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Testing the universality of the many-body metal-insulator transition by time evolution of a disordered one-dimensional ultracold fermionic gas

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It is now possible to study experimentally the combined effect of disorder and interactions in cold atom physics. Motivated by these developments we investigate the dynamics around the metal-insulator transition (MIT) in a one-dimensional Fermi gas with short-range interactions in a quasiperiodic potential by the time-dependent density-matrix renormalization group technique. By tuning disorder and interactions we study the MIT from the weakly to the strongly interacting limit. The MIT is not universal as time evolution, well described by a process of anomalous diffusion, depends qualitatively on the interaction strength. By using scaling ideas we relate the parameter that controls the diffusion process with the critical exponent that describes the divergence of the localization length. In the limit of strong interactions theoretical arguments suggest that the motion at the MIT tends to ballistic and critical exponents approach mean-field predictions.

Studies of the interplay of interactions and disorder have flourished in recent years [1–5]. The reasons for this renewed interest include cold atom experiments [1], more quantitative numerical simulations [2], and novel theoretical techniques [3,4]. Adding further appeal to this problem, numerical results of the many-body metal-insulator transition by time evolution of a disordered one-dimensional Hubbard model,

\[ V(n) = \lambda \cos(2\pi \omega n + \theta), \]  

with \( \omega \) irrational, \( \theta \in [0, 2\pi) \), and \( \lambda > 0 \). In the noninteracting limit a 1D tight-binding model with this potential and a hopping parameter \( J = 1 \) undergoes a metal-insulator transition (MIT) at \( \lambda_c = 2 \) [7]. As attractive interactions are turned on, \( \lambda_c \) decreases [8]. It is thus possible to study the role of interactions at the MIT from the weak- to the strong-coupling limit. We employ the term MIT instead of superconducting-insulator transition because according to Ref. [8] quasi-long-range order is already broken when the insulator transition occurs.

The model. We employ tDMRG [9] to study the dynamics of the \( L \)-site spin-1/2 Hubbard model,

\[ \mathcal{H} = -J \sum_{i=1,s}^{L-1} (\hat{c}_{i-1,s} \hat{c}_{i,s} + \text{H.c.}) + U \sum_{i=0}^{L-1} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} + \sum_{i=0}^{L-1} V(i) \hat{n}_i, \]  

in which \( \hat{c}_{i,\sigma} \) annihilates an atom at site \( i \) in spin state \( \sigma (\uparrow, \downarrow) \), \( \hat{n}_{i,\sigma} = \hat{c}_{i,\sigma} \hat{c}^{\dagger}_{i,\sigma} \), \( \hat{n}_i \equiv \hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow} \), \( U < 0 \) is the on-site interaction, and \( V(i) \) is given by (1) with \( \omega = (\sqrt{5} - 1)/2 \). The angle \( \theta \) is chosen so that \( V(i) \) is symmetric relative to the center of the system.

The tDMRG provides an efficient way to simulate the time evolution of a wave function obtained with DMRG. Our initial configuration (\( t = 0 \)) is the ground state of the Hamiltonian where the disordered potential (1) is replaced by a simple potential well of width \( \ell = 64 \) and depth \( D = 10 \) centered at the origin,

\[ V_{\ell < 0}(i) = D \Theta(|x_i| - \ell/2), \]  

where \( \Theta \) is the Heaviside function and \( x_i = i - (L - 1)/2 \) is the location of the site relative to the center of the system. For \( t > 0 \) we compute the real-time evolution (\( t > 0 \)) of this ground state under the Hamiltonian \( \mathcal{H} \) for \( L = 256 \) after the potential well is replaced by the quasiperiodic potential (1). \( \mathcal{H} \) is broken into terms affecting only two neighboring lattice sites. The time evolution operator \( e^{-i\mathcal{H}t} \), decomposed using the second-order Suzuki-Trotter breakup, is iteratively applied on the ground state obtained by finite system DMRG. The time step \( \Delta t \), measured in units of \( h/J \), satisfies \( 0.01 \leq \Delta t \leq 0.05 \) and \( m = 200 \) states have been kept in the DMRG simulation unless noted otherwise.

Before we proceed with the calculation we provide a brief overview of previous research on this model. In the noninteracting limit, \( U = 0 \), the MIT is described by a process

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of anomalous diffusion [10] controlled by the multifractal dimensions of the spectrum [7]. The localization length $\xi \propto |\lambda - \lambda_c|^{-\nu}$ diverges at the transition with $\nu \approx 1$ [11]. For $\lambda = 0$ the model is exactly solvable [12] for all $U$’s. For $|U| \gg 1$ it is mapped onto a weakly interacting hard-core Bose gas with a rescaled hopping parameter $J' \approx J^2/|U|$ [13]. This suggests that the MIT will occur at $\lambda_c \sim J^2/|U|$. For finite disorder and interactions there are already several studies about the static properties of Eq. (2) [8,14,15] and related models [16–20]. The dynamics of an interacting 1D Bose gas in a quasiperiodic potential was first investigated numerically in Ref. [16]. For a more recent study in which interactions are treated in a mean-field fashion we refer to Ref. [17]. In Refs. [8,15] it was found that, in a 1D Fermi gas with attractive interactions, $\lambda_c = \lambda_c(U)$ depends on the interaction and that weak disorder can enhance superfluidity. Renormalization group techniques were employed in Ref. [20] to study the weak disorder limit of spinless fermions in the Fibonacci chain, a quasiperiodic potential that is critical for each value of the coupling constant. For sufficiently weak interactions it was found in Ref. [14] that the spectrum of the Fibonacci chain is still multifractal. However, in the case of the potential (1) the system is already an insulator for $U < 0$ and $\lambda = 2$.

Results. In order to investigate the dynamics of (2) we first compute the $n$th order moment defined as

$$\langle x^n(t) \rangle = \left[ \frac{\sum_i |\Psi(t)\rangle |\hat{\delta}_i| \langle \Psi(t)\rangle}{\sum_i \langle \Psi(t)\rangle |\hat{\delta}_i| \langle \Psi(t)\rangle} \right],$$

in which $|\Psi(t)\rangle$ is the many-body wave function at time $t$. Here, $i = 0, 1, \ldots, L - 1$ runs over the site index and $\hat{\delta}_i = \sum_{\sigma} \hat{c}_i^{\dagger} \hat{c}_{i+1}^{\dagger}$ is the number operator at site $i$. We set $J = 1$, the number of fermions per spin to $N = 12$ and $L = 256$. Initially fermions are confined to sites 96–159 by the potential well $V_{i<\text{conf}}(i)$ (3). Then we study the time evolution after the potential well is removed and the quasipotential $V(i)$ is switched on at $t = 0$.

The results for $\langle x^2(t) \rangle$ and different $\lambda$’s are depicted in Fig. 1. The values $U = -6, -10$ correspond to the regime of strong coupling where the interaction energy is larger than the kinetic and potential energy due to the quasiperiodic potential. We clearly observe in Fig. 1 arrest of diffusion for sufficiently large $\lambda$. The critical disorder $\lambda_c < 2$ for which the MIT occurs decreases as $|U|$ increases. We have estimated $\lambda_c$ directly from $\langle x^2(t) \rangle$ by identifying a narrow region of $\lambda$’s for which the dynamics becomes substantially slower than in the metallic region and also by an explicit calculation of the participation ratio [8]. In the latter the critical $\lambda_c$ at which MIT occurs, for a fixed $(L,U)$, is identified as a maximum of the participation ratio as a function of $\lambda$. We have also found that $\lambda_c$ does not strongly depend on the filling factor provided that the chemical potential is far from the band edge.

In order to fit the numerical data we employ the ansatz,

$$\langle x^2(t) \rangle = x_0^2 [1 + (t/t_0)^\alpha],$$

where $x_0$, $t_0$, and $\alpha$ are fitting parameters. We note that this fitting function is only an educated guess. We choose it because, despite its simplicity, it led to a good description of the data. Other functions recently used in the literature [1] were also tried but the fitting was qualitative worse. Results of the best fit (see Fig. 1) are presented in Fig. 2 for different values of $U$ at $\lambda \approx \lambda_c$. It is observed that $\alpha$ depends on $U$ and it is different from the one for $U = 0$, $\alpha \approx 1 \approx 2dH$, where $dH$ is the Hausdorff dimension of the spectrum [7]. Therefore strong interactions modify substantially the dynamics at the MIT.

This is an important result. According to the one-parameter scaling theory [21] the parameter $\alpha$ is related to the critical exponent $\nu$ that labels the universality class of the MIT. Therefore different $\alpha(U)$ at the MIT correspond to different

FIG. 1. (Color online) $U = -10$: tDMRG calculation of $\langle x^2(t) \rangle$ Eq. (4) for, from top to bottom, $\lambda = 0.1, 0.15, 0.28$. Diffusion is clearly suppressed at $\lambda = 0.28$. The dashed line is the best, $\alpha \approx 1.54$, fitting function (5) around the MIT $\lambda = \lambda_c \approx 0.15$. $U = -6$: tDMRG calculation of $\langle x^2(t) \rangle$ (4) for, from top to bottom, $\lambda = 0.15, 0.25, 0.40$. The dashed line is the best, $\alpha \approx 1.48$, fitting function (5) around the MIT $\lambda = \lambda_c \approx 0.25$. In both figures $L = 256$ and $N = 12$. The maximum time $t_{\text{max}}$ that we can explore is dictated either by the stability of the DMRG simulation $(U,\lambda) = (-10.0.28),(-6.0.40)$ or by the growing importance of finite size effects for $t > t_{\text{max}}$ in the rest of the cases.

FIG. 2. (Color online) $\alpha$ [see text around (5) for details] vs the critical exponent $\nu$ that labels the universality class of the MIT. Therefore different $\alpha(U)$ at the MIT correspond to different

$\nu$. The latter is obtained by fitting (7) to $\Delta E = a e^{b(U-\lambda,\nu)}$ with $a,b, \nu$ fitting parameters, $L = 13$, and $\omega = 5/13$ in (1). Fitting is restricted to a small region $\lambda > \lambda_c$ such that $\xi < L$. Error bars were obtained by considering the stability of the results under small changes in $\lambda_c$ and the fitting interval. From left to right, the points correspond to $(U,\lambda_c) = (-10.0.15),(-6.0.25),(-3.0.47),(-2.0.70),(-1.1.01),(0.2)$. Quantitative agreement with the expression $\nu = \frac{\alpha}{dH}$ (solid line) is observed.
universalit
classes. An important concept of this theory is the dimensionless conductance \( g = E_T / \delta \), where \( E_T \), the Thouless energy, is the energy related to the typical time for a particle to cross a sample of size \( L \) and \( \delta \) is the mean level spacing. For a disordered metal (normal diffusion) \( g(L) \propto L^{D-2} \to \infty \) for \( L \to \infty \) since \( E_T \propto 1 / L^2 \) and \( \delta \propto 1 / L^D \). Analogously for an insulator \( g(L) \propto e^{-L/\xi} \) decays exponentially. A MIT is characterized by a scale independent \( g(L) = g_c \). Two mechanisms can lead to this scale invariance: localization effects that slow down the motion \((\chi^2(t)) \propto t^\alpha\) at the MIT and a multifractal spectrum [7], with the Hausdorff dimension \( d_H \), that induces an anomalous scaling of \( \delta \propto 1 / L^{D/d_H} \). Based on these arguments it was predicted in Ref. [21] that in \( D = 1 \) a MIT will occur provided that \( 2d_H = \alpha \). In the noninteracting limit this relation was verified in Refs. [7,10].

In the presence of repulsive interactions it has been suggested [22] that the scaling theory must include two parameters, \( g \) and the ratio between an energy related to interactions and the mean level spacing. For attractive interactions, especially in a quasiperiodic potential, the situation is less clear. In any case the above arguments, together with the numerical results above, provide a rather compelling albeit qualitative picture of the role of interactions: As \(|U|\) increases, \( \alpha > 1 \) increases and the motion becomes superdiffusive. According to the scaling theory, the MIT can occur only if \( d_H \) also increases. Physically that means that interactions smooth out the fractal properties of the spectrum at the MIT. The smoothing will be substantial when the interacting energy is much larger than the typical size of the subbands induced by the quasiperiodic potential around the Fermi energy. In this large \(|U|\) limit, corresponding to hard-core bosons, the spectrum is no longer fractal \((d_H \approx 1)\) and therefore the dynamics at the MIT \( \alpha = 2d_H \approx 2 \) approaches the ballistic limit. The numerical findings of Ref. [14] and the semi analytical results of Ref. [20] for spinless fermions fully support this picture. We note that [3] many features of the many-body MIT are similar to those of a single particle in a Cayley tree [23]. For this model \( \alpha = 2 \) and \( \nu = 1/2 \) around the MIT. It is thus tempting to speculate that these results also applies to the Hamiltonian (2) in the limit \(|U| \to \infty\).

Before we turn to the next observable a few comments are in order: (a) The fitting interval is long enough for disorder and interactions to strongly influence the motion. (b) The motion is slower as \(|U|\) increases. The length of the fitting interval (see below) increases accordingly. As a result, for \(|U| > 1\) the value of \( \alpha \) is more dependent on the interval. It is thus likely that additional transient terms are present in (5). We stick to (5) because the addition of more terms with a clear physical motivation would lead to ambiguous results. (c) The maximum time that we represent in the figures, and that it is used in the fittings, was chosen so that both the numerical error accumulation \((t \lesssim 1000)\) and finite-size effects that obscure localization are negligible. For the latter the maximum time strongly depends on \( U, \lambda \). This maximum time \( t_{\text{max}} \) for which finite-size effects are not important is chosen by imposing that the occupation number of the last five sites remains less than 0.01 and no sharp increases occur for smaller times. For instance, around \( \lambda \approx \lambda_c \), \( t_{\text{max}} \approx 650 \) for \( U = -10 \) but only \( t_{\text{max}} \approx 75 \) for \( U = -1 \).

![FIG. 3.](https://repository.kulib.kyoto-u.ac.jp/download/031602-3) (Color online) Participation number \( P(t) \) (6) for the same parameters as Fig. 1. A nonincreasing \( P(t) \) for \( t \to \infty \) is a signature of localization.

In order to obtain information of the time evolution of the full many-body wave function we have also computed the time-dependent participation number [24],

\[
P(t) = \frac{\left( \sum_i |\Psi(t)|^2 \right)^2}{\sum_i |\Psi(t)|^4},
\]

which, up to normalization factors, gives an estimation of the number of sites which, at a given time, are occupied (see Ref. [25] for more information). In an insulator \( P(t) \) will be constant for sufficiently long times but in a metal it will always increase with time. Even a steady increase indicates that at least some parts of the wave packet can escape localization. Therefore \( P(t) \) is an indicator of localization of the full wave packet. In Fig. 3 we plot \( P(t) \) for \( U = -10, -6 \) and different \( \lambda \)’s. The results are fully consistent with the previous calculation of moments. The transition is located around the same \( \lambda_c \) and no increase in time is observed for \( \lambda > \lambda_c \).

We note that it is feasible to study experimentally both \( \langle \chi^2(t) \rangle \) and \( P(t) \) in cold atom settings by single site-sensitive measurements that extract the probability of each site being occupied [26]. Therefore we expect that in the near future our theoretical findings about the location and dynamics of the MIT in strongly interacting 1D cold Fermi gases will encourage experimental research in this problem.

We now turn to further substantiate the nonuniversality of the MIT by an explicit calculation of the critical exponent \( \nu \). For that purpose we study the sensitivity of the ground state to a change of boundary conditions [18],

\[
\Delta E = E_P - E_L,
\]

where \( E_P \) and \( E_L \) stand for the ground state for periodic and antiperiodic boundary conditions, respectively. As the MIT is approached from the insulator side, \( \Delta E \propto e^{-L/\xi} \) with \( \xi \propto |\lambda - \lambda_c|^{-\nu} \). We exploit this relation to find \( \nu \), with \( L = 13 \). In Fig. 2 we present results for \( \nu(U) \) for different \( \alpha(U) \) at \( \lambda = \lambda_c \). It is observed that, as \( U \) increases, \( \nu \) decreases from its noninteracting value \( \nu \approx 1 \). This is an additional indication that the MIT in many-body systems is not universal. However, the expected approach to the mean-field limit \( \nu = 1/2 \) for \( U \gg 1 \) seems to be slow. Theoretical arguments [21,27] suggest that
the anomalous diffusion, through $\alpha(U)$, at the MIT is directly related to the critical exponent $\nu(U)$ that labels the universality class of the MIT. The simplest expression consistent with ideas and techniques employed in the noninteracting limit [11,14,27] is $\nu = 2$, which is in qualitative agreement (see Fig. 2) with the numerical results. Finally we note that the calculation of $\nu$ is rather crude and subjected to substantial uncertainties in the fitting procedure. This is especially true for the $U = -6, -10$ for which the value of $\alpha$ is rather sensitive to both the fitting interval and the details of the fitting function (5). For instance, for smaller intervals and fitting functions including additional transient terms, the values of $\alpha$ tend to be larger.

In conclusion, we have carried out a DMRG study of the MIT in an interacting 1D Fermi gas in a quasiperiodic potential. The main results of the paper are as follows: (a) The dynamics around the MIT is well described by a process of superdiffusion. (b) The MIT is not universal—critical exponents depend on the interaction strength and slowly approach mean-field predictions for sufficiently strong interactions. (c) Based on scaling arguments [21] we propose that for strong interactions the dynamics tends to ballistic and the localization length $\xi$ diverges at the MIT as $\xi \propto |\lambda - \lambda_c|^{-\nu}$ with $\nu \approx 1/2$. (d) Our results can be tested experimentally in cold atom settings.

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