Many-body localization transition in random quantum spin chains with long-range interactions

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Abstract – While there are well-established methods to study delocalization transitions of single particles in random systems, it remains a challenging problem how to characterize many-body delocalization transitions. Here, we use a generalized real-space renormalization group technique to study the anisotropic Heisenberg model with long-range interactions, decaying with a power $\alpha$, which are generated by placing spins at random positions along the chain. This method permits a large-scale finite-size scaling analysis. We examine the full distribution function of the excitation energy gap from the ground state and observe a crossover with decreasing $\alpha$. At $\alpha_c$ the full distribution coincides with a critical function. Thereby, we find strong evidence for the existence of a many-body localization transition in disordered antiferromagnetic spin chains with long-range interactions.

Introduction. – Long-range interactions between local quantum degrees of freedom, such as spins and quantum rotors, are ubiquitous in real materials, such as doped semiconductors and glassy systems. Anomalous magnetic properties of doped semiconductors, e.g. the low-temperature power-law divergence of their magnetic susceptibility, are thought to arise from local magnetic moments, positioned randomly [1–6]. These moments are coupled in the insulating phase within a finite range, limited by the localization length. In the metallic phase the coupling becomes long-ranged, decaying with a power of the distance between magnetic moments [7]. Low-temperature properties of a wide range of glassy systems can be modeled by 2-level systems describing the excitations of ions tunneling between local potential minima [8–11]. Dipole-dipole interactions between their dipole moments and elastic coupling between them lead to an effective model of random long-range coupled Heisenberg spins. Recently, there have been experimental indications of a novel quantum phase transition to a collective state in such a system [11]. Thus, a systematic analysis of long-range coupled quantum models is called for.

The random spin-(1/2) Heisenberg chain is considered to be the paradigm of disordered systems whose low-energy universal behavior is controlled by an infinite-randomness fixed point where all spins are bound to randomly located singlets, if the interactions are antiferromagnetic and short-ranged [12–15]. In real materials the interaction between local magnetic moments is longer ranged. Thus, it is an important open question of practical importance, if the strong disorder fixed point becomes destabilized and a delocalization transition to extended spin excitations is induced with increasing interaction range.

Dynamics and relaxation in disordered systems are characteristically different from ordered systems, as they involve distributions of relaxation times and activation energies. As noted earlier on, the physics of random systems is fully described by probability distributions of quantities like the activation energy [2]. An analysis based only on averages is likely to miss relevant physical processes such as rare events [16]. In this article we implement the real-space renormalization group method to investigate random quantum spin models with long-range couplings by analyzing full distribution functions of their excitation...
energy gaps from the ground state, $\epsilon_1$. When states are localized at different positions in space, they are uncorrelated and one expects the spacing between neighboring energy levels, such as $\epsilon_1$, to follow the Poisson level spacing distribution. In contrast, extended states overlap, causing power-law level repulsion, which results in the Wigner surmise distribution function of $\epsilon_1$. Therefore, the position and critical properties of delocalization transitions can be characterized by analyzing the distributions of level spacings in their vicinity [17].

The non-interacting Anderson model of disordered fermions with long-range hoppings, decaying with distance as $R^{-\alpha}$, is well known to show an insulator-metal transition as a function of the decay exponent $\alpha$. When $\alpha > d$, ($d$ is the dimension), all states are localized [18]. Localization means in this case that for length scales $r > \xi$, ($\xi$ the localization length), the eigenfunctions decay as $\psi(r) \sim r^{-\alpha}$. For $\alpha < d$, the eigenstates are extended, $\psi(r)$ does not decay with distance. One can detect the transition by calculating the inverse participation ratio $I_\alpha = \int |\psi(r)|^d \sim L^{-\xi_\alpha}$ [19–21]. For $\alpha < \alpha_c = d$, one finds $\tau_\alpha = d$ corresponding to extended states, whereas for $\alpha > d$, $\tau_\alpha = 0$, corresponding to localized states [18]. When $\alpha = d$ the system is critical and eigenfunction intensities exhibit multifractality, $\langle |\psi|^{2\alpha} \rangle \sim L^{-d_{\alpha, q}(q-1)-d}$, where $d_{\alpha}$ is the multifractal dimension of the $q$-th moment [21,22]. The critical inverse participation ratio scales with $L$ with power $\tau_\alpha = 3d - 2\alpha_0$, where $\alpha_0 > d$ is the multifractality parameter, which depends on system dimension and symmetries. We note that there are other classes of random models with long-range interaction, which do show a delocalization transition at $\alpha < d$. One such system is the model of non-interacting fermions with non-random long-range coupling and diagonal disorder [23]. Another example are the hierarchical models studied in ref. [24]. Random banded matrices with critical long-range coupling have been studied for $d = 1$ as paradigmatic models of Anderson metal-insulator transitions (MIT), allowing large length, numerical finite-size scaling.

**Random quantum spin chains.** – Here, we study random quantum spin chains [25] with long-range couplings $J_{ij} = J|\mathbf{r}_i - \mathbf{r}_j|^{-\alpha}$, where $0 < \alpha < \infty$. It is expected that there occurs a many-body transition between localized and delocalized states, at a critical $\alpha_c$. However, it is not yet known if $\alpha_c$ is equal to the non-interacting value $\alpha_0^d = d = 1$. It has been shown rigorously for clean spin chains with long-range exchange couplings that the ground state has long-range order when $\alpha < \alpha^* = 2d = 2$, based on an extension of the Mermin-Wagner theorem [26]. Since disorder tends to suppress long-range order, $\alpha^*$ is expected to decrease with disorder towards smaller values or even to vanish. Thus, one can expect that delocalization occurs first at an upper critical $\alpha_c$, before the transition to an ordered state happens at smaller $\alpha$, allowing for an intermediate phase, such as a spin glass phase. The aim of this article is to identify and characterize the delocalization transition.

We consider the Hamiltonian of the random XXZ Heisenberg model

$$H = \sum_{i,j} J_{x;ij} (S_{xi} S_{xj} + S_{yi} S_{yj}) + J_{z;ij} S_{zi} S_{zj},$$

(1)

with $r_i, r_j$ representing the $N$ sites, where a spin is placed, as chosen randomly from a lattice of sites at fixed density $N/L = 0.1$ with periodic boundary conditions. We assume antiferromagnetic coupling between all pairs of sites $i,j$ with $J_{ij} = J|\mathbf{r}_i - \mathbf{r}_j|^{-\alpha}$. Thus, the couplings $J_{ij}$ are randomly distributed with the typical coupling between nearest-neighbor spins $J_{nn} = J(L/N)^{-\alpha}$. The coupling between any spins in the chain cannot become smaller than the minimal coupling $J_{min} = J(L/2)^{-\alpha}$.

**Jordan-Wigner transformation.** It is insightful to use the Jordan-Wigner transformation which maps the spin chain equation (1) onto the Hamiltonian of interacting fermions. For $J_{z} = 0$ one thereby finds

$$H = \sum_{i,j} J_{z;ij} \left( c_i^+ c_j e^{i\pi \hat{n}_{ij}} + c_j^+ c_i e^{-i\pi \hat{n}_{ij}} \right),$$

(2)

where the operator $\hat{n}_{ij} = \sum_{i<j} \epsilon_n c_n^+ c_n$ counts how many fermions are encountered while hopping between the sites $i$ and $j$. For nearest-neighbor hopping this is exactly the Hamiltonian of non-interacting fermions with random hopping, which is known to show the Dyson anomaly: the eigenfunctions in the center of the band decay spatially with a stretched exponential, $\psi(x) \sim \exp(-\sqrt{2/t_0})$, where $t_0$ is a small length scale [27]. Away from the band center the eigenfunctions decay exponentially with localization length $\xi$, which diverges at the band center as $\xi \sim -\ln |\epsilon|$. The density of states is singular at half-filling, $\rho(\epsilon) = |\epsilon|^{-1} \ln |\epsilon|^{-3}$ [28]. Therefore, the expectation value of the nearest level spacing shifts to the small value $\Omega_N \sim \exp(-\sqrt{N})$. For longer-range hopping the interaction between the fermions manifests itself through the fluctuating phase factors in the hopping amplitudes, making this a challenging many-body problem.

**Real-space renormalization group.** – Let us therefore return to eq. (1) and apply the real-space renormalization group (RSRG) [12–15,25,29,30] procedure, which enables us to study larger systems numerically than with exact diagonalization [31]. One starts with the strongest coupled pair, say $(i,j)$, which in its ground state forms a singlet. Taking the expectation value of eq. (1) in that singlet state, performing second-order perturbation theory in the coupling with other spins [32], one obtains an effective Hamiltonian where the coupling between spins $(l,m)$ is renormalized. For the coupling between $x$- (or $y$)- and $z$-components one gets

$$\begin{align*}
(J_{x,m}^l)' &= J_{x,m}^l - (J_{i}^l - J_{i}^j)(J_{x,m}^l - J_{x,m}^j)/(J_{x,m}^i + J_{x,m}^j), \\
(J_{z,m}^l)' &= J_{z,m}^l - (J_{i}^l - J_{i}^j)(J_{z,m}^l - J_{z,m}^j)/2J_{x,m}^j.
\end{align*}$$

(3)
These renormalization rules are anisotropic and are valid as long as \( J_z \gg 0 \). For \( J_x \to 0 \), the Ising limit, the ground state becomes degenerate between the two Néel states, and degenerate perturbation theory yields the correct RG rules. When initially all couplings have the same anisotropy \( \gamma = J_{ij}^2/J_{ij}^0 \), the renormalization rules in eqs. (3) changes the anisotropy of the renormalized pair \( l_m \) to

\[
\gamma_{lm} = \gamma^{1+\gamma}/2.
\]

(4)

Thus, while the isotropic chain \( \gamma = 1 \) is a fixed point, any anisotropy drives the chain to i) the XX random singlet phase \( \gamma \to 0 \) for \( \gamma < 1 \), ii) the Ising antiferromagnet with staggered magnetization in the \( z \)-direction, \( \gamma \to \infty \) for \( \gamma > 1 \). We will focus here on the regime \( \gamma \to 0 \), \( J_z \to 0 \), the XX limit with long-range interactions in order to see if the random singlet phase is stable when longer-range interactions are added and to search for a possible many-body localization transition.

We implement the RSRG by iterating the RG rules in eqs. (3) for each realization of bare coupling parameters until the system has been completely decimated to one remaining effective bond whose energy excitation gap \( \epsilon_1 \) is recorded. The resulting distribution functions of such exit gaps for up to 300000 random realizations are subsequently analyzed as a function of the decay exponent \( \alpha \) and number of spins \( N \).

In fig. 1 we show the distribution functions of \( \epsilon_1 \) for random XX chains (\( J_z = 0 \), \( N = 128 \)) with antiferromagnetic interactions of power \( \alpha = 0.5 \). Results for true long-range coupling (brown curve) are compared with short-ranged couplings as obtained by including only nearest-neighbor (black), next-nearest-neighbor (red), next-next-nearest-neighbor (green) and next-next-next-nearest-neighbor (blue) interactions.

The distribution of \( \epsilon_1 \) of random spin chains of \( N \) spins with nearest-neighbor interactions is then known to be well described by the Weibull distribution

\[
P_W(\epsilon_1) = u_0^{1/z}N\epsilon_1^{1/z-1} \exp(-u_0\epsilon_1^{1/z}N),
\]

where \( 0 < z < \infty \), \( P_W \) is normalized, \( \int_0^\infty d\epsilon_1 P_W(\epsilon_1) = 1 \), and the expectation value of the excitation energy is \( \langle \epsilon_1 \rangle_W = \Gamma(1+1/z)/u_0^{1/z}N^{1/z} \), where \( \Gamma(x) \) is the Gamma function. At the infinite-randomness fixed point (IRFP) \( \zeta \) goes with system size \( N \) to infinity, \( \zeta \to \sqrt{N\alpha_0/l_0}/\ln N \) yields for the expectation value of the Weibull function, \( \langle \epsilon_1 \rangle \sim \exp(-\sqrt{N\alpha_0/l_0}) \), which is known to be the typical value of the excitation energy of model equation (2) with random nearest-neighbor hopping. We checked that nearest-neighbor results (black curves) are for all \( \alpha > 0 \) well modeled by the IRFP distribution, eq. (5), with \( z = \sqrt{N\alpha_0/l_0}/\ln N \). This is demonstrated in fig. 2 for values from \( \alpha = 0.1 \) to \( \alpha = 1 \) in steps of 0.1 for \( N = 64 \), where we find that the length scale \( l_0 \) in units of the initial distance between the spins \( \alpha_0 \) increases continuously with decreasing \( \alpha \) as shown in the inset. This is due to the fact that the initial distribution of exchange couplings narrows with decreasing \( \alpha \), so that the flow to the strong disorder fixed point occurs at larger length scales \( L > l_0 \). The parameter \( u_0 \), which shifts the center of the distribution function, is fitted and found to decrease as \( \alpha \) is increased.

The distribution changes strongly when couplings to farther sites are added [39]. Chains with both nearest- and next-nearest-neighbor couplings correspond to zig-zag chains, which have been studied in ref. [40], where it was concluded that the distribution is given by eq. (5) with a finite \( \zeta \). Similarly, one may expect that chains with further, but finite-range couplings are given by eq. (5) with another finite \( \zeta \). We note that \( \zeta = 1 \) corresponds to the distribution function of localized levels, the Poisson level spacing distribution \( P(\epsilon) = \exp(-\epsilon_1/\Delta) \). It is well known that
the level spacing of extended states is well described by the Wigner surmise, which for time reversal invariant systems (GOE) gives

$$P_{\text{GOE}}(\epsilon_1) = \frac{\pi}{2} \frac{\epsilon_1}{\Delta} \exp(-\frac{\pi}{4}(\epsilon_1/\Delta)^2).$$  \tag{6}

$P_{\text{GOE}}$ is normalized such that $\int_0^\infty d\epsilon_1 P_{\text{GOE}}(\epsilon_1) = 1$ and $\int_0^\infty d\epsilon_1 \epsilon_1 P_{\text{GOE}}(\epsilon_1) = \Delta$. At the delocalization transition critical states are known to obey critical level spacing distributions, conjectured to be of the form [41],

$$P_c(\epsilon_1/\Delta) = B(\epsilon_1/\Delta^2) \exp(-A(\epsilon_1/\Delta)^3).$$  \tag{7}

Note that this distribution is normalized $\int_0^\infty d\epsilon_1 P_c(\epsilon_1) = 1$ and the first moment is $\langle \epsilon_1 \rangle = \Delta$. We will further analyse random spin chains with a finite-range interaction in ref. [42]. Here, we concentrate on random spin chains with truly long-range, antiferromagnetic interactions. In fig. 3 we show results for distribution functions of $\epsilon_1$, scaled by their first moments. We observe that by lowering the decay exponent $\alpha$, rendering the interactions more long-ranged, the distribution functions are moved towards higher energies and become more narrow. Strikingly, a sharp cutoff is observed at large $x = -\log(\epsilon_1)$ for all $\alpha$ considered. This cutoff coincides exactly with the excitation energy of a singlet of spins which are coupled by the bare coupling at maximal distance $L/2$, which for XX chains depends on chain length $L$ as $\epsilon_{\text{min}} = 1/2J(L/2)^{-\alpha}$. Thus, that lower limit to the excitation energy has to be taken into account in deriving the distribution function. Therefore, we conjecture that for all $\alpha$ the distributions are modified by a cutoff factor of form $\exp(-c/(x_{\text{max}} - x))$, with an essential singularity at $x_{\text{max}} = \alpha \log(L/2) + \log(2/J)$.

In fig. 3(b) we show numerical results for $\epsilon_1$ as obtained from the RSRG from the 3rd last RG step\footnote{Here, we took the excitation energy of the strongest singlet pair of the 3rd last RG step. Accordingly $x_{\text{max}} = \log[2] + \alpha(\log L/6)$. We found that the distribution of the excitation energy from the singlet in the last RG step of the chain with true long-ranged coupling is masked too much by the cutoff function, so that one cannot determine $\alpha_c$ accurately.} together with a plot of the analytical critical distribution functions eq. (7) with $\Delta = N^{-\beta}$, with $\beta = 1$, $A = 2$ and $B = 4$ (red curve in fig. 3(b)), multiplied with the cutoff function ($c = 4$) and normalized. We find that for $N = 128$ it fits the data very well at $\alpha = 1.6$ (red line). Thus, this crossover in the level distribution function could be an indication of a many-body localization-delocalization transition at $\alpha_c = 1.6$. We performed the calculations also for larger system sizes $N = 320$. The result is shown in fig. 4 together with the critical distribution function multiplied with the cutoff function ($c = 8$) with $x_{\text{max}}(L = 3200)$ and normalized (red curve) fits the data well for $\alpha = 1.6$. As additional evidence for the delocalization transition we plot in fig. 4 the Poisson level distribution function multiplied with the same cutoff function ($c = 8$) and normalized (blue curve) for $\alpha = 2.2$, which confirms that states are localized there, while for $\alpha = 0.8$ the data fits the orthogonal Wigner surmise multiplied with the cutoff function (orange curve), indicating that the states are extended. For $\alpha = 0.6$ the unitary Wigner surmise (brown curve) multiplied with the cutoff function fits the data well. This can be explained by the fact that the phase factors in eq. (2), correspond to random magnetic-field factors, when neglecting their quantum dynamics, which break time reversal symmetry and change the universality class to the unitary one. For $\alpha < 1$ the density of states at small energies becomes more sparse and deviations from the Wigner surmise are seen. This can be an indication of a reduction of the density of states, due to the long-range interactions. In fact a mean-field theory analysis yields a logarithmic Coulomb gap for $\alpha = d = 1$ and a power-law pseudogap for $\alpha < 1$ [9,43].

Turning on the $z$-coupling towards the isotropic Heisenberg chain the RG rules are still given by eqs. (3) and we do not find a qualitative change of this delocalization

![Fig. 3](image-url) (Colour on-line) Distributions of $\epsilon_1$ in random long-range coupled XX spin chains for (a) $\alpha = 0.5, 1.0, 2.0$ and $N = 32, 64, 128, 256$ (black, red, green, blue line), rescaled by their first moments. (b) $\alpha = 1.2$ to $\alpha = 2$ (from left to right) in steps of 0.1, $N = 128$. Red line: critical function, eq. (7), multiplied with a cutoff function, $\exp(-c/(x_{\text{max}} - x))$, $c = 4$ for $\alpha = 1.6$.

![Fig. 4](image-url) (Colour on-line) Distribution function for $N = 320$ together with the critical distribution function multiplied with the cutoff function ($c = 8$) with $x_{\text{max}}(L = 3200)$ for $\alpha = 1.6$ and normalized (red curve), the Poisson level distribution function (blue curve) for $\alpha = 2.2$, the orthogonal Wigner surmise for $\alpha = 0.8$ (orange curve), and the unitary Wigner surmise for $\alpha = 0.6$ (brown curve), all multiplied with the same cutoff function ($c = 8$) and normalized.
physics. The excitation gap becomes enhanced by a factor 2 changing only the quantitative value of $\alpha_c$. In the Ising limit, the renormalization rules change (see footnote 1) since the ground state becomes degenerate. Random Ising spin chains with long-range coupling have been studied in ref. [44], where it was found that all excitations are short-ranged for $\alpha > 2$, while a correlated spin glass phase with $T_c = 0$ exists for $1 < \alpha < 2$. Recently, a quantum Ising model with long-range interactions has been considered finding a strong disorder fixed point with a dynamical exponent $z = \alpha$ [45].

Conclusions and discussion. – In conclusion, we analyzed the full distribution functions of the first excitation energy $\epsilon_1$ from the ground state of the anisotropic Heisenberg model with long-range interactions, decaying with a power $\alpha$, as generated by placing spin sites at random positions along the chain. In the XX regime we find critical values $\alpha_c$ where the distribution of excitation energies coincides with the critical distribution function, indicating that for smaller $\alpha < \alpha_c$ there is an extended phase.

We will perform in ref. [42] a more extensive finite-size scaling analysis of the spectral statistics using previously developed methods [17] in order to establish the criticality and to extract the critical parameters.

Since one of our motivations for this work was to contribute to an understanding of the anomalies in the magnetic properties of doped semiconductors, we may ask if the crossover in the distribution function of excitation energies can be experimentally detected by measuring the temperature dependence of the magnetic susceptibility $\chi(T) = n_{FM}(T)/T$, where $n_{FM}(T)$ is the number of free magnetic moments at temperature $T$. At the IRFP, one obtains with the singular behavior of $\rho(\epsilon) = |\epsilon|^{-1} \ln |\epsilon|^{-3}$, that $n_{FM}(T) \sim n_{M} \int_{0}^{T} d\epsilon \rho(\epsilon) \propto n_{M}/\ln^{2} T$. Thus, one finds a logarithmic reduction of the paramagnetic susceptibility. We expect, when interactions range beyond nearest neighbor, a crossover to Poissonian distribution and to the constant density of states $\rho(\epsilon) = \rho_0$. Accordingly, one expects that $\chi(T) \to n_{M}\rho_0$, which is independent of temperature. Thus, we conclude that the suppression of the singularity of the density of states, when increasing the range of the interaction, weakens the singularity in the magnetic susceptibility. Thus, we may expect a decrease of the magnetic susceptibility as the doping is increased from the insulator towards the metal phase. On the other hand, the many-body delocalization transition in the spin degrees of freedom cannot be observed in such thermodynamic measurements since the average density of states is unchanged at this quantum phase transition. Rather, in order to detect the delocalization transition we suggest time-dependent measurements such as spin echo experiments.

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