Coulomb Gaps in One-Dimensional Spin-Polarized Electron Systems

Gun Sang Jeon and M.Y. Choi
Department of Physics and Center for Theoretical Physics
Seoul National University
Seoul 151-742, Korea

S.-R. Eric Yang
Department of Physics
Korea University
Seoul 136-701, Korea

We investigate the density of states (DOS) near the Fermi energy of one-dimensional spin-polarized electron systems in the quantum regime where the localization length is comparable to or larger than the inter-particle distance. The Wigner lattice gap of such a system, in the presence of weak disorder, can occur precisely at the Fermi energy, coinciding with the Coulomb gap in position. The interplay between the two is investigated by treating the long-range Coulomb interaction and the random disorder potential in a self-consistent Hartree-Fock approximation. The DOS near the Fermi energy is found to be well described by a power law whose exponent decreases with increasing disorder strength.

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The effects of electron interactions are particularly strong in one-dimensional (1D) systems, leading to Luttinger liquids or to various instabilities. Random disorder also has strong effects in 1D systems: Regardless of disorder strength, all states are known to be localized with the localization length comparable to the mean free path. The interplay of electron interactions and random disorder in low-dimensional systems is of great current interest. It has been shown recently that in the absence of disorder the long-range Coulomb interaction between electrons reduces quantum fluctuations so that the ground state acquires quasi-long range order much close to a 1D Wigner crystal. This reduction of quantum fluctuations is reflected in the density of states (DOS), which vanishes faster than any power as the Fermi energy $\mu$ is approached:

$$ g(E) \sim \exp\{-A[\ln(E_c/|E-\mu|)]^{3/2}\}, $$

where $A$ and $E_c$ are appropriate constants. In the strongly localized regime, where the overlap of electron wave functions is negligible, electrons may be treated classically and the DOS exhibits a Coulomb gap of the form:

$$ g(E) \sim [\ln(E_c/|E-\mu|)]^{-1}. $$

When the Thouless length is shorter than the localization length, the system is in the disordered Fermi liquid regime, where the overlap of electron wave functions can be significant. In this case the electron interactions can be included perturbatively within the weak localization theory, and the first-order correction to the DOS near the Fermi level is given by:

$$ \delta g(E) \sim |E-\mu|^{-1/2}, $$

except in the limit $E \to \mu$, where the perturbation theory is expected to breakdown.

In this work we employ a self-consistent Hartree-Fock (HF) method to investigate the DOS at zero temperature in the quantum regime where the localization length is comparable to or larger than the inter-particle distance. Both the long-range Coulomb interaction and disorder are expected to reduce quantum fluctuations: The Coulomb interaction pushes the system to the classical limit, where quantum fluctuations can be neglected except for the redefinition of the strength of the impurity potential, and disorder is expected to restore the Fermi liquid behavior. Thus a HF mean-field approximation may provide a reasonable description of the interplay between disorder and the Coulomb interaction. This interplay is especially interesting with spin-polarized electrons since the Fermi wave vector is equal to $\pi/a$, where $a$ is the period of the Wigner lattice. In the presence of weak disorder we expect that the processes leading to the Coulomb gap interact with the Bragg scattering leading to a gap in the DOS of a Wigner crystal. Such a spin-polarized system of electrons can be realized in organic chains or in quasi-one-dimensional quantum wires in a strong magnetic field. We find in the quantum regime that the DOS can be fitted well with a power-law, and that the exponent decreases as the strength of disorder is increased.

A prototype model in which the interplay between disorder and the Coulomb interaction can be investigated is a 1D jellium model with $N$ spin-polarized electrons, interacting with each other via the long-range Coulomb interaction in the presence of random impurities. We perform a finite-size calculation in a cell of length $L$ with...
periodic boundary conditions. When the effects of the image charges are taken into account the Coulomb interaction can be written as

\[ V_C(x_1 - x_2) = \sum_{l=-\infty}^{\infty} \frac{e^2}{\epsilon((x_1 - x_2 - lL)^2 + d^2)^{1/2}}, \]

where \( d \) is the cut-off length corresponding to the transverse dimension of the system and \( \epsilon \) is the dielectric constant. For simplicity, we assume that the impurity at position \( x_i \) is characterized by the \( \delta \)-function potential with random strength \( W_i \). This gives the total impurity potential of \( N_I \) impurities in the form

\[ W_I(x) = \sum_{l=-\infty}^{\infty} \sum_{i=1}^{N_I} W_i \delta(x - x_i - lL), \]

where \( W_i \) and \( x_i \) are quenched random variables distributed uniformly in the range \([-W_{\text{max}}/2, W_{\text{max}}/2]\) in the interval \([-L/2, L/2]\), respectively. The electron-electron interaction is treated self-consistently within a HF approximation in the momentum space. We expand the HF single-particle wavefunction for state \( \alpha \) as follows:

\[ \Psi_{\alpha}(x) = \sum_k c_{k\alpha} \phi_k(x), \]

where the basis states are

\[ \phi_k(x) = \frac{1}{\sqrt{L}} \exp(ikx) \]

and the wavevector \( k \) takes integer multiples of \( 2\pi/L \). The expansion coefficients \( c_{k\alpha} \) satisfy the equations

\[ \sum_{k'} \langle k|H_0 + W_I + U + V_{\text{HF}}|k'\rangle c_{k'\alpha} = \epsilon_{\alpha} c_{k\alpha}, \]

where the matrix elements are evaluated by integrating the coordinate over the interval \([-L/2, L/2]\). Here \( H_0 \) is the kinetic energy and the HF matrix elements are given by

\[ \langle k'|V_{\text{HF}}|k'\rangle = \sum_{\alpha} n_\alpha [\langle k, \alpha|V_C|k', \alpha\rangle - \langle k, \alpha|V_C|\alpha, k'\rangle], \]

where the first and second terms are the Hartree and exchange potentials, respectively. The potential \( U \) is due to the uniform positive background charge and \( n_\alpha \) is 1/0 for occupied/unoccupied states \( \alpha \). The HF matrix elements in Eq. (8) depend on the expansion coefficients via

\[ \langle k, \alpha|V_C|k', \alpha\rangle = \sum_{k_1,k_2} c_{k_1,\alpha}^* c_{k_2,\alpha} \langle k, k_1|V_C|k', k_2\rangle, \]

where the Coulomb matrix elements are given by

\[ \langle k_1, k_2|V_C|k'_1 k'_2\rangle = \delta_{k_1+k_2,k'_1+k'_2} K(k_1 - k'_1) \]

with

\[ K(k) = \frac{1}{L} \sum_{l=-\infty}^{\infty} \int_{-L/2}^{L/2} dx \frac{e^2}{\epsilon((x - lL)^2 + d^2)^{1/2}} \exp(-ikx). \]

In our numerical work, the electron number \( N \) is fixed to \( L/d \), so that the inter-particle distance is equal to \( d \). We measure the strength of the Coulomb interaction and impurity potential using dimensionless parameters \( V = V_I/E_K \) and \( W = V_D/E_K \), where \( V_I = e^2/\epsilon d \), \( V_D = W_{\text{max}}/d \), and \( E_K \equiv \hbar^2 k_0^2/2m_\epsilon \) with \( k_0 \equiv 2\pi/d \). The impurity number \( N_I \) is set equal to 5\( N \) while the dimension of the Hamiltonian matrix is taken to be \( 2N+1 \) for \( W = 0.1, 3N+1 \) for \( W = 0.4 \), and \( 5N+1 \) for \( W = 1.0 \). The convergence of the obtained results has been tested by increasing the dimension of the matrix. Figure 1 displays the probability distribution function of an electron at the Fermi energy in strongly localized (\( W = 1.0 \)), intermediate (\( W = 0.1 \)), and disorder free (\( W = 0 \)) regimes. We see that the localization length decreases with the disorder strength, and particularly, in the absence of impurities, observe 1D crystalline order rather than an electron liquid. This mean-field result is in qualitative agreement with the result obtained through the use of the bosonization technique, which has predicted quasi-long-range-order with the correlation function decaying slower than any power, regardless of the strength of the long-range Coulomb interaction. At \( W = 0.1 \) the electrons are in the quantum regime since the localization length extends over several times the inter-particle distance. We note that even at \( W = 1.0 \) the electrons the localization length is comparable to the inter-particle distance.

The average DOS integrated over the system size is given by

\[ \bar{g}(E) = \frac{\langle \Delta D(E) \rangle}{\Delta E}, \]

where \( \Delta D(E) \) represents the number of eigenenergies in the energy range of width \( \Delta E \) around energy \( E \) and the double angular brackets denote the disorder average. Here we set the value of \( \Delta E \) to be 0.05 in units of \( E_K \), and compute the DOS by means of Eq. (13). Figure 2 displays \( \bar{g}(E) \) at \( W = 0.1 \) for five different system sizes \( L/d = 30, 40, 50, 60, \) and 80. We observe that a large reduction of the DOS occurs near the Fermi energy. Since there is an energy range where no significant DOS is present, we need to average over many disorder realizations to get accurate values of the DOS. We find that for
$W = 0.1$ the number $N_D$ of disorder realizations between 1001 and 3844 is quite sufficient. To analyze the shape of the gap quantitatively, we fit the DOS near the Fermi energy to a power law:

$$g(E) \propto |E - \mu|^{\alpha},$$  \hspace{1cm} (14)

where the DOS $g(E)$ is related to the obtained (average) DOS $\bar{g}(E)$ via

$$\bar{g}(E) = \frac{1}{\Delta E} \int_{E-\Delta E/2}^{E+\Delta E/2} dE \, g(E).$$  \hspace{1cm} (15)

This fit of the DOS for $W = 0.1$ is shown in Fig. 3. The power law fits our numerical results quite well, with $\mu = -0.29 \pm 0.02$ and $\alpha = 5.80 \pm 0.16$. For comparison, we have also fitted $\bar{g}(E)$ to a logarithm, given by Eq. (2), only to find substantial disagreement: The function, Eq. (2), is a sublinear function of $E$ while the numerical data form a superlinear function; see Fig. 2.

Figure 4 shows the system size dependence of the exponent $\alpha$ for two different values of disorder strength, $W = 0.1$ and 0.4. The values of $(L/d, N_D)$ for $W = 0.1$ are as in Fig. 2, while for $W = 0.4$ four new values are chosen. The numbers of disorder realizations for $W = 0.4$, which have been chosen between 199 and 477, can be much smaller than those for $W = 0.1$ since there are many more states near the Fermi energy due to stronger disorder. The obtained results of the size dependence tend to bend up in the large system, and yield finite extrapolated values of $\alpha$ in the limit $L/d \to \infty$, which provides an evidence for the algebraic gap formation in the thermodynamic limit. As expected, the exponent $\alpha$ decreases with $W$, implying that the gap softens as the strength of disorder is increased. On the other hand, we expect that in the very clean limit ($W \ll 0.1$) the power law will fail, leading to the gap of the form in Eq. (1).

In summary, we have investigated the density of states of interacting spinless electrons in the presence of random disorder in one dimension. We find numerical evidence for the formation of a gap near the Fermi level: The density of states can be fitted with a power law in the quantum regime, where the localization length is comparable to or larger than the inter-particle distance. The magnitude of the exponent describing the algebraic gap decreases with increasing disorder.

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[14] The effects beyond the HF approximation may be estimated by screening the exchange interaction within the GW approximation. Since the electrons are all localized here, the screened interaction will be essentially identical to the bare interaction except for the simple change in the dielectric constant $\epsilon$. Thus we expect that the GW approximation would not yield qualitatively different results. Indeed the HF calculation is known to be exact in the strong-disorder limit, regardless of the dimension. See Ref. [10].
FIG. 2. Density of states as a function of energy for various system sizes. The data marked by diamonds(◇), plus signs(+), squares(□), crosses(×), and triangles(△) correspond to \((L/d, N_D) = (30, 1924), (40, 3740), (50, 3108), (60, 3844)\) and \((80, 1001)\), respectively. The disorder strength \(W\) and the electron density \(n\) are fixed to 0.1 and \(1/d\), respectively.

FIG. 3. Power-law fit of \(\bar{g}(E)\) in a system of size \(L/d = 60\) and disorder strength \(W = 0.1\).

FIG. 4. Exponent \(\alpha\) as a function of the inverse of the system size for two values of disorder strength, \(W = 0.1\) and 0.4. While the parameters \((L/d, N_D)\) for \(W = 0.1\) are the same as those in Fig. 2, for \(W = 0.4\) we have used \((L/d, N_D) = (30, 477), (40, 296), (50, 252),\) and \((60, 199)\). The electron density is fixed to \(1/d\). The lines are guides to the eye.
Figure 1

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