Localization of two interacting particles in a one-dimensional random potential

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We investigate the localization of two interacting particles in a one-dimensional random potential. Our definition of the two-particle localization length, ξ, is the same as that of von Oppen *et al.* [Phys. Rev. Lett. **76**, 491 (1996)]. ξ's for chains of finite lengths are calculated numerically using the recursive Green's function method for several values of the strength of the disorder, W, and the strength of interaction, U. When $U=0$, ξ approaches a value larger than half the single-particle localization length as the system size tends to infinity and behaves as $\xi \sim W^{-\nu_0}$ for small W with $\nu_0 = 2.1 \pm 0.1$. When $U \neq 0$, we use the finite size scaling ansatz and find the relation $\xi \sim W^{-\nu}$ with $\nu = 2.9 \pm 0.2$. Moreover, data show the scaling behavior $\xi \sim W^{-\nu_0} g(b|U|/W^{\Delta})$ with $\Delta = 4.0 \pm 0.5$. [S0163-1829(97)07543-7]

Recently, there has been intensive attention[1–10] focused on the problem of the localization of two interacting particles in a one-dimensional (1D) random potential. With a few assumptions on the statistical nature of single-particle localized states, Shepelyansky[1] has mapped the problem approximately to a random band matrix model and obtained an expression for the two-particle localization length, ξ, as

$$\xi \simeq U^2 \frac{\xi_1^2}{32}, \tag{1}$$

where U is the on-site interaction in unit of the hopping energy between nearest neighbor pair sites, and ξ_1 the single-particle localization length. This expression is surprising because it implies that ξ can exceed ξ_1 at sufficiently small disorder, i.e., sufficiently large ξ_1. Later Imry[2] has provided a support for Eq. (1) by invoking the Thouless scaling argument. However, the methods employed in Refs. 1 and 2 are partly approximate and the strict validity of the expression of Eq. (1) is questionable as discussed in, e.g., Refs. 3–8 and 10.

Many authors[3–6] have tried to find more refined expressions than Eq. (1) by improving the assumptions of Shepelyansky. However, at this stage, there exist controversies yet as to the quantitative expression for ξ like Eq. (1). Frahm *et al.*[3] obtained the relation $\xi \sim \xi_1^{1.65}$ by the transfer matrix method while an approximate calculation of Green function by von Oppen *et al.*[5] leads to the hypothesis $\xi = \xi_1/2 + c|U|\xi_1^2$, where c is a constant depending on the statistics of the particles. With the assumption that the level statistics of two interacting particles is described by a Gaussian matrix ensemble, Weinmann and Pichard[6] argued that ξ increases initially as $|U|$ before eventually behaving as U^2. Moreover, very recently, Römer and Schreiber have claimed the disappearance of the enhancement as the system size grows (see Refs. 7 and 8).

Some of these discrepancies, especially between numerical studies, are due to different definitions for two-particle localization length between authors and also to lack of careful analysis of the finite size effect of the system size. The system under study is a ''quantum mechanical two-body problem'' in a sense. Motion of the two particles can be decomposed into the motion of the center of mass (CM) and that of the relative coordinate. We are interested in the CM motion since the wave function describing the relative motion would not be different from that arising from the single-particle localization problem in the thermodynamic limit if the interaction is short ranged. Therefore, in this paper, we use the same definition for ξ as introduced by von Oppen *et al.*[5] for the measure for localization length of the CM:

$$\frac{1}{\xi} = -\lim_{|n-m|\to\infty} \frac{1}{|n-m|} \ln|\langle n,n|G|m,m\rangle|. \tag{2}$$

Here, G is the Green function and $|i,j\rangle$ is a two-particle state in which the particle 1 (2) is localized at a site i (j). The above definition is reasonable for a description of the CM motion as long as U is smaller than or of the order of the hopping energy between sites.[5] In practice, we calculate ξ_N defined below in Eq. (4) for chains of finite lengths *without any approximation* for several values of W and U. We then estimate ξ by extrapolating ξ_N using the finite size scaling ansatz. When $U=0$, we find $\xi \sim W^{-\nu_0}$ with $\nu_0 = 2.1 \pm 0.1$. Data for $U \neq 0$ lead to the relation $\xi \sim W^{-\nu}$, with $\nu = 2.9 \pm 0.2$. Also the data lead us to propose a scaling form $\xi \sim W^{-\nu_0} g(b|U|/W^{\Delta})$, where $g(y)$ is a scaling function with the property $g(y \to 0) = \text{const}$ and $g(y \to \infty) \sim y^{(\nu-\nu_0)/\Delta}$. Δ is given as 4.0 ± 0.5.

We work within the tight-binding equation given by

$$\psi_{m+1,n} + \psi_{m-1,n} + \psi_{m,n+1} + \psi_{m,n-1} = (E - \epsilon_m - \epsilon_n - U\delta_{m,n})\psi_{m,n}, \tag{3}$$

where $\psi_{i,j} = \langle i,j|\psi\rangle$, E is the energy of the two particles, and $\delta_{m,n}$ the Kronecker delta. m and n are the site indices of a chain of length N and range from 1 to N, ϵ_m is the random site energy chosen from a box distribution with interval $[-W/2, W/2]$ (Ref. 11), and the hard wall boundary condition, i.e., $\psi_{0,n} = 0$ and so on, is used. As was previously noted,[3,7] if one interprets (m,n) as Cartesian coordinates of a square lattice of size $N \times N$, the Hamiltonian describes a single particle in a two-dimensional random potential. In Eq.

(2), the thermodynamic limit is first taken and then the limit $|n-m|\to\infty$. To estimate this quantity, we define a sequence ξ_N as

$$\frac{1}{\xi_N}=-\left\langle\left\langle \frac{1}{N-1}\ln|\langle 1,1|G_N|N,N\rangle|\right\rangle\right\rangle, \tag{4}$$

where G_N represents the Green function for a chain of length N and the double brackets represent the configurational average. To be specific, calculation of G_N amounts to evaluation of the inverse of the matrix, $(E-\mathcal{H})$, the size of which is $N^2\times N^2$. One can calculate several elements of G_N, i.e., the elements involving the sites of two opposite edges of the square lattice, very efficiently using the recursive algorithm of MacKinnon and Kramer.[12] We assume that ξ_N approaches ξ as $N\to\infty$.

The on-site interaction of the Hamiltonian given by Eq. (3) is relevant only to the spatially symmetric states, which would be realized, say, for a pair of electrons with total spin zero. One can easily see that the contributions to Eq. (2) are only from the spatially symmetric states from the following consideration. The Green's function represents the transition amplitude from an initial state to a final state and since the Hamiltonian, Eq. (3), is invariant under the exchange operation of two particles, the parity of the wave function is conserved during the time evolution. Since the initial state of Eq. (2) is a doubly occupied state, i.e., a spatially symmetric state, we are treating only the contributions from symmetric states.

Numerical calculations of ξ_N for various values of W, U, and N are performed for $E=0$ without approximation. N is varied within the range $10\leqslant N\leqslant 200$ and for a given parameter set, the configurational average is performed over sufficiently many different realizations to control the uncertainties of ξ_N within 1%.

We first examine the case of $U=0$, i.e., the noninteracting two particles. In this case, when the total energy of the system is fixed to E, the two-particle wave function is a superposition of the products of two single-particle states of energy E' and $E-E'$, and the Green function is given by the convolution of two single-particle Green functions as

$$\langle i,i|G(E)|j,j\rangle\sim\int dE'\langle i|G_0(E')|j\rangle\langle i|G_0(E-E')|j\rangle. \tag{5}$$

It is a nontrivial problem to calculate $\xi(U=0)$ since there exist contributions from various energies. Some authors[4,5] have assumed the relation $\xi(U=0)=\xi_1/2$, i.e., half the single-particle localization length, which should be, however, seriously examined. Our numerical data presented in Fig. 1 show that the assumption is not strictly valid. The filled symbols on the $N=\infty$ axis represent $\xi_1/2$ calculated from the expression $\xi_1\simeq 105/W^2$,[13] while the empty symbols are our numerical results for ξ_N. Taking into account the fact that the uncertainty of each data point is smaller than the symbol size, ξ_N does not seem to extrapolate to $\xi_1/2$ as N tends to infinity. Moreover, the discrepancy between the two quantities becomes larger as W gets smaller. Therefore, we conclude that within the definition of Eq. (2), the single-particle localization length is not an adequate parameter, if it is qualitatively, for a quantitative description of two-particle

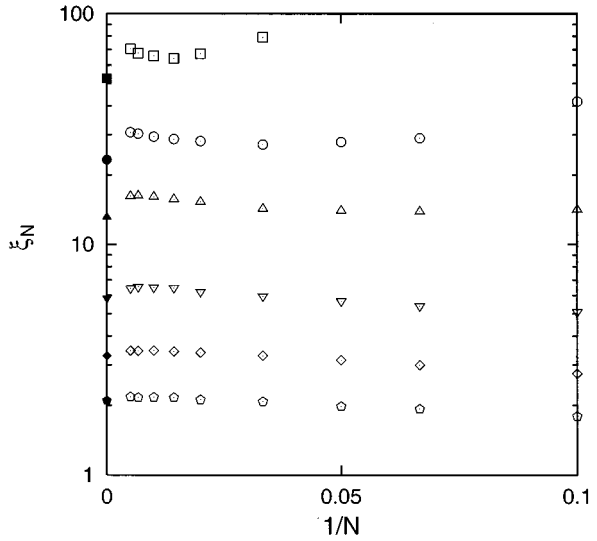

FIG. 1. ξ_N (open symbols) as a function of $1/N$ for $U=0$ and $\xi_1/2$ (filled symbols) calculated from the expression $\xi_1\simeq 105/W^2$: $W=1.0$ (box), 1.5 (circle), 2.0 (uptriangle), 3.0 (downtriangle), 4.0 (diamond), and 5.0 (pentagon), from top to bottom. The uncertainty of each data point is less than the symbol size.

localization problem. From the data of $N=200$, we get $\xi(U=0)\simeq 70/W^{\nu_0}$ with $\nu_0=2.1\pm 0.1$.

Next, we discuss the case of $U\neq 0$. Figure 2(a) shows the results for $U=1.0$ and W ranging from 0.5 to 10.0. The y axis label represents the renormalized localization length, i.e., ξ_N divided by the system size. For larger values of W and N, ξ_N/N behaves as $\sim 1/N$, which implies the convergence of ξ_N's to their constant limiting values. This means that the condition $N\gg\xi$ is well satisfied for these data. However, for smaller values of W, i.e., for W ranging from 0.5 to 1.5, it is not easy to deduce the value of ξ since ξ_N's increase steadily within the range of the N presented. Therefore we rely on the scaling idea,[12] which states that ξ_N/N is given by a function of a single parameter, i.e., N/ξ:

$$\xi_N/N=f(N/\xi). \tag{6}$$

The implication of Eq. (6) is that on a log-log plot all data points of Fig. 2(a) fall on a single curve when translated by $\ln\xi(W)$ along the x axis. As a result, $\xi(W)$'s can be obtained as fitting parameters. The result of data collapsing is shown in Fig. 2(b) for the data set $N\geqslant 50$. $\xi(W=5.0)$ has been obtained to be 2.87 ± 0.01 by fitting the data set for $W=5.0$ and $N\geqslant 50$ to the formula $\xi_N=\xi-A/N$,[14] where A is a constant. Other remaining values of $\xi(W)$'s are obtained by examining the amount of relative translations with respect to the data set of $W=5.0$. The scaling plot is quite good and one can see that the scaling function $f(x)$ behaves as

$$f(x)\sim\begin{cases}1/\sqrt{x} & \text{if } x\ll 1,\\ 1/x & \text{if } x\gg 1.\end{cases} \tag{7}$$

As was previously mentioned, the asymptotic behavior for $x\gg 1$ represents the convergence of ξ_N's to ξ. On the other hand, the behavior for $x\ll 1$ is very interesting since the same asymptotic behavior has been found for noninteracting disordered 1D systems.[13] For the noninteracting case, the resis-

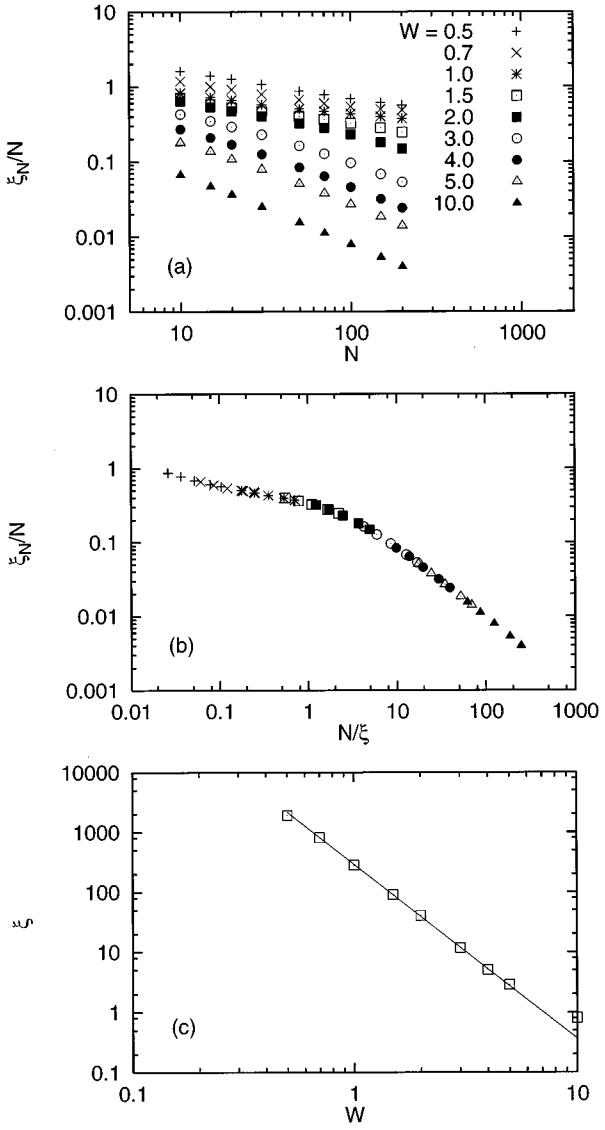

FIG. 2. (a) ξ_N/N as a function of N for $U=1.0$. (b) Scaling plot constructed from the data of (a) for $N \geqslant 50$. $\xi(W)$'s are obtained as fitting parameters by this procedure. (c) ξ as a function of W. The data for $W \leqslant 5.0$ fit well to a straight line of $\sim W^{-2.9}$ as shown.

tance ρ_N^0 of a chain of length N is related to the single-particle localization length ξ_N^0 as[13]

$$\rho_N^0 = [\cosh(2N/\xi_N^0) - 1]/2. \tag{8}$$

For $N/\xi_N^0 \ll 1$, the right hand side of Eq. (8) reduces to $\sim (N/\xi_N^0)^2 \sim N/\xi_1$. Therefore for the noninteracting case, the asymptotic behavior for $N \ll \xi_1$ represents the metallic behavior of the resistance, i.e., the linear increase of the resistance as the chain length in the metallic regime. Though no explicit expression like Eq. (8) is present for the system under study in this paper, we believe that the same asymptotic behavior for the two cases found here is a strong indication that the definition in Eq. (2) is a physically reasonable one.

The ξ's thus obtained as a function of W are plotted in Fig. 2(c).[15] For $0.5 \leqslant W \leqslant 5.0$ they are reasonably well fitted to the form of $\sim W^{-\nu}$, where ν is given by 2.9 ± 0.1. Within the error, this value for ν is different from $\nu_0 = 2.1 \pm 0.1$, i.e., the critical exponent for $U=0$, and from 4.0, which is the value expected by Eq. (1).

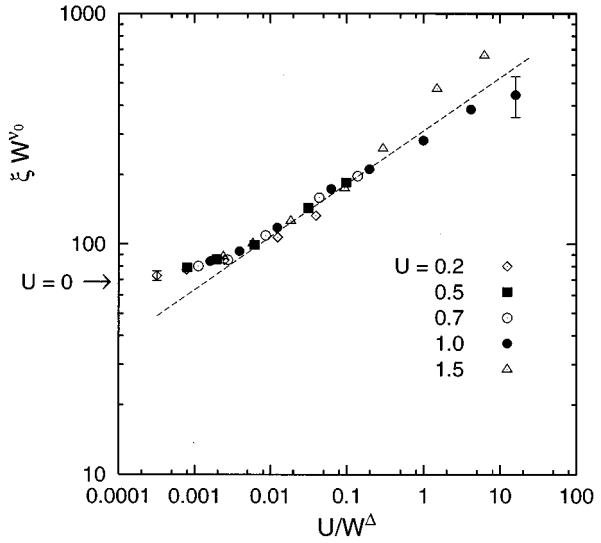

FIG. 3. The scaling plot of ξW^{ν_0} versus U/W^{Δ} with $\nu_0 = 2.1$ and $\Delta = 4.0$. The typical uncertainty of data for $W < 1.5$ ($W \geqslant 1.5$) is shown for the rightmost (leftmost) data point. The straight line is $\sim x^{0.23}$.

Further calculations and similar scaling analyses have been performed for other values of U, i.e., 0.2, 0.5, 0.7, and 1.5 up to system size $N=200$. It is difficult to determine ξ for $W<1.5$ and $U<1.0$ since the corresponding data of ξ_N's do not show scaling behaviors due to the fact that sufficiently large system sizes have not been reached for these parameters. The resulting ξ's (for $1.5 \leqslant W \leqslant 5.0$ if $U<1.0$ and for $0.7 \leqslant W \leqslant 5.0$ if $U>1.0$) give $\nu = 2.7$, 3.0, 2.9, and 3.1 for $U = 0.2$, 0.5, 0.7, and 1.5, respectively. Since we do not expect that ν depends on U, we interpret the variation of the values for ν as resulting from numerical uncertainties. Therefore our final result for the critical exponent of ξ is 2.9 ± 0.2.

Our result for ν implies that introduction of nonzero U changes the critical behavior of ξ and, in analogy with thermal critical phenomena, the point $W=U=0$ may be regarded as a multicritical point and the line $W=0$ as a critical line in the $W-U$ plane. Then, one may assume a scaling form for ξ as follows:

$$\xi = W^{-\nu_0} g(b|U|/W^{\Delta}), \tag{9}$$

where $g(y)$ is a scaling function, Δ a crossover exponent, and b a constant. Here, we used the fact that Eq. (3) is symmetric for $E=0$ so that ξ depends only on the absolute value of U. The scaling function should satisfy $g(y \to 0) = \text{const}$ and $g(y \to \infty) \sim y^{(\nu - \nu_0)/\Delta}$ for consistency. We obtain reasonably good scaling plots within the range $\Delta = 4.0 \pm 0.5$. The scaling plot for $\Delta = 4.0$ is shown in Fig. 3, where $\xi W^{2.1}$ is plotted against U/W^4 for various values of W and U. Although the data for $W<1.5$ may appear to deviate from the scaling curve, taking into account rather large numerical uncertainties of these data, one can expect that they are consistent with the scaling behavior of other data points. We expect that the crossover between the two asymptotic

behaviors occurs at $y\sim 1$ so that the constant b is estimated to be of the order of 100 from Fig. 3. Data within the range $0.01<U/W^{\Delta}<1.0$ $(1<y<100)$ approximately obey the form $\simeq y^{0.23}$, which is shown as a straight line. Since we expect the asymptotic behavior $\sim y^{(\nu-\nu_0)/\Delta}$ for this regime, we obtain $(\nu-\nu_0)/\Delta\simeq 0.23$, i.e., $\nu\simeq 3.0$, which is in good agreement with our previous estimate, i.e., $\nu=2.9\pm 0.2$. At this stage, we have not found a physical mechanism regarding the scaling parameter, U/W^{Δ} with $\Delta=4.0\pm 0.5$. The quantity $\xi(U)-\xi(U=0)$ might be also of interest. Our data show that this is consistent with a form $\xi(U)-\xi(U=0)\sim W^{-2.1}(U/W^4)^{1/2}$ in the region $bU/W^{\Delta}<1.0$. This behavior shows that the first correction to $g(y)$ for $y\ll 1$ is given as $\sim y^{1/2}$. On the other hand, our result confirms the enhancement of localization lengths due to the interaction. The arrow of Fig. 3 represents the value of ξW^{ν_0} for $U=0$, so that it is clearly seen that ξ monotonically increases with respect to U.

Finally, we point out differences between our work and some of those previously reported. References 3 and 7 deal with exactly the same system as ours but use a different definition for the two-particle localization length. As mentioned before, the problem can be considered as that of a noninteracting single particle in a two-dimensional potential. These authors study the evolution of a state along one of the edges of the square lattice. However, in this paper, we are concerned with the ''pair propagation,'' more generally, the propagation of the CM of the two particles. The definitions for ξ given by Eqs. (2) and (4) describes the propagation along one of the diagonals of the square lattice, instead of that along the edge. Our definition of ξ is exactly the same as that of von Oppen *et al.*[5] However it should be noted that in their work, calculation of ξ involves an approximation; the approximation scheme used in Ref. 5 fails for small values of U while our results are valid for all values of U.

In summary, we have investigated numerically the localization of two interacting particles in 1D random potential using the definition introduced previously for the two-particle localization length. While we find the enhancement of ξ by the interaction, critical properties of ξ are different from those reported in previous studies. We ascribe the differences to the approximation used in one case and, in the other cases, to a different definition of ξ. Further works are needed to connect the resistance and the two-particle localization length and to elucidate the relation between ξ and ξ_1.

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[11] Note that the definition of W in some previous studies, i.e., Refs. 1, 3, 4, and 6, is different from ours by a factor of 2.
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[14] Although this functional form is not theoretically based, the data fit quite well to this form. Therefore no significant error in our results is expected by using this form.
[15] The numerical uncertainty in ξ is somewhat larger for $W<1.5$ $[\delta(\ln\xi)\sim\delta\xi/\xi\sim 0.2]$ than that for $W\geqslant 1.5$ $[\delta(\ln\xi)\sim 0.05]$. This is because the data for $W<1.5$ lie in a rather flat range, as shown in Fig. 2(b), so that the scaling plot obtained by translations remains reasonably good within a comparatively broad range of ξ. Nevertheless, for Fig. 2(c), uncertainty of each data point is less than the symbol size.