УДК 539.21:537.1

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SPATIAL LOCALIZATION AND QUANTUM DIFFUSION OF INTERACTING ELECTRONS IN LOW-DIMENSIONAL DISORDERED SOLIDS

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The density of states of many-particle excitations is calculated using the Hubbard model. For interacting electrons in a one-dimensional disordered system the coulomb repulsion between strongly localized electrons results in the delocalization.

***Key words**: disordered systems, electronic transport, quantum localization, electron-electron interaction.*

1. Introduction. In the beginning of the 21st century, considerable advances in the controlled fabrication of sub-micron solid state structures, as well as the common availability of low temperature facilities, have allowed for a systematic investigation of artificially made structures whose electronic properties are modified or even dominated by quantum interference effects. This makes it possible to perform experiments in the mesoscopic regime which directly probe quantum properties of phase coherent many-body systems. While a variety of phenomena can be understood within a weakly interacting quasi-particle approach [1], the always present strong Coulomb interaction between electrons can have a dramatic influence on the transport properties when the electrons are confined in low-dimensional systems. A prominent example is the Coulomb blockade effect and the resulting conductance oscillations in the transport through quantum dots [2].

Insights towards lower dimensions or very dilute limits results in a poorer screening of the electron-electron interaction, enhancing the role of Coulomb repulsions. When the disorder is strong, quantum interference leads to Anderson localization [3] of the electron wave functions. The resulting suppression of the mobility of the charge carriers becomes also detrimental to screening, thereby further amplifying the role of interactions. On can therefore expect important effects of the electron-electron interaction and. Even a breakdown of the Fermi-liquid quasi-particle approaches in confined and disordered systems might be expected.

Recent experiments [4,5] have asked for reexamination of the scaling theory of localization, which predicts only localized states in one or two spatial dimensions (2D). This result has been obtained when neglectting coulomb interactions. Interplay between disorder and interaction can lead also to the breakdown of the one-parameter scaling hypothesis.

In this paper we consider two interacting electrons as a staring point for treating interactions in a random potential. Some researches suggested that a suitably defined localization length of the two-particle states λ_2 in one-dimensional disordered potential can me much larger than the one-particle localization length λ_1. Numerically an enhancement of the localization length was found by considering, for example, a transfer matrix calculations for finite samples and for a 'bag model' [6] or direct diagonalization [7], but a unifying picture does not exist yet.

2. Localization length enhancement. Here, we report results of extensive numerical calculations for the spectrum of the two-electron energies and the localization length. For the latter, one can use the center-of-mass (CM) coordinate system and apply the transfer matrix method to the bag model, in contrast to the earlier investigations [6,7]. The two-electron density of states shows a behavior, which is very similar to that of the one electron behavior in two-dimensional disordered solids. Near the centre of the spectral band the energy level statistics shows a crossover from the Poisson law towards the Wigner-Dyson statistics when interaction energy is increased. This was found in paper [7] by applying a powerful technique of the

probability calculation of the fluctuations in the discrete spectra of the electron states near the ground state. For the localization length we find that many-particle localization length exceeds the single-particle localization length at the same strength W of the disordered impurity potential:

$$\lambda_2(W,b) > \lambda_1(W). \tag{1}$$

These findings were similar to the previous results in papers [5-7]. However, this enhancement is almost independent of the interaction as long as the range of the latter is much smaller than the 'bag size'. Therefore the largest relative coordinate is defined by the following relation:

$$b \equiv r_{\max}, \tag{2}$$

where b is the 'bag size', which the largest interparticle distance.

Using the finite size scaling we extract the localization length for the limiting case $b \to \infty$. Therefore we present strong evidence for the two-dimensional system that the disorder scaling of the localization length in the infinite system at the thermodynamic limit is governed by the following exponential expression:

$$\lambda_2(W,\infty) \sim \exp(1/W^2), \tag{3}$$

independent of whether or not a finite range interaction is present. We used the Schrodinger equation discretized in the CM coordinates

$$-\psi_{R+1,r} - \psi_{R,r\pm1} + [V_{R+r} + V_{R-r} + U(r)]\psi_{R,r} = E\psi_{R,r}, \tag{4}$$

where $R = (x_1 + x_2)/2$, and $r = (x_1 - x_2)/2$, are the center-of-mass and the relative coordinates, respectively. Here $U(r)$ is the interaction and V is the random potential. Apart from correlations in the random potential, $(V_{R-r}+V_{R+r})$, the equation (4) can also be considered as the Schrodinger equation for a particle in two-dimensional non-interacting system. Alternatively, one can view on expression (1) as describing two degrees of freedom, which "interact" via a random coupling $(V_{R-r}+V_{R+r})$, while one of the particles subject to a potential energy U. Considering a finite range of the relative distance, $|r| < b$, we obtain the bag model in the CM coordinates, for which we perform a transfer-matrix analysis [8]. The inverse of the smallest Lyapunov exponent defines the localization length of the two electrons, λ_2. In Fig. 1 (inset), λ_2^{-1} is shown as a function of the disorder, W, for different bag sizes b at $E = 0$. With these data we performed a finite size scaling, as shown in the main Figure. All points collapse in one common monotonic curve. The scaling works perfectly with an accuracy of 1%. The plot of Fig. 2 demonstrates the disorder dependence of the scaling parameter λ_1 in comparison with the single-particle results in 1D and 2D, as well with results obtained within the bag model using particle coordinates [8]. For larger disorder our findings coincide with previous ones, however for small W they behave as λ_{2D}, that is the result for a single particle in 2D.

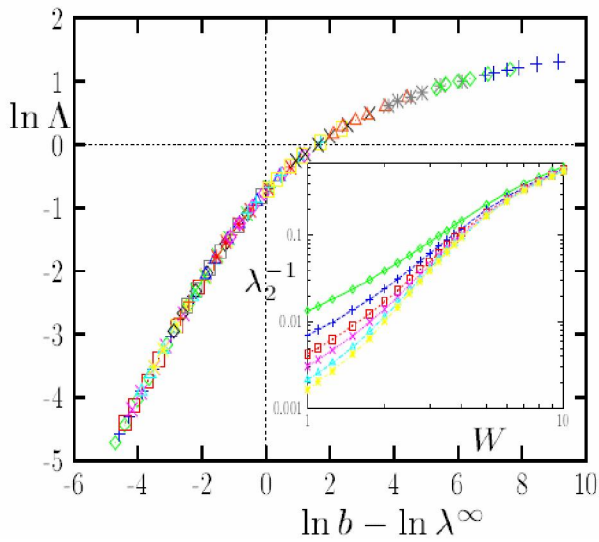

Fig. 1. Scaling curve for the reduced renormalized localization length of two interacting particles $\Lambda = \lambda_2/b$. Inset: raw data $\lambda_2(W)$ for b = 10, 20, 40, 70,100 and 200 (top to bottom)

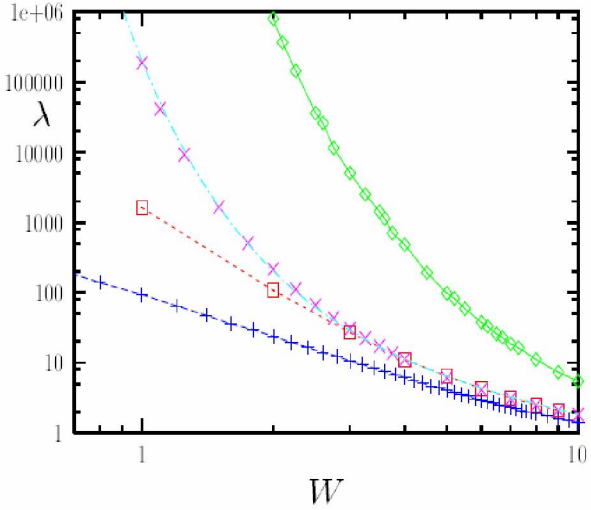

Fig. 2. Localization length λ_{2D} for one-electron approximation in two-dimensional disordered system (◊); scaling parameter λ_∞ fitted by $13.6/W\exp(9.6/W^{1.5})$, shown by symbol (x); λ_2 in single particle coordinates (□) and λ_1 (+)

From the above numerical results, we conclude in agreement with earlier suggestions, that the localization length of two particles in a random potential is enhanced by the interaction. However, in contrast to earlier work, we find for smaller disorder ($W < 4$) a much stronger delocalization effect. This might be an effect of the discretization in CM coordinates which induces a strong correlation between the particles. On the other hand, the description with discretized CM coordinates becomes asymptotically correct for small disorder such that the disorder potential can be considered as representing a coupling between two degrees of freedom.

3. Quantum diffusion. Using a decomposition method 8, we calculated the time evolution of two-particle wave functions in particle coordinates. For short times, the mean radius, of the wave function grows ballistically, for intermediate times it grows logarithmically before it saturates for $t\to\infty$. The saturation value was used to estimate the localization length, shown in Fig. 3 as a function of disorder W and interaction strength U. In the range $2 < W < 6$ we observe the power-law behavior $\lambda_2 \sim W^{-\alpha}$.

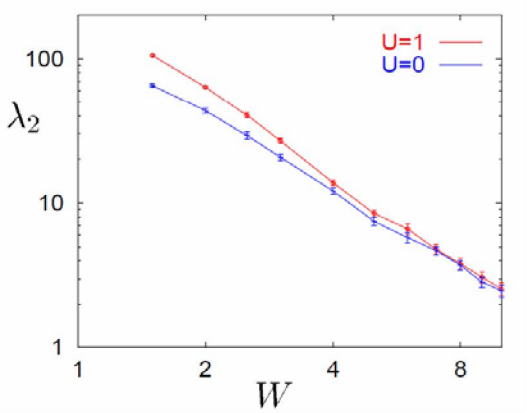

Fig. 3. Two-electron localization length $\lambda_2(W)$ obtained from time evolution calculations with and without interaction

For $U = 0$ the fit yields $\alpha=1.95 \pm 0.11$, that corresponds to the correct zero-interaction limit. The interaction-induced enhancement is smaller than that obtained earlier in paper [4], since many states with smaller λ_2 contribute also to the quantum diffusion. For $U = 1$, we find $\alpha = 2.27\pm0.09$. Using only the extension in the CM direction, the enhancement is more pronounced,

$$\lambda_{2CM}(U = 1) \sim W^{-2.4}.$$

We also determined the localization length by using the inverse participation ratio and the mean relative extension. Independently of the method, λ_2 is enhanced at small U and decreases at large U. The maxima of λ_2 are located at $|U| \approx 2$, consistent with the results from the level statistics.

4. Energy level statistics. In order to study the spectral properties we consider the Hamiltonian of the two electrons in a disordered one-dimensional potential regular lattice of the length L with the repulsive on-site interaction $U\delta_{i,j}$. In fact, we deal with the well-known Hubbard model for correlated electrons on a single lattice site. Consider the spectrum of quantum particles in a random potential using the Anderson model with interaction. The Hamiltonian of the model on a simple 1D lattice is given by

$$H = \sum_{j,\sigma} e_j c_{j\sigma}^{+} c_{j\sigma} + \sum_{j,m\neq 0,\sigma} t_m (c_{j\sigma}^{+} c_{j+m,\sigma} + c_{j\sigma} c_{j+m,\sigma}^{+}) + \frac{U}{2} \sum n_{j,\sigma} n_{j,-\sigma}, \tag{4}$$

where $c_{j\sigma}^{+}$ creates an electron on the j-th site of a lattice. $n_{j,\sigma} = c_{j\sigma}^{+} c_{j,\sigma}$ ist he operator of the occupation number on the j-th site with the spin σ. The random potential is introduced via the on-site energies e_n (diagonal disorder). They are uniformly and independently distributed in the interval from $-W/2$ to $W/2$, i.e. according to the `box' distribution. Thus, the disorder parameter W is given as a width of the uniform distribution of random bear energies. The Hamiltonian matrix is constructed in the basis of the $L(L+1)$ symmetrized products of single-electron wave functions. The total spin of the electron problem in question is equal to zero. The model Hamiltonian has been diagonalized with periodic boundary conditions. The density of multi-electron states $\rho_2(E)$ has been determined for various disorder degree W and Hubbard interaction potential U. The results of our numerical calculations are demonstrated on Fig. 4. The obtained two-electron density of states in one-dimensional disordered system is strikingly similar to that of a single particle in a two-dimensional disordered square lattice. For fixed degree of the disorder W the density of states decreases only slightly near the middle of the spectral band, when interaction energy is increased. This is in favor of the Hubbard band which separates by detaching from the main spectrum for sufficiently large interaction U. It contains order of $\sim 1/L$ states and vanishes for the infinite sizes. This is because the total number of electrons is fixed (the dilute limit). The form of the main band is quite insensitive to the strength of the electron-electron interaction.

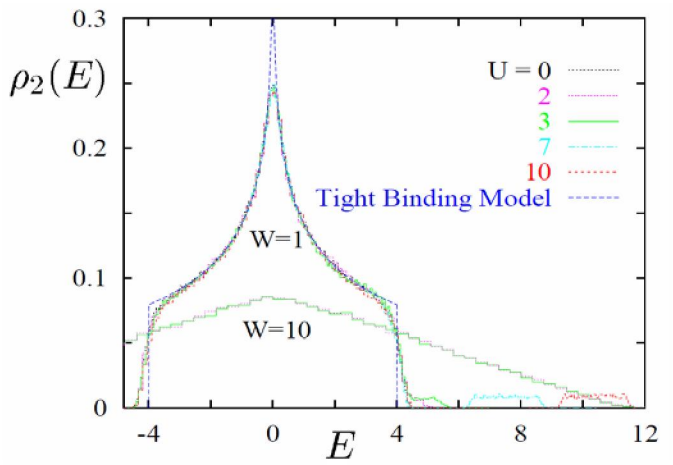

Fig. 4. Two-electron density of states $\rho_2(E)$ of a one-dimensional system of length L=100 with various interaction energies U

However the statistics of the energy levels at the band centre E=0 changes drastically with increasing Hubbard interaction energy U for certain given pairs of disorder W and system size L. The nearest level spacing distribution $P(s)$ shows a crossover from Poisson distribution to the Wigner-Dyson distribution and other way around, both with increasing the interaction energy U, as depicted in the Fig. 5. This transition of the level statistics is measured by the parameter

$$\gamma = \frac{\langle s^2 \rangle - \langle s_W^2 \rangle}{\langle s_P^2 \rangle - \langle s_W^2 \rangle}, \tag{5}$$

which defines the relative deviation from the Wigner distribution. Here

$$\left\langle s^2 \right\rangle = \int_0^\infty s^2 P(s) ds \tag{6}$$

is the spacing variance. The subscript labels indicate the Poisson (P) and Wigner-Dyson (W) distribution are used. The level spacing is measured in units of the mean level spacing for two-particle spectrum Δ_2. The disorder has been chosen such that

$$L \approx \lambda_1 = 105/W^2, \tag{7}$$

Results are shown in the inset of Fig. 5.

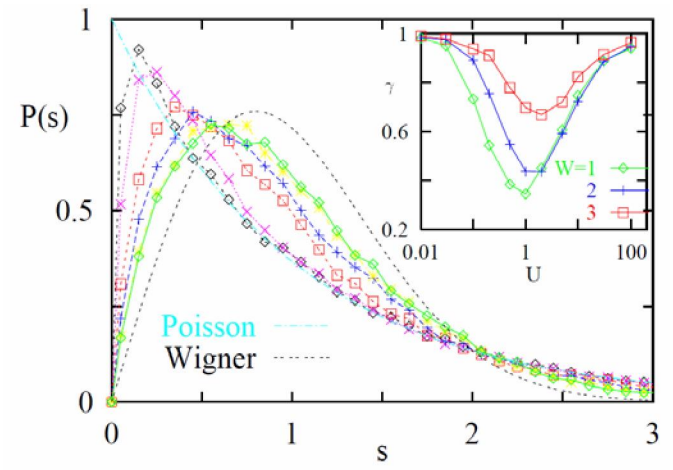

Fig. 5. Level spacing distribution $P(s)$ for the interaction energy U=0.01,0.03,0.1,0.2,0.5,1.0 (left to right) at the centre of the spectral band E=0 for disorder degree W=1. Inset: parameter γ (see text) vs. U for various W

4. Conclusions. We investigate the influence of the interplay between disorder and interaction on several properties that give insight into transport of charge carriers in a one-dimensional random potential. These are the quantum diffusion of wave packets, the statistical correlations of the electron energy levels and the localization length. We apply various numerical approaches: the direct large-scale diagonalization method, the solution of the time-dependent Schrцdinger equation, the transfer-matrix technique and the finite-size scaling *analysis.* For few fermions it is found that short-range interactions leads to an enhancement of the localization length, so that some many-body states can coherently propagate for a distance larger than the non-interacting localization length. The level correlations of the two-electron spectrum exhibit a continuous crossover from the intermediate statistics towards the Poisson distribution in the limits of strong and weak interaction, while for the larger number of electrons a saturation to the Wigner statistics is obtained.

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ТӨМЕНӨЛШЕМДІ РЕТТЕЛМЕГЕН ҚАТТЫ ДЕНЕЛЕРДЕГІ ЛОКАЛИЗАЦИЯ ЖӘНЕ ӨЗАРА ӘРЕКЕТТЕГІ ЭЛЕКТРОНДАРДЫҢ КВАНТТЫҚ ДИФФУЗИЯСЫ

Хаббарданың моделін пайдаланып көпбөлшекті қозулардың тығыздық жағдайлары есептеліп шығарылған. Бірбөлікті реттелмеген жүйеде өзара қимылдардағы электрондар үшін күшті локализацияланған электрондар арасындағы кулондық итеріс делокализацияға әкелінеді.

И.Х. Жарекешев

ЛОКАЛИЗАЦИЯ И КВАНТОВАЯ ДИФФУЗИЯ ВЗАИМОДЕЙСТВУЮЩИХ ЭЛЕКТРОНОВ В НИЗКОРАЗМЕРНЫХ НЕУПОРЯДОЧЕННЫХ ТВЕРДЫХ ТЕЛАХ

Используя модель Хаббарда, вычислена плотность состояний многочастичных возбуждений. Для взаимодействующих электронов в одномерной неупорядоченной системе кулоновское отталкивание между сильно локализованными электронами приводит к делокализации.

Ключевые слова: неупорядоченные системы, электронный транспорт, квантовая локализация, электрон-электронное взаимодействие.