c. We associate this transition with the IM transition.[5]

For the finite system the following results can be obtained directly using the perturbation theory with respect to J:

(i) the ground state and the lowest excited states have a large common negative shift which is proportional to J^2 and to the total number of particles N. This shift is the same for all low-lying states and does not affect the excitation spectrum of the system;

(ii) at $\nu = 1/2$ the splitting of the ground state appears in the N-th order and is proportional to J^N. At other filling factors the splitting is proportional to J^K with K being proportional to N;

(iii) the flux dependence of the ground state for the flux in x-direction appears in the L_x-th order and is proportional to J^{L_x} in 2D case. In 1D the flux dependence appears in the N-th order and is proportional to J^N.

Thus, we conclude that both lifting of the ground-state degeneracy and appearance of the flux sensitivity occur very sharply and they can be used as convenient criteria for the structural and the IM transitions respectively. Note that the correlation function is a less sensitive criterion for small clusters[7, 8] since it does not exhibit sharp behavior in the transition region.

THE MECHANISM OF TRANSITION

Our data suggest the following mechanism of the transition. The width of the band of the defect in the WC increases with J such that its lowest edge comes close to the energy of the ground state.[8, 9] Strong mixing between the crystalline and defect states with the same quasimomentum occurs at this point and an avoided crossing appears between the ground state and the states in the defect band.

One can interpret the avoided crossing in terms of the ground state which acquires a large admixture of defect states. This interpretation reminds the idea of zero-point defectons proposed by Andreev and Lifshitz.[10]

In principle, one can imagine that the state with a quasimomentum $\mathbf{P}$ different from those generated by the WC icon becomes the ground state via a branch crossing. However, in all cases we have considered, we observe the avoided crossing between the crystalline state and the state in the defect band with the same $\mathbf{P}$. Assuming that this is the case for larger clusters, we conclude that the phase transition is not of the first order.

The proposed mechanism implies that critical value of J is determined by the energy Δ of the lowest defect at $J = 0$. Our data suggest the following simple empirical rule for J_c:

$$J_c = \beta\Delta \tag{3}$$

where β is some number which is close to 0.5 for all 2D and 1D systems we have studied.

For the exactly soluble 1D problem with nearest-neighbor interaction[11–13] β is exactly equal to 0.5. For the 1D Coulomb problem $\Delta = 2\ln 2 - 1 = 0.386$. Our computations[9] show that for the Coulomb interaction J_c is between 0.17 and 0.3, which gives $0.44 < \beta < 0.77$. Note that this result clearly contradicts to the statement by Poilblanc et al.[14] that 1D Coulomb system is metallic at all J.

We have found Eq. (3) to be extremely useful[15] when applied to the 1D problem with the nearest neighbor interaction V_1 and the next-nearest neigbor interaction V_2. This problem has been studied[16] in connection with the spin version of the Hamiltonian Eq. (1). The IM phase diagram for this model has been studied recently in Ref. 14.

In this case Δ is a function of V_1 and V_2, so that Eq. (3) gives the IM phase diagram in the (V_1,V_2)-space. We have found that the phase diagram obtained in such a way is consistent with our extensive numerical simulations. It predicts the existence of metallic phase at arbitrarily large values of interaction. The ground state in this phase represents a mixture of two degenerate crystalline phases.

GAP AT NONZERO J

At large enough J, the excitation gap in the spectrum is determined by the confinement quantization. On the other hand, the gap Δ at $J = 0$ is the energy of defect and it has a non-zero limit in macroscopic system. Thus, an important question arises, whether or not the gap has a non-zero limit right after the IM transition. The non-zero gap would mean that the state after the transition is superconducting.

We have made a lot of computational efforts to answer this question but the results are still inconclusive. We have found that the gap for the 4×8 cluster is less than for 4×4 cluster but the ratio is significantly larger than 0.5 as would be expected from the confinement quantization solely.

CONCLUSIONS

We have performed a numerical study of the structural and IM phase transitions in 2D fermionic systems with Hamiltonian Eq. (1). We argue that the structural transition on a lattice is not of the first order in all cases considered. We think that the origin of the transition is an avoided crossing of the ground state and the defect states in the Wigner crystal with the same total quasimomentum. This simple picture implies that the critical value of J is determined by the defect with the lowest energy Δ at $J = 0$. To illustrate our point the data for 1D systems with Coulomb interaction and with next-nearest neighbor interactions are also presented. The possibility of the delocalized phase above the transition to be superconducting is discussed.

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