

Technische Universität Chemnitz-Zwickau

Sonderforschungsbereich 393

Numerische Simulation auf massiv parallelen Rechnern

R. A. Römer and M. Schreiber

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Preprint SFB393/97-18

Preprint-Reihe des Chemnitzer SFB 393

SFB393/97-18

August 1997

Author's addresses:

Rudolf A. Römer and Michael Schreiber, Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz

<http://www.tu-chemnitz.de/sfb393/>

Weak delocalization due to long-range interaction for two electrons in a random potential chain

Rudolf A. Römer and Michael Schreiber

Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

(Version: April 25, 1997; printed August 25, 1997)

Abstract

We study two interacting particles in a random potential chain by a transfer matrix method which allows a correct handling of the symmetry of the two-particle wave function, but introduces an artificial “bag” interaction. The dependence of the two-particle localization length λ_2 on disorder, interaction strength and range is investigated. Our results demonstrate that the recently proposed enhancement of λ_2 as compared to the results for single particles is vanishingly small for a Hubbard interaction. For longer-range interactions, we observe a small enhancement but with a different disorder dependence than proposed previously.

71.55.Jv, 72.15.Rn, 72.10.Bg

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Shepelyansky [1] recently argued that the Hubbard interaction between two particles in a random potential chain would reduce the localization in comparison with independent particles. In particular, he obtained an enhancement of the two-interacting-particle (TIP) localization length λ_2 independent of the statistics of the particles and of the sign of the interaction such that

$$\lambda_2/\lambda_1 \approx U^2\lambda_1/32 \quad (1)$$

in the band center. Here λ_1 ($\approx 105/W^2$ for small W [14]) is the single-particle (SP) localization length in one dimension (1D) and U the Hubbard interaction in units of the nearest-neighbor hopping strength. A Gaussian form was assumed for the distribution of the interaction matrix elements thereby ignoring possible correlations between these.

Support for this result was given by Imry [2] with the help of a Thouless-type block-scaling argument. Frahm *et al.* [3] used the transfer matrix method (TMM) to study the TIP problem without any approximations and found numerically that $\lambda_2/\lambda_1 \sim \lambda_1^{0.65}$. They also measured the distribution of the matrix elements of the Hubbard interaction in the disorder-diagonal basis of localized SP eigenstates and found a strongly non-Gaussian behavior contrary to Shepelyansky's assumption. An approximate calculation of λ_2 with a Green function method lead Oppen *et al.* [4] to the hypothesis $\lambda_2/\lambda_1 = 1 + C\frac{|U|}{\pi}\lambda_1$, with $C \approx 0.34$ for bosons and 0.36 for fermions. They also identified a scaling parameter $U\lambda_1$. Weinmann *et al.* [5] obtained delocalized states with $\lambda_2 \approx 25 > \lambda_1 \approx 11$ by an exact diagonalization study of the TIP Hamiltonian for disorder $W = 3$.

Following the approach of [3], we recently studied the TIP problem by a different TMM [6] and found that (i) the enhancement $\lambda_2(U)/\lambda_1$ decreases with increasing system size M , (ii) the enhancement $\lambda_2(1)/\lambda_2(0)$ is constant for given M and small W , (iii) $\lambda_2(0) = \lambda_1$ in the limit $M \rightarrow \infty$ only, and (iv) $\lambda_2 \approx \lambda_1$ for $M \rightarrow \infty$, i.e. the enhancement also vanishes completely in this limit. Unfortunately, the symmetry of the wave function remains unspecified in this TMM. Also, reconsidering the original approach of Shepelyansky [1] and Imry's block-scaling picture [2], we have recently shown [7] that the neglect of phase correlations leads to erroneous results in well-understood similar problems and thus may not capture the relevant physics of TIP. In this Letter, we first briefly review an alternative TMM also introduced already in [3] which allows a correct treatment of the symmetry of the electron wave function. We find in agreement with [6] that the enhancement $\lambda_2(1)/\lambda_2(0)$ is vanishingly small for a Hubbard interacting system. Finite- and long-range interactions lead to a somewhat larger enhancement, but the data nevertheless suggests that as before $\lambda_2(1)/\lambda_2(0) \approx \text{const.}$ for small disorder.

The Schrödinger equation for the TIP problem with Hubbard interaction is written in a suggestive form as

$$\psi_{n+1,m} = [E - (\epsilon_n + \epsilon_m) - U\delta_{n,m}]\psi_{n,m} - \psi_{n,m+1} - \psi_{n,m-1} - \psi_{n-1,m}, \quad (2)$$

where $n, m = 1, \dots, M$ are the two site indices of the particles, E is the total energy of both particles, and ϵ_n is the random potential at site n . In the following, we use a box distribution $[-W/2, W/2]$ for the ϵ_n . If one interprets (n, m) as Cartesian coordinates on a finite lattice with $M \times M$ sites, the problem becomes identical to a non-interacting Anderson model in 2D [8] but with a disorder potential symmetric with respect to the diagonal $n = m$ and hard-wall boundary conditions [3]. However, the symmetry of the fermionic electron wave function

remains unspecified. Therefore, we now define the center-of-mass coordinate $R = n + m$ and the particle distance $r = n - m$ and study the transfer in the R direction, that is along the diagonal, with a finite maximal two-particle distance r_{\max} . By the additional restriction $r \geq 0$, the symmetry $\psi_{n,m} = \psi_{m,n}$ of the spatial part of the electron wave function is now included. Unfortunately, the finite r_{\max} introduces an artificial “bag” interaction [1,3]: the particles feel an infinite attractive force whenever they are a distance r_{\max} apart. Obviously, the present task includes the distinction of any true interaction effect from the effects of the “bag”. As the latter occurs also for $U = 0$, we propose that $\lambda_2(1)/\lambda_2(0)$ and not $\lambda_2(1)/\lambda_1$ measures the enhancement due to U .

Applying the Hamiltonian to the wave function on the r th site of the R th layer in order to determine the amplitudes at the \tilde{r} th site in the $(R + 1)$ th layer, one has also to consider the as yet unknown amplitude at the $(\tilde{r} \pm 1)$ th site. This behavior can be encoded into a matrix $I(R)$. The explicit form of $I(R)$ for the present TIP problem is the same as for a SP Anderson model defined on a triangular lattice [12] but with hard-wall boundaries. We have to distinguish further between odd and even R , since the onsite Hubbard interaction at $r = 0$ occurs only for R even. The TIP problem (2) then reads

$$I(R + 1)\Psi(R + 1) = [E\mathbf{1} - \chi(R) - H_{\perp}]\Psi(R) - I(R - 1)\Psi(R - 1), \quad (3)$$

where $\Psi(R) = (\psi_{R,1}, \dots, \psi_{R,r}, \dots, \psi_{R,r_{\max}})$ is the wave vector of layer R , H_{\perp} is the SP hopping term for the transverse (r) direction and $[\chi(R)]_{i,r} = [\epsilon_{n(R,r)} + \epsilon_{m(R,r)} + U\Theta(s - |r| + \frac{1}{2})]\delta_{i,r}$ codes the random potentials and the interaction [3]. The step function Θ reflects the range s of the interaction. E.g., $s = 0$ corresponds to a Hubbard onsite interaction, $s = 1$ to a nearest-neighbor interaction for R odd and onsite interaction for R even, and so on. The transfer matrices $T(R)$ are then given by

$$T(R) = \begin{pmatrix} I(R)^{-1}[E\mathbf{1} - \chi(R) - H_{\perp}] & -\mathbf{1} \\ \mathbf{1} & \mathbf{0} \end{pmatrix}, \quad (4)$$

and the evolution of the state is determined by the matrix product $\tau(N) = \prod_{R=1}^N T(R)$ applied to an orthonormal set of initial vectors $[\Psi(1), \Psi(0)]^T$. In order to avoid numerical rounding errors, these vectors have to be reorthonormalized after about every 10th matrix multiplication as usual [8]. The eigenvalues $\exp[\pm 2\gamma_i(N)]$ of $[\tau^{\dagger}(N)\tau(N)]^{1/N}$ exist for $N \rightarrow \infty$ due to Oseledec’s theorem [9] and are obtained by summing the norms calculated in each orthonormalization. The smallest Lyapunov exponent γ_{\min} determines the slowest possible decay of the wave function and thus the largest localization length $\lambda_{\max} = 1/\gamma_{\min}$. We now *define* the TIP localization length $\lambda_2 = \lambda_{\max}/\sqrt{2}$. The factor accounts for the distance between successive layers in the R direction [10]. As usual, the accuracy of the numerical estimates for λ_2 is obtained not from the statistics of the exponents, but rather from the statistics of the changes [8].

In Fig. 1 we show results obtained by the present TMM to an accuracy of 5% for $W \leq 2$ and $r_{\max} = 600$ and at least 2% otherwise. We first note that the data for $r_{\max} = 600$ and $s = 20$ agree well with the results obtained [3] for $W \leq 4$ [10]. A simple power-law fit for $1.5 \leq W \leq 4$ yields $\lambda_2 \sim W^{-3.4 \pm 0.4}$. The λ_2 data for $r_{\max} = 200$ and $s = 0$ are smaller than the results obtained [6] by the TMM for unsymmetrized particles. Fitting a power-law behavior to these data for $1.4 \leq W \leq 4$, we find $\lambda_2 \sim W^{-3.9 \pm 0.2}$. We can also fit these

data reasonably well by $\lambda_2 = \lambda_1 + A\lambda_1^\alpha/(B + W)$ with $\alpha = 2$, $A = 0.5$ and $B = 1.3$ and $1.4 \leq W \leq 10$. Without W dependence or with an exponent $\alpha = 3/2$ as suggested in [13] the fits become considerably worse.

In Fig. 1 we have also plotted the behavior for $U = 0$, where the system reduces to two non-interacting particles in 1D. The following could be expected: For $U = 0$, the SP will localize independently at two arbitrary sites, say n_0, m_0 , with localization length λ_1 . The wave function can then be written as a symmetrized product of two SP wave functions with exponentially decaying envelope, i.e. $\psi_{n,m}^{(0)} \sim \exp[-|n - n_0|/\lambda_1] \exp[-|m - m_0|/\lambda_1] + \exp[-|m - n_0|/\lambda_1] \exp[-|n - m_0|/\lambda_1]$. Here, the SP eigenenergies $\pm E_0$ are chosen such that $E = 0$; then $\lambda_1 \equiv \lambda_1(E_0) = \lambda_1(-E_0)$. Two points are worth mentioning: (i) Suppose that $m < m_0 < n_0 < n$ and thus $r > r_0 = n_0 - m_0$. Then we have $\psi_{n(R,r),m(R,r)}^{(0)} = \exp[(r_0 - r)/\lambda_1] + \exp[-(r_0 + r)/\lambda_1]$ independent of R . The same happens for $m_0 < m < n < n_0$ ($r < r_0$). Thus the TMM in the R direction will necessarily encounter regions where the wave function is *constant*. This will lead to an overestimation of $\lambda_2(0)$ and thus an apparent enhancement already for $U = 0$. (ii) The non-interacting two-particle wave function $\psi_{n(R,r),m(R,r)}^{(0)}$ is not isotropic in the 2D plane (R, r) . Since the TMM will not necessarily measure the decay directly in the R direction, we expect that γ_{\min} will also contain information about the decay in other directions. These decay lengths of $\psi_{n(R,r),m(R,r)}^{(0)}$ are longer and thus we again expect $\lambda_2(0) \geq \lambda_1$.

Fig. 1 shows that the TMM indeed overestimates $\lambda_2(0)$. Consequently, the interaction-caused enhancement $\lambda_2(1)/\lambda_2(0)$ is much smaller than the previously [3] reported $\lambda_2(1)/\lambda_1$ and there is hardly any enhancement visible beyond the statistical fluctuations.

From Fig. 1 we see that for $W \geq 6$, the present data for $U = 0$ and $U = 1$ coincide with the SP TMM data already quite well. An enhancement λ_2/λ_1 shows only for small disorder ($W \leq 4$). However, in this region, the computed values of λ_2 become comparable to the size of the system such that an increasing part of the wave function reaches the “bag” boundary. We therefore studied the size dependence of the enhancement $\lambda_2(1)/\lambda_2(0)$ for various W and s . Typical data are presented in Fig. 2. For Hubbard interaction $s = 0$ and $r_{\max} \geq 200$ there is only a vanishingly small, if any enhancement within the numerical accuracy. Our data show nearly no dependence on the bag size for $r_{\max} \geq 200$, which confirms that the results in Fig. 1 are not influenced by the choice $r_{\max} = 200$. For $r_{\max} \geq 200$ we obtained $\lambda_2(0) \approx 22$ independent of r_{\max} . Thus λ_2 does not approach λ_1 for larger systems. We attribute this discrepancy from [6] to the artificial “bag” because the regions in which $\psi_{n,m}^{(0)}$ is independent of R as discussed above grow with increasing r_{\max} . Thus the decreasing influence of the hard-wall boundary conditions [6] is counterbalanced.

In [3] it was argued that a (constant) finite-range interaction gives a strong enhancement. Indeed, Figs. 1 and 2 show an enhancement for $s > 0$ independent of r_{\max} , but it is rather weak. In [11] it was argued that long-range interaction also leads to a strong enhancement. Our results for a Hubbard interaction with a tail $U/|r| >$ for $r \neq 0$ in Fig. 2 show an enhancement, but it is also only weak. It is comparable to the case $s = 8$ also for other $W \leq 4$.

The W dependence of our data for *small* $W < 4$ is the same within the numerical accuracy for all s and also for the long-range case. Thus the enhancement $\lambda_2(1)/\lambda_2(0)$ is the same for all such W , i.e., it does not grow with further decreasing W as suggested by Eq. 1. The case $W = 3$ shown in Fig. 2 is representative.

In summary, we have studied the interaction-induced enhancement of the localization length for two fermions in a 1D random potential by a TMM which appropriately takes into account the symmetry of the wave function. For a Hubbard interacting system we find a vanishingly small enhancement already for small system sizes $r_{\max} \geq 200$. Finite- and long-range interactions lead to a weak enhancement which persists even for large system sizes. However, this enhancement is much smaller than previously proposed. It is important that we compare with the localization length $\lambda_2(0)$ in the bag model and not with the SP result λ_1 as in [3], because only in this way we can account for the artificial “bag” interaction inherent in the symmetrized TMM. We note that similar results for the bag model have recently been obtained in Ref. [15]. Furthermore, the results of Ref. [15] suggest that after a discretization of the Schrödinger equation in more suitable center-of-mass and relative coordinates the enhancement vanishes completely even for longer range interactions.

ACKNOWLEDGMENTS

We gratefully acknowledge fruitful discussions with T. Vojta. This work has been supported by the Deutsche Forschungsgemeinschaft as part of Sonderforschungsbereich 393.

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FIGURES

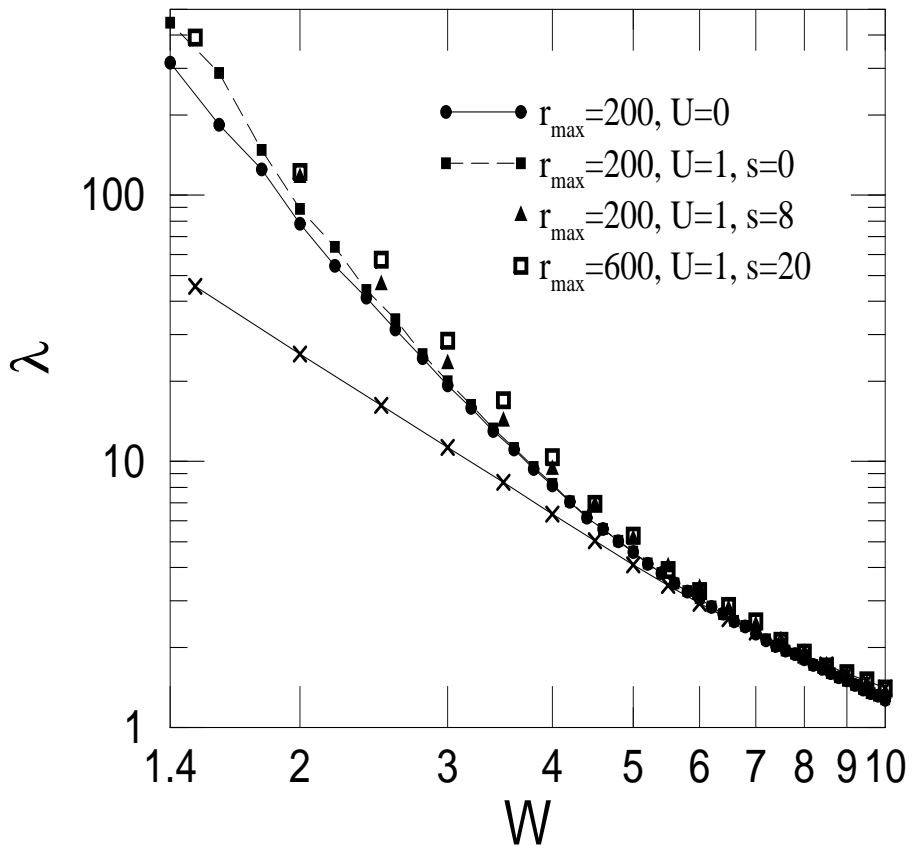


FIG. 1. Two-particle localization length λ_2 at energy $E = 0$. We also show TMM data (\times) for SP. The $U = 0$ data for $r_{\max} = 600$ and $r_{\max} = 200$ are so close that we only show the latter.

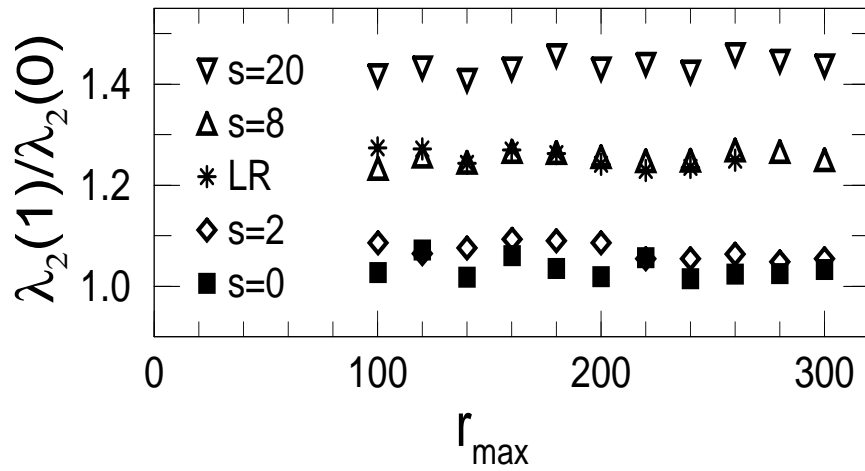


FIG. 2. TIP enhancement as a function of the “bag” size at $W = 3$ and $E = 0$ for various finite-range interactions and also a long-range interaction (LR).