Quantum Coulomb gap

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Abstract. We study numerically strongly-localized systems with long-range interactions. We obtain the density of states for 1-D Anderson Hamiltonian with $r^{-1/2}$ interactions by exact diagonalization. The limit in which the hopping term is zero has been well studied and leads to a linear gap near the Fermi energy. We find the same linear dependency for non zero hopping however the slope decreases. The effects of possible numerical problems, like finite size effects or the use of a limited set of eigenvalues, is analyzed.

1. Introduction
From the work of Mott [1] dealing with the transport properties of disorder system a vast field of solid state physics has merged. That field is known as Variable Range Hopping (VRH) and its main concern is the characterization of the conduction properties of disorder interacting systems at finite temperature.

A fundamental step in that task is to understand the density of states (DOS) of disorder and interacting system. In 1971 Pollak [2] suggested the existence of a gap in the DOS when Coulomb like interactions are present in disordered and completely localized electronic systems. This phenomenon is better known as the Coulomb gap and should produce dramatic consequences in the low temperature conduction. The existence of that gap has been experimentally observed in [3] and [4].

Although the theory in which the Coulomb gap appears has been already established by Efros and Shklovskii [5, 6], it has been always assumed that the systems under study are well represented by classical laws. At a first stage, it could be thought that in the strongly-localized regime it is possible to renormalize the localization length of electrons and obtain that they are completely localized. Nevertheless it is clear that quantum effects must play a role at least near the metal-insulator transition. Quantum effects in the coulomb gap has been poorly studied [7, 8, 9, 10], just because it is a long-range effect and within an exact quantum treatment it is impossible to deal with large systems. In these studies different approximations were used and obtained opposite results, in some cases the authors claimed that the Coulomb gap opens due to quantum effects and in others either remains the same or closes.

In this work we study the generalization of the Coulomb gap when quantum effects are taken into account. The DOS near the Fermi energy for a 1-d lattice with up to 20 sites is calculated. As a Coulomb interaction $(1/r)$ produces a logarithmic Coulomb gap when dealing with 1-D system, we use a $1/√r$ interaction which gives a linear gap similar to the usual Coulomb gap in two dimensions.

2. The model
We consider a one-dimensional lattice system with the following Hamiltonian:

$$H = \sum_i \phi_i n_i - t \sum_{i<j} c_i^\dagger c_j + V \sum_{i\neq j} \frac{(n_i - K)(n_j - K)}{\sqrt{r_{ij}}},$$

(1)
where \( \phi \) is a random site energy, with a uniform distribution in the interval \([-W/2, W/2]\), \( t \) is the hopping parameter, \( V \) is the strength of interaction and \( K \) is the compensation constant; \( <i,j>\) indicates a sum over all nearest neighbors pairs. As mentioned above, we have chosen an interaction potential decaying as \(1/\sqrt{T}\) in order to obtain a classical linear gap. In the following we fix the disorder amplitude to \(W = 2\) and the interaction strength to \(V = 1\).

The main goal of this work is to study the single-particle density of states (DOS) for a given number of electrons \(N\) and size of the system \(L\). We split this DOS into two contributions, one for holes, extracting an electron out of the system, and one for electrons, adding an electron to the system. The local DOS for holes at site \(k\), which by assumption have negative energies, is

\[
\rho^N_h(\epsilon, k) = \sum_\alpha \delta(\epsilon + E^{N-1}_\alpha - E^N_0) \left| \langle \psi^{N-1}_\alpha | c_k | \psi^N_0 \rangle \right|^2,
\]

while the DOS for particles is

\[
\rho^N_p(\epsilon, k) = \sum_\alpha \delta(\epsilon - E^{N+1}_\alpha + E^N_0) \left| \langle \psi^{N+1}_\alpha | c_k | \psi^N_0 \rangle \right|^2,
\]

where the superindex in the energy refers to the number of electrons in the sample and the subindex to the energy level (zero referring to the ground state). We shall employ the grand canonical ensemble, search for the ground state of the hamiltonian for different number of electrons and keep the number \(N\) that minimizes the grand potential \(\Omega = H - \mu N\). In the classical limit this is a rather expensive procedure compared to other procedures (see for example [11]), but as we will see it is not so expensive in the quantum case and in this way we ensure that the electron energies are always positive (and the hole energies negative).

In order to compute the density of states, Eqs. 3 and 2, we also need to partially diagonalize the Hamiltonian for holes obtaining only a set of the smallest eigenvalues and their eigenvectors in each case. Then, Eqs.3 and 2 are computed and the results stored in an histogram.

As we are interested only in the DOS near the Fermi level we need to get a small number, \(ns\), of low energy states with one more and one less electron than in the ground state. This part is the most expensive. Nevertheless we do not need to perform full diagonalization of the Hamiltonian which would be much more expensive. All the numerical data were obtained using an eigensolver based on ARPACK libraries. Those libraries are specially suited to work with sparse matrices and to compute a few eigenvectors rather than fully diagonalize the Hamiltonian. We use system sizes from \(L = 10\) to \(L = 20\) and for the disorder average we compute over 30000 samples.

As an example we show in FIG 1 the classical DOS \((t = 0)\) using this procedure for different values of \(ns\). We see that all curves overlap near the center of the gap and for \(ns > 20\) the gap is properly represented. For this system size, with \(ns > 60\) we already reproduce the full single-particle DOS. Another more rigorous procedure to establish a range of energies in which our computation is valid is the following. For a given \(ns\), we set up a maximum energy \(\epsilon_{max}(ns)\) in such a way that all the samples used in the computation obey \(E_{ns} > \epsilon_{max}(ns)\). Then, the error due to the truncation in the range \([-\epsilon_{max}, \epsilon_{max}]\) will be exactly zero. We found that this condition is too strong. Instead, we adopt \(\epsilon_{max}\) in such a way that only 1% of the samples violate the inequality \(E_{ns} > \epsilon_{max}\). This error is small enough to explore the relevant physics of the problem. The different values of \(\epsilon_{max}\) are shown in the figure as vertical dashed lines. For all calculations of the DOS we have performed the same analysis, similar vertical lines will be plotted in other figures in this work. Another way to show the effect due to the truncation in the number of eigenvectors used is to check the area, \(A\), of the numerical DOS. We observe in the legend of FIG 1 that, for this system size, \(ns = 60\) is enough to provide accurate results in the whole energy range.

We may notice in FIG 1 that the DOS presents some filling of the gap near zero, this is a well-known finite size effect. In the classical case, the DOS near the Fermi energy is completely dominated by long...
Figure 1. The classical single-particle DOS obtained retaining only a number of states \( n_s \). The size of the system is \( L = 10 \) and \( K = 1/2 \). Different colors represent different values of \( n_s \). The black solid line has been obtained using the LAPACK algorithm which calculates all the spectrum and thus, this is an exact computation. In the legend is specified the area, \( A \), of each curve. See text for further explanations.

distance correlations, so for small systems this part of the DOS cannot be properly obtained. As the sizes available with our method are rather small we need a careful analysis of the effect of increasing \( L \). In Fig. 2 different system sizes are used to compute the classical Coulomb gap. Though the finite size effects are important at a region close to the Fermi energy we can observe that for an intermediate part of the gap they are quite small. This is the region where we will concentrate our analysis. Again we may notice the vertical lines which correspond to \( \epsilon_{\text{max}} \) for each case, we see that the region of interest is well inside the interval \( [-\epsilon_{\text{max}}, \epsilon_{\text{max}}] \).

Figure 2. Several system sizes are depicted for the classical DOS. The dashed vertical lines indicate again the accurate energy range as described in the text related to FIG 1. The case \( L = 1000 \) has been computed using a classical algorithm, which allows for much bigger system sizes.
Related to FIG. 2, we should mention that, according to the self-consistent theory [6] the slope of the DOS should be $1/2$. The intermediate part of the gap (excluding the region near zero) fits very well to a straight line with slope 0.8. This subject deserves more attention, but it would require to study much larger systems, so here we will concentrate in the quantum effects.

3. Quantum Effects

Once we have clarified the role of the two main sources of error we introduce a small hopping $t$ in order to estimate the quantum effects. The results are shown in FIG. 3. It clearly shows that in a strongly localized regime, quantum effects tend to open the gap. The gap remains fairly linear but with a smaller slope. This is the main result of this work. This result is in contradiction with previous works.

FIG. 3 is not affected by the truncation in the number of eigenvalues used. In fact only the region $(-\epsilon_{\text{max}}, \epsilon_{\text{max}})$ is plotted for each case, but it is important to verify that it is not affected by finite size effects either. In FIG. 4 we show the results for $t = 0.2$ for different system sizes. We observe that although the finite size effects are important at a region close to the Fermi energy, for an intermediate part of the gap they are quite small. In fact the effects seem to be smaller that in the classical case, FIG. 2.

Figure 3. Single-particle DOS versus energy $L = 20$ and several values of $t$. The black line corresponds to the classical DOS for a large system size.

One possible explanation for the opening of the gap, could be the tendency to form a periodic structure. Without disorder, the ground state would correspond to a kind of anti-ferromagnetic order, with charges of opposite sign placed in nearest neighbors. Obviously, in the classical limit we do not get such long-range order. But, it is true that the disorder selected is not very large, our system sizes are small, so a correlation length of the order of the system size would be seen as a long-range order. Also, the hopping term could partially favor this anti-ferromagnetic order as an electron with the neighbors empty can delocalize and reduce its energy; similarly to the anti-ferromagnetic order in the Hubbard model [12]. So it is necessary to check that this is not the situation in FIG. 3. We have calculated the correlation function

$$C_{i,j} = \langle \psi_{\text{gs}} \vert n_i (1 - n_j) \vert \psi_{\text{gs}} \rangle,$$

where $\psi_{\text{gs}}$ is the ground state and $n_i = C_i^\dagger C_i$. We have checked that certainly there is short-range correlation but it tends to zero as sites $i$ and $j$ separate apart. Another way to check that this effect is
Figure 4. Single-particle DOS versus energy for several system sizes and $t = 0.2$. The dashed vertical line indicates again the accurate energy range as described below. The case $L = 1000$ corresponds to the classical limit and is shown only for comparison.

Not affecting our results is to study systems with an odd number of sites (see FIG. 5). We can see that, certainly, in the intermediate part of the gap the system is not affected by any kind of finite size effect. In the center of the gap there are differences between odd and even system sizes, the latter slightly favor correlations and produce a slightly deeper gap. Although, in the center the tendency indicates that the depth decreases as we increase system size, due to the large finite size effect, it is not possible to conclude anything concrete about the shape of the gap very near the Fermi level, although the DOS seems to go to zero at $E_F$.

Figure 5. Single-particle DOS versus energy for several system sizes and $t = 0.2$. An odd-even effect can be appreciated near the Fermi level, this effect disappears for intermediate energies inside the gap. The case $L = 1000$ corresponds to the classical limit and is shown only for comparison.
4. Estimation of the localization length

In order to better understand the results of the previous sections it is necessary to estimate the localization length, $\xi$, of the system for the range of $t$ used. In order to extract this length we have used two equivalent methods. On one hand, we can compute the sensibility to a change in the boundary conditions. Let us denote $E(\phi)$ the energy of a system under boundary conditions $c_{L+1} = e^{i\phi}c_1$, and $\Delta E = E(\pi) - E(0)$ the difference between periodic and anti-periodic boundaries. In a similar way as in [13] [14], the localization length could be extracted from:

$$\lim_{L \to \infty} \log (\Delta E(-1)^N) = -\frac{L}{\xi} + b,$$

where $N$ is the number of electrons in the sample and $b$ a constant. On the other hand a two points correlator could be used. In this case, the localization length is given as in [15] by:

$$\lim_{L \to \infty} \log \langle \psi_{gs}|c_L c_1^\dagger|\psi_{gs}\rangle = -\frac{L}{\xi} + b'.$$

![Figure 6. Average of the log $\Delta E$ versus system size, $L$, for several values of $t$. In the legend we can see the localization length for each case. The straight lines show the fit to eq. 5 for the final points in each case.](image)

We have checked that both methods lead to equivalent results. We have found that with the method of twisting the boundary conditions we get slightly better numerical precision. We performed two diagonalizations to compute the ground state energy for periodic and anti-periodic boundary conditions and average over 500 samples. In Fig. 6 the average of the log $\Delta E$ is represented and from there the localization length is computed.

We see that in some cases, for our system sizes we do not get a perfect straight line. Nevertheless, for $t = 0.1$ and $t = 0.2$ we can estimate the localization length by roughly 0.8 and 1.0 respectively, of the order of the nearest neighbors distance.

5. Conclusions

We have studied numerically a quantum strongly-localized systems with long-range interactions. We have calculated the single-particle DOS for systems with localization length of the order of nearest neighbors distance.
In our case, the limit in which the hopping term is zero has been well studied and leads to a linear gap near the Fermi energy. We find the same linear dependency for non zero hopping however the slope decreases. We have analyzed the possible numerical problems, like finite size effects or the use of a limited set of eigenvalues, showing that the behavior in the intermediate part of the gap is not affected by such problems.

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6. Bibliography

[1] N. F. Mott. Phil. Mag. 19:835 (1969)
[2] M. Pollak. Discuss. Faraday Soc. 50 (1970)
[3] J. G. Massey and M. Lee, Phys. Rev. Lett. 75, 4266 (1995)
[4] V. Y. Butko, J. F. Ditusa, and P. W. Adams, Phys. Rev. Lett. 84, 1543 (2000)
[5] A. L. Efros and B I Shklovskii, J. Phys. C : Solid State Phys. 8, L49 (1975)
[6] A. L. Efros, J. Phys. C: Solid State Phys. 9, 2021 (1976)
[7] G. Vignale and W. Hanke, Phys. Rev B 34, 3003 (1986)
[8] Q. Li and P. Phillips, Phys. Rev B 48, 15035 (1993)
[9] F. Eppelein, M. Schreiber and T. Vojta, Phys. Rev B 56, 5890 (1997)
[10] G. Sang Jeon, H-W. Lee and M. Y. Choi, Phys. Rev B 59, 3033 (1999)
[11] S. D. Baranovskii, A. L. Efros, B. L. Gelmont and B I Shklovskii, J. Phys. C: Solid State Phys. 12, 1023 (1979)
[12] G. D. Mahan, Many-Particle Physics, page 416, Kluwer, New York (2000).
[13] P. Schimteckert, T. Schulze, C. Shuster, P. Schwab and U. Eckern, Phys. Rev. Lett. 80, 560 563 (1998)
[14] P. Schmitteckert, R. A. Jalabert, D. Weinmann, and J.L. Pichard, Phys. Rev. Lett. 81, 2308 2311 (1998)
[15] J. M. Carter and A. Mackinnon, Phys. Rev. B 72, 024208 (2005)