

# Excitation transfer in disordered spin chains with long-range exchange interactions

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## 1 Abstract

2 We examine spin excitation or polarization transfer via spin chains with long-range ex-  
 3 change interactions in the presence of diagonal and off-diagonal disorder. To this end,  
 4 we determine the mean localization length of the single-excitation eigenstates of the  
 5 chain for various strengths of the disorder. We then identify the energy eigenstates of  
 6 the system with large localization length and sufficient support at the chain boundaries  
 7 that are suitable to transfer an excitation between the sender and receiver spins con-  
 8 nected to the opposite ends of the chain. We quantify the performance of two transfer  
 9 schemes involving weak static couplings of the sender and receiver spins to the chain,  
 10 and time-dependent couplings realizing stimulated adiabatic passage of the excitation  
 11 via the intermediate eigenstates of the chain which exhibits improved performance.

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## 1 Introduction

Excitation or polarization transfer in interacting few- and many-body quantum systems plays a key role in many branches of science and technology, ranging from photosynthesis, where photon energy is transferred from a light-absorbing center to a reaction center via collections of near-resonant two-level systems (spins) [1], nuclear magnetic resonance of large molecules involving many interacting spins [2], or quantum state transfer in various spin chains realized, e.g., by dopants in solids [3–5], arrays of polar molecules [6, 7], superconducting qubits [8], ions in traps [9, 10] or Rydberg atoms in microtraps [11]. Whereas spin chains are commonly described in the nearest-neighbour approximation, experimentally relevant systems often possess long-range exchange interactions, or hopping, scaling with distance  $r$  as  $J \sim 1/r^\nu$  with the resonant dipole-dipole interaction,  $\nu = 3$ , being most frequently the case [1, 2, 5–7, 11].

Many of such systems are inherently disordered. Diagonal disorder leads to exponential (Anderson) localization of all the eigenstates of one-dimensional systems [12–14], which would suppresses excitation transfer in sufficiently long spin chains. Off-diagonal disorder also leads to localization which, however, may be weaker than exponential [15–17]. The localization properties of the system with long-range exchange interaction are more subtle [18–23] and many features still merit further investigation, which is one of the motivations of the present work.

Specifically, we study disordered spin chains – collection of two-level atoms, molecules or spins arranged in nearly periodic quasi one-dimensional array and coupled with each other by the resonant dipole-dipole exchange interaction. We raise the questions whether or not, and to what degree, such a disordered system can serve for excitation or spin polarization transfer between the sender and the receiver spins coupled to the opposite ends of the chain in a controllable way. To that end, we first determine the (single-excitation) localization properties of the system and their dependence on the energy, comparing and contrasting spin systems with long-range and nearest-neighbor exchange interactions. Obviously, only chains of length smaller or comparable to the longest localization length can transfer excitation between the two ends. Next we identify the energy eigenstates that have sufficient support at the two ends of the chain to strongly couple to the sender and receiver spins. We then explore two excitation transfer protocols, one that involves static resonant couplings of the sender and receiver spins to the most suitable eigenstate of the chain [24, 25, 25], and the other inspired by stimulated Raman adiabatic transfer [26–28] that involves counterintuitive time-dependent couplings of the sender and receiver spins to the corresponding eigenstate of the chain. We find that the adiabatic coupling, despite being slower than the static coupling scheme, leads to a much higher probability of excitation transfer as it is more robust to various sources of disorder.

The paper is organized as follows. In Sec. 2 we introduce the Hamiltonian of the system involving a collections of spins (two-level systems) with long-range resonant dipole-dipole exchange interactions and formulate the transfer problem. In Sec. 3 we consider disordered spin chains and numerically determine the localization lengths for different single-excitation eigenstates of the system in the presence of energy (diagonal) and position (off-diagonal) disorder. In Sec. 4 we present two excitation transfer protocols between the sender and receiver spins resonantly coupled to a suitable energy eigenstate of a spin chain with no disorder. In Sec. 5 we extract the mean transfer probability for chains of different length with different strength and type of disorder. Our conclusions are summarized in Sec. 6.

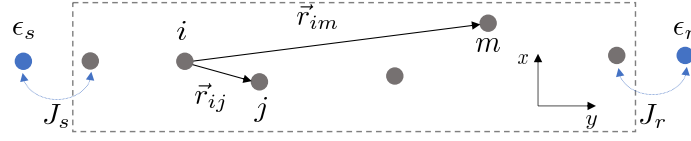


Figure 1: Schematic of a position (and energy) disordered chain of spins  $i, j, \dots, m, \dots$  in the  $xy$  plane. The spin chain is coupled with rates  $J_{s,r}$  to the sender (s) and receiver (r) spins having energies  $\epsilon_{s,r}$ .

## 67 2 The system

68 We consider a chain of  $N$  spins – two-level systems – interacting with each other via the long-  
 69 range exchange interactions  $J_{ij} = C_3(1 - 3 \cos^2 \theta_{ij})/|\vec{r}_{ij}|^3$ , where  $C_3 \propto |\vec{\phi}|^2$  is the electric  
 70 or magnetic dipole-dipole interaction coefficient,  $\vec{r}_{ij}$  is the position vector between spins  $i$   
 71 and  $j$ , and  $\theta_{ij}$  is the angle between the direction of the dipole moments  $\vec{\phi}$  and the position  
 72 vector between the spins. We account only for the near-field part of the total dipole-dipole  
 73 interaction potential and neglect the retardation and spontaneous radiative decay of the spin  
 74 excitations [29,30], assuming that the typical distance between the spins is much smaller than  
 75 the wavelength of the transition between the spin-up and spin-down states. The Hamiltonian  
 76 of the system is

$$\mathcal{H} = \frac{1}{2} \sum_{i=1}^N \epsilon_i \hat{\sigma}_i^z + \sum_{i \neq j}^N J_{ij} (\hat{\sigma}_i^+ \hat{\sigma}_j^- + \hat{\sigma}_j^+ \hat{\sigma}_i^-), \quad (1)$$

77 where  $\epsilon_i$  is the excitation energy of spin  $i$ ,  $\hat{\sigma}_i^{x,y,z}$  are the Pauli spin operators and  $\hat{\sigma}_i^\pm = \frac{1}{2}(\hat{\sigma}_i^x \pm i\hat{\sigma}_i^y)$   
 78 are the raising and lowering operators. We assume that all the spins are positioned in one  
 79 ( $xy$ ) plane (see Fig. 1) and their dipole moments ( $\vec{\phi} \parallel \hat{z}$ ) are perpendicular to that plane,  
 80  $\theta_{ij} = \pi/2 \forall i, j$ , thus  $J_{ij} = C_3/|\vec{r}_{ij}|^3$ .

81 We assume that a sender and a receiver spins are coupled in controllable way to the oppo-  
 82 site ends of a finite spin chain, see Fig. 1. The spin chain is assumed initially fully polarized,  
 83 with all the spins unexcited. Our aim is to transfer an excitation between the sender and  
 84 receiver spins via the spin chain. To this end, we need to identify and employ extended eigen-  
 85 states of the disordered chain having sufficient support at its two ends in order to strongly  
 86 couple to sender and receiver spins and mediate the transfer. To selectively couple the sender  
 87 and receiver spins to the suitable eigenstates of the chain, we assume that their energies  $\epsilon_s$ ,  
 88  $\epsilon_r$  and couplings  $J_s, J_r$  to the first and last spins of the chain can be precisely controlled, un-  
 89 like the energies and couplings of the spins in the disordered chain. Initially, the excitation is  
 90 localized at the sender spin, while the spin chain contains no excitations, and our aim will be  
 91 to retrieve the excitation from the receiver spin at a specific time  $\tau$  to be determined below.

92 We next examine the localization length of the single-excitation eigenstates of spin chains  
 93 in the presence of diagonal disorder corresponding to energy disorder of individual spins, and  
 94 off-diagonal disorder in the interspin couplings stemming from the position disorder of the  
 95 spins.

## 96 3 Localization lengths in disordered spin chains

97 We impose diagonal disorder corresponding to random variations of the spin excitation en-  
 98 ergies  $\epsilon_j = \epsilon_0 + \delta\epsilon_j$  around some  $\epsilon_0$  (which can be set to 0) with  $\delta\epsilon_j$  having a Gaussian  
 99 probability distribution  $P(\delta\epsilon) = \frac{1}{\sqrt{2\pi\sigma_\epsilon^2}} e^{-\frac{\delta\epsilon^2}{2\sigma_\epsilon^2}}$  with the mean  $\langle \delta\epsilon \rangle = 0$  and variance  $\sigma_\epsilon^2$ . Next,

100 the position of each spin  $j$  is given by the coordinates  $(x_j, y_j)$ . In an ideal 1D lattice with period  
 101  $a$ , we would have  $x_j = aj$  and  $y_j = 0$  for all spins  $j = 1, 2, \dots, N$ , and the exchange interaction  
 102 strength between the nearest-neighbor spins would be  $J = C_3/a^3$ , the next-nearest neighbors  
 103  $J/2^3$ , etc. We impose the position disorder via  $x_j \rightarrow aj + \delta x_j$  and  $y_j \rightarrow \delta y_j$ , where the  
 104 random variables  $\delta x_j$  and  $\delta y_j$  have a Gaussian probability distribution  $P(\delta\mu) = \frac{1}{\sqrt{2\pi\sigma_\mu^2}} e^{-\frac{\delta\mu^2}{2\sigma_\mu^2}}$   
 105 ( $\mu = x, y$ ) around mean  $\langle \delta\mu \rangle = 0$  with variance  $\sigma_\mu^2$ . The position disorder then translates to  
 106 off-diagonal (interspin coupling) disorder in the Hamiltonian (1).

107 In the limit of  $N \rightarrow \infty$ , disorder leads to (Anderson) localization of all the eigenstates of  
 108 the system [12–14]. The wavefunction  $\psi_k(x)$  of each single-excitation eigenstate  $|\psi_k\rangle$  is then  
 109 localized around some position  $\mu_k$  with the localization length  $\xi_k$ . An important characteristic  
 110 of the system is the dependence of the localization length  $\xi_k$  on the energy  $E_k$  of the eigenstates  
 111 to be used for the excitation transfer. To determine the localization length, we numerically  
 112 diagonalize the Hamiltonian for sufficiently long chains ( $N = 1000$  spins) to neglect the finite  
 113 size effects, and then for each eigenstate we identify the position  $\mu_k$  corresponding to the  
 114 maximum (in absolute value) of the wavefunction  $\psi_k(x)$  and subsequently fit an exponential  
 115 function

$$|\psi_k(x)| \propto e^{-\frac{|x-\mu_k|}{\xi_k}} \quad (2)$$

116 to the spatial profile of the eigenstate, extracting thereby the localization length  $\xi_k$ . We note  
 117 that the thus obtained localization length is a convenient measure of the spatial extent of the  
 118 wavefunction even if it is not exponentially localized (see below).

119 A more common measure to quantify the localization properties of the eigenstates is the  
 120 inverse participation ratio (IPR) [31]. It is, however, not suitable for our purposes, since IPR  
 121 cannot determine whether a wavefunction is spatially localized on a number of neighboring  
 122 sites or is delocalized on a similar number of remote sites [32]. We use, therefore, an alterna-  
 123 tive method to verify that the localization length  $\xi_k$  extracted from the exponential fit (2) is  
 124 a reliable quantity to characterize our system. We can partition the chain into two halves and  
 125 for each eigenstate  $|\psi_k\rangle = \sum_{i=1}^N v_i^{(k)} |i\rangle$  calculate the excitation number variance in one of the  
 126 halves [35],

$$\Delta n_k^2 = \langle \hat{n}^2 \rangle - \langle \hat{n} \rangle^2, \quad (3)$$

127 where  $\hat{n} = \sum_{i=1}^{N/2} \hat{\sigma}_i^+ \hat{\sigma}_i^-$  is the excitation number operator with eigenvalues  $n = 0, 1$  since we  
 128 consider only single-excitation states. The variance is therefore given by

$$\Delta n_k^2 = p_k - p_k^2, \quad (4)$$

129 where  $p_k = \sum_{i=1}^{N/2} |v_i^{(k)}|^2$  is the probability to find the excitation in the left half of the chain.

130 Clearly, for a strongly localized state with  $\xi/a \ll N/2$ , the probability  $p$  is either close to  
 131 0 or close to 1 (unless the wavefunction is localized near the center of the chain,  $\mu/a \simeq N/2$ ,  
 132 the probability of which is  $2\xi/(aN) \ll 1$ ), and the number variance is small,  $\Delta n^2 \rightarrow 0$ . In the  
 133 opposite limit of a completely delocalized wavefunction  $\xi/a > N$ , the probability is  $p \simeq 1/2$   
 134 and the number variance approaches the maximum  $\Delta n^2 \rightarrow 1/4$ . Assuming an exponentially  
 135 localized wavefunction  $\psi(x)$  of the form (2), we can calculate  $p$  for any position of the peak  
 136  $\mu$ , and upon averaging over the peak positions  $\mu/a \in [1, N]$  we obtain a relation between  
 137  $\Delta n^2$  and  $\xi/N$  shown in the inset of Fig. 2. For small  $\xi/a < N/2$ , the number variance grows  
 138 approximately linearly with the localization length as  $\Delta n^2 \approx \frac{3}{8} \frac{\xi}{aN}$ , and it starts to saturate  
 139 thereafter. We note that an equivalent measure of localization of a single-excitation wave-  
 140 function in one partition of the system is the entanglement entropy  $S$  [35, 36] related to the  
 141 number variance via  $S \geq (4 \ln 2) \Delta n^2$ .

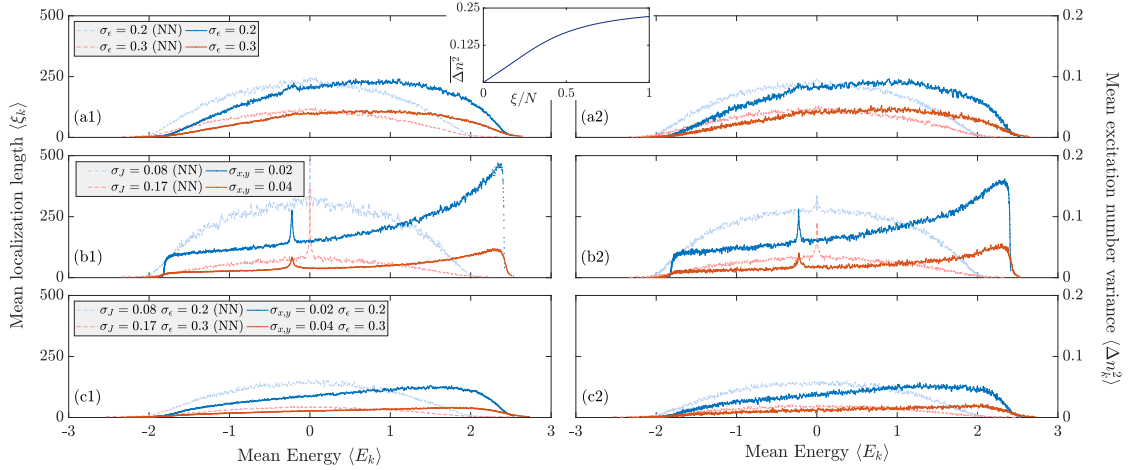


Figure 2: Mean localization length  $\langle \xi_k \rangle$  (in units of lattice spacing  $a = 1$ ) [left panels (a1), (b1), (c1)], and mean excitation number variance  $\langle \Delta n_k^2 \rangle$  [right panels (a2), (b2), (c2)] vs the mean energy  $\langle E_k \rangle$  (in units of  $J = C_3/a^3$ ) of the  $k$ -th eigenstate of a chain of  $N = 1000$  spins obtained upon averaging over 1000 independent realizations of disordered chains with long-range exchange interactions (solid lines with filled circles) and nearest-neighbor interactions (dashed lines), for (a) energy (diagonal) disorder with standard deviation  $\sigma_\epsilon$ , (b) position (off-diagonal) disorder with standard deviation  $\sigma_{x,y}$  or  $\sigma_J$ , and (c) combination of energy and position disorder. For illustrative purposes, we use in (a) and (b) the strength of the diagonal  $\sigma_\epsilon$  and off-diagonal  $\sigma_{x,y}$  (or  $\sigma_J$ ) disorders that lead to comparable localization lengths. Inset shows the averaged number variance  $\overline{\Delta n^2}$  vs  $\xi/N$ , as described in the text.

142 In Fig. 2 (left panels: a1, b1, c1), we show the mean localization length  $\langle \xi_k \rangle$  versus the  
 143 mean energy  $\langle E_k \rangle$  of the eigenstates of spin chains with long-range exchange interactions for  
 144 three different cases: (a) diagonal (energy) disorder, (b) off-diagonal (position) disorder, and  
 145 (c) combination of diagonal and off-diagonal disorders. The corresponding mean excitation  
 146 number variances  $\langle \Delta n_k^2 \rangle$  are shown in Fig. 2 (right panels: a2, b2, c2). For each case we  
 147 consider two different strengths of the disorder determined by the standard deviations  $\sigma_\epsilon$  and  
 148  $\sigma_{x,y}$ .

149 For comparison, we also consider chains with nearest-neighbor exchange interactions and  
 150 the same effective disorder as described by Hamiltonian

$$\mathcal{H}_{\text{nn}} = \frac{1}{2} \sum_{i=1}^N \epsilon_i \hat{\sigma}_i^z + \sum_{i=1}^{N-1} J_i (\hat{\sigma}_i^+ \hat{\sigma}_{i+1}^- + \hat{\sigma}_{i+1}^+ \hat{\sigma}_i^-), \quad (5)$$

151 where  $\epsilon_i$  are the random spin energies as above, while  $J_i = J + \delta J_i$  are the exchange couplings  
 152 with  $J = C_3/a^3$  and  $\delta J_i$  being Gaussian random variables with the mean  $\langle \delta J \rangle = 0$  and standard  
 153 deviation determined by the uncertainty propagation formula

$$\sigma_J \approx |\partial_x D(x, y)| \sigma_x + |\partial_y D(x, y)| \sigma_y,$$

154 where  $D(x, y) = C_3/(x^2 + y^2)^{3/2}$ .

155 Note that, in an ideal lattice with no disorder, the single excitation spectrum of Hamilto-  
 156 nian (1) is given by

$$E_k = 2 \sum_{m=1}^N \frac{J}{m^3} \cos \frac{\pi k m}{N+1}, \quad (6)$$

157 while the spectrum of the system with only the nearest-neighbor interactions, Eq. (5), corre-  
 158 sponds to the  $m = 1$  term in the above sum, i.e.  $E_k^{(\text{nn})} = 2J \cos \frac{\pi k}{N+1} \in [-2J, 2J]$ . One can  
 159 treat perturbatively the  $m > 1$  terms of Eq. (6) near the band edges and deduce [37, 38] that  
 160 the lower edge of the energy band is shifted from  $-2J$  to approximately  $-1.8J$  while upper  
 161 edge is shifted from  $2J$  to approximately  $2.4J$ . Thus, the long-range character of the exchange  
 162 interaction affects the energy band structure and the density of states.

163 **Diagonal disorder.** Consistent with the above discussion, for a chain with long-range ex-  
 164 change interactions and diagonal disorder, we observe in Fig. 2(a1) and (a2) that the profile  
 165 of the mean localization length  $\langle \xi_k \rangle$  and the nearly identical profile of the mean excitation  
 166 number variance  $\langle \Delta n_k^2 \rangle$  are shifted and skewed towards the higher energies  $\langle E_k \rangle$ , as com-  
 167 pared to the nearest-neighbor interacting chains. For the presently considered dipole-dipole  
 168 interactions,  $J_{ij} \propto 1/|r_{ij}|^3$ , the localization length  $\langle \xi_k \rangle$  remains finite for all energies  $\langle E_k \rangle$ . We  
 169 note, however, that for power-law interaction  $J_{ij} \propto 1/|r_{ij}|^\nu$  with decreasing  $\nu$  a localization-  
 170 delocalization transition occurs at  $\nu = 3/2$  near the (shifted) upper edge of the energy band  
 171  $\langle E_k \rangle \approx 5J$  [39].

172 **Off-diagonal disorder.** Even though the wavefunctions of the eigenstates of a chain with  
 173 off-diagonal disorder may not be exponentially localized for all energies, for consistency and  
 174 comparison with diagonal disorder, we still use the exponential fit of Eq. (2) to deduce the  
 175 localization length and verify its applicability by the corresponding excitation number variance.  
 176 For the nearest-neighbor interacting chain with only off-diagonal disorder, the first feature to  
 177 note in Fig. 2(b1, b2) is the sharp peak of the localization length at zero energy. This peak is  
 178 related to the well-known divergence of the density of states  $\rho(E) \sim \frac{1}{E|\ln E|^3}$  [40, 41] leading to  
 179 the localization length divergence as  $\xi \sim |\ln E|$  that follows from the Thouless relation [42].  
 180 But unlike the case of diagonal disorder, the eigenstates near zero energy are localized as  
 181  $|\psi(x)| \propto e^{-\sqrt{x/\xi}}$  rather than exponentially [15–17]. We note the relevant early studies of  
 182 Dyson [43, 44] and the insightful connection to the graph theoretical concepts [16, 45].

183 The long-range exchange interactions in the chain with off-diagonal disorder [38, 46, 47]  
 184 lead to certain modification of the localization spectrum. The zero-energy peak of the nearest-  
 185 neighbor interacting chain is now displaced to  $\langle E_k \rangle \simeq -0.22J$ , which follows from the per-  
 186 turbative treatment of Eq. (6) near the center of the band [38], and is suppressed, since  
 187 the underlying lattice is weakly non-bipartite due to the weak next-nearest-neighbor interac-  
 188 tions [45], which is in complete agreement with our numerical results in Fig. 2(b1, b2). We  
 189 note again that the use of IPR [32] is inadequate to quantify the localization length in the  
 190 vicinity of  $\langle E_k \rangle \simeq -0.22J$ , as it would indicate more, rather than less, localized states [38].  
 191 That is why we still use the localization length  $\langle \xi_k \rangle$  obtained from the exponential fit of Eq. (2)  
 192 and verify its applicability by the corresponding excitation number variance  $\langle \Delta n^2 \rangle$ .

193 Another feature is that, perhaps counterintuitively, disordered chains with long-range ex-  
 194 change interactions exhibit shorter localization length in the central part of the spectrum, as  
 195 compared to chains with only nearest-neighbor interactions [18, 20, 21]; in effect the long-  
 196 range interactions amplify the disorder. But for larger energies the localization length  $\langle \xi_k \rangle$   
 197 (and the excitation number variance  $\langle \Delta n_k^2 \rangle$ ) gradually increases [38, 48] and it exhibits a sharp  
 198 peak near the upper edge of the energy band,  $\langle E_k \rangle \approx 2.4J$ . The states near the upper edge  
 199 of the energy band are in fact completely delocalized,  $\langle \xi_k \rangle \approx N/2$ , at least for not too strong  
 200 off-diagonal disorders that we consider. This behaviour is reminiscent to the emergence of ex-  
 201 tended states at the band edge for spin chains with diagonal disorder and long-range hopping  
 202  $J_{ij} \propto 1/|r_{ij}|^\nu$  with decreasing power  $\nu$ , but for our case of off-diagonal disorder and  $\nu = 3$ ,  
 203 the sharp peak is much more pronounced.

204 **Combined diagonal and off-diagonal disorder.** Finally in Fig. 2(c1, c2) we show the mean  
 205 localization length and the mean excitation number variance versus the mean energy for the  
 206 chains with both diagonal and off-diagonal disorders that concurrently localize the system  
 207 eigenstates. Now the (shifted) zero-energy peak is completely suppressed [45] while the eigen-  
 208 states with the longest localization length reside between the center and the upper edge of the  
 209 band skewed by the long-range exchange interactions.

210 To summarize, the important information gained by our analysis of the localization lengths  
 211 in disordered spin chains is the maximum length of a finite chain that can support excitation  
 212 transfer through an extended eigenstate. Conversely, when the chain length exceeds the maxi-  
 213 mum localization length of the eigenstates, we expect the transfer to be completely suppressed.  
 214 We note that in all cases when the obtained mean localization length is sufficiently shorter than  
 215 the chain length,  $\langle \xi_k \rangle < aN/2$ , the relation  $\langle \Delta n_k^2 \rangle \approx \frac{3}{8} \frac{\langle \xi_k \rangle}{aN}$  holds to a very good approxima-  
 216 tion, which justifies our approach to characterizing the localization properties of disordered  
 217 spin chains with long-range exchange interactions.

## 218 4 Excitation transfer schemes

219 The large localization length of single-excitation eigenstates in a spin chain is necessary but  
 220 not yet sufficient to ensure efficient transfer of excitation between the sender and receiver  
 221 spins. Rather, the extended eigenstates of the chain should have sufficient support at the two  
 222 ends of the chain in order to strongly couple to the sender and receiver spins.

223 To illustrate the procedure for excitation transfer, in this section we consider spin chains  
 224 with long-range interactions but no disorder. Solving the eigenvalue problem

$$\mathcal{H} |\psi_k\rangle = E_k |\psi_k\rangle, \quad (7)$$

225 we obtain the eigenstates  $|\psi_k\rangle = \sum_i v_i^{(k)} |i\rangle$  which couple to the sender and receiver spins at  
 226 the two ends of the chain with the corresponding strengths

$$\Omega_s^{(k)} = J_s v_1^{(k)}, \quad \Omega_r^{(k)} = J_r v_N^{(k)}, \quad (8)$$

227 where  $J_s$  and  $J_r$  are the coupling strength of the sender and receiver spins to the first and the  
 228 last spins of the chain. Hence, in order to efficiently transfer the excitation from the sender  
 229 to the receiver spin via a particular eigenstate  $|\psi_k\rangle$  of the chain, this eigenstate should have  
 230 large amplitudes  $|v_{1,N}^{(k)}|$  at both ends of the chain.

231 In Fig. 3 we show the absolute value of the product  $|v_1^{(k)} v_N^{(k)}|$  of the boundary amplitudes  
 232 of the different energy eigenstates  $|\psi_k\rangle$  of the chain. This figure reveals that the eigenstates  
 233 most suitable for the transfer are in the middle of the spectrum,  $E_k \sim 0$ , while the eigenstates  
 234 at the upper edge of the spectrum,  $E_k \lesssim 2.4J$ , would only weakly couple to the sender and  
 235 receiver spins and are thus unsuitable for the excitation transfer, despite having large (or even  
 236 divergent) localization length in disordered chains. Having in mind the chains with both diag-  
 237 onal and off-diagonal disorder exhibiting the localization peak in the vicinity of  $E = -0.22J$ ,  
 238 we shall tune the energies of the sender and receiver spins to  $\epsilon_{s,r} \approx -0.22J$ .

239 Another critical issue for the efficient transfer via the selected eigenstates of the chain is the  
 240 small leakage of the excitation, initially at the sender spin, to all other non-resonant eigenstates  
 241 of the chain [24, 25]. In a chain of  $N$  spins, the average distance between the energy eigenstates  
 242 is  $\Delta E \simeq 4J/N$ . Therefore the coupling strength of the sender and receiver spins, tuned to  
 243 resonance to a particular eigenstate, should satisfy  $\Omega_{s,r} < \Delta E$ . Since the amplitudes of the  
 244 edge states for the most delocalized eigenstates are  $v_{1,N}^{(k)} \sim 1/\sqrt{N}$ , we obtain from (8) that the  
 245 coupling rates should satisfy  $J_{s,r} \lesssim J/\sqrt{N}$  in order to avoid the leakage of the excitation to the  
 246 undesired states of the chain and attain high transfer probability [49].

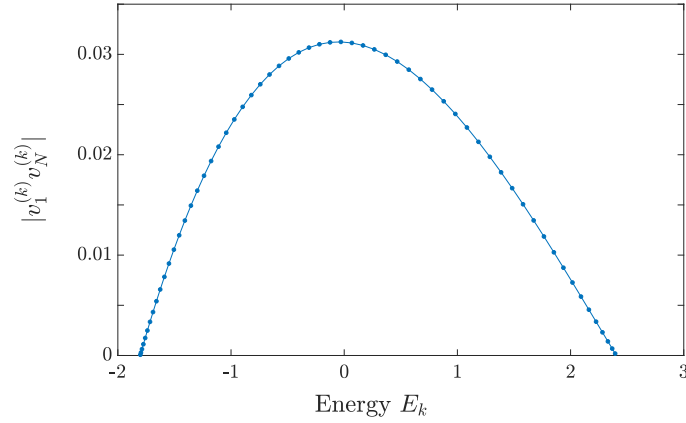


Figure 3: Absolute value of the product  $|v_1^{(k)} v_N^{(k)}|$  of the boundary amplitudes of  $k$ -th eigenvector of the chain vs the eigenenergy  $E_k$  (in units of  $J$ ), for an ordered chain of  $N = 61$  spins with long-range exchange interaction.

247 **Static coupling to the chain.** To illustrate the ongoing discussion, in Fig. 4 we show the  
 248 dynamics of excitation transfer between the sender and receiver spins via spin chains of dif-  
 249 ferent length  $N$  with no disorder. For convenience, we chose chains with odd number of spins,  
 250  $N = 11, 21, \dots$ , and tune the energies of the sender and receiver spins  $\epsilon_{s,r}$  to the energy of the  
 251 “fittest” eigenstate closest to  $E = -0.22J$ .

252 The state of the system in the single excitation subspace can be written as  $|\Psi\rangle = \alpha_s |s\rangle + \sum_{i=1}^N \alpha_i |i\rangle + \alpha_r |r\rangle$ ,  
 253 where  $\alpha_j$  are the amplitudes and  $|j\rangle$  denotes the state with the excitation at position  $j = s, r$   
 254 or  $i \in [1, N]$ . Initially the excitation is localized at the sender spin,  $|\Psi(0)\rangle = |s\rangle$ , and the  
 255 couplings  $J_{s,r}$  are set to the constant values  $J_{s,r} \simeq 0.5J/\sqrt{N}$ . The state of the system  $|\Psi(t)\rangle$   
 256 evolves according to the Hamiltonian (1), and the transfer probability to the receiver spin  
 257  $P_r(t) = |\langle r|\Psi(t)\rangle|^2$  is shown in Fig. 4(a). In a three-state system, complete transfer would  
 258 occur at time  $\tau = \pi/(2\sqrt{2}\Omega_{s,r})$ . Our multilevel system now behaves as an effective three-state  
 259 system with a single intermediate eigenstate of the chain, and the transfer time scales as  $\tau \propto N$   
 260 consistently with  $\Omega_{s,r} \propto 1/N$ , see Fig. 4(b). We note that the linear scaling of the transfer  
 261 time with the length of the chain stems from our requirement to avoid the leakage of excitation  
 262 into the undesired states. But this scaling is consistent with the Lieb-Robinson bound [50–52]  
 263 which is in fact a much lower bound for the achievable transfer time although with a reduced  
 264 transfer probability due to the leakage. In Fig. 4(c) we show the dynamics of probabilities of  
 265 excitation of the sender spin,  $P_s(t) = |\langle s|\Psi(t)\rangle|^2$ , the chain,  $P_c(t) = \sum_{i=1}^N |\langle i|\Psi(t)\rangle|^2$ , and the  
 266 receiver spin,  $P_r(t)$ , during one full transfer cycle.

267 **Time-dependent adiabatic couplings.** In a three-state system, a more efficient excitation  
 268 transfer can be achieved using an analog of stimulated Raman adiabatic passage (STIRAP)  
 269 [26–28]. It involves time-dependent couplings and must be sufficiently slow in order to be  
 270 adiabatic, but is robust and avoids populating the intermediate – here the spin-chain – state(s).

271 Consider an effective three-state system  $|\Psi\rangle = \alpha_s |s\rangle + \alpha_k |\psi_k\rangle + \alpha_r |r\rangle$  governed by the  
 272 Hamiltonian

$$\mathcal{H}^{\text{eff}} = \Delta\epsilon_k |\psi_k\rangle \langle \psi_k| + (\Omega_s^{(k)} |s\rangle \langle \psi_k| + \Omega_r^{(k)} |r\rangle \langle \psi_k| + \text{H.c.}) \quad (9)$$

273 where  $\Delta\epsilon_k = E_k - \epsilon_{s,r}$  is a possible energy mismatch between the selected eigenstate of the  
 274 chain  $|\psi_k\rangle$  and the sender and receiver spins. This Hamiltonian has a zero-energy coherent  
 275 population trapping (or dark) eigenstate  $|\Psi_0\rangle \propto \Omega_r^{(k)} |s\rangle - \Omega_s^{(k)} |r\rangle$  that does not involve the  
 276 intermediate state  $|\psi_k\rangle$  of the spin chain. With the excitation initially localized on the sender



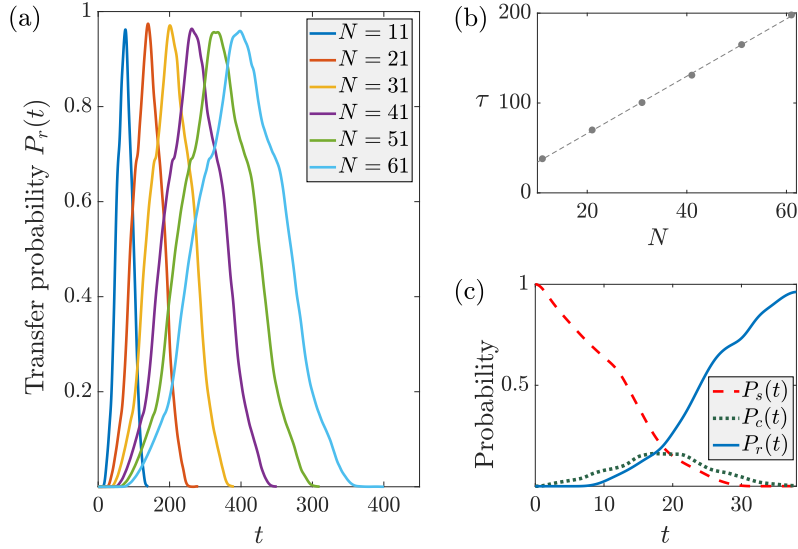


Figure 4: Excitation transfer via static couplings of the sender and receiver spins with rates  $J_{s,r} = 0.49J/\sqrt{N}$  to the chain of  $N$  spins with long-range exchange interactions and no disorder. (a) Transfer probability  $P_r(t)$  vs time  $t$  (in units of  $1/J$ ) for different chain lengths  $N$ . The energies of the sender and receiver spins  $\epsilon_{s,r}$  are tuned to the energy of the eigenstate of the chain closest to  $E = -0.22J$ . (b) Transfer time  $\tau$  (gray filled circles), corresponding to the first peak of the transfer probability in (a) for each chain length  $N$ . Dashed line shows the linear fit  $\tau J = 3.2N + 2.3$ . (c) Time-evolution of the excitation probability for the sender  $P_s(t)$ , receiver  $P_r(t)$  and intermediate chain  $P_c(t)$ , for a chain of  $N = 11$  spins.

277 spin, we set the coupling  $|\Omega_r^{(k)}| \gg |\Omega_s^{(k)}|$  such that the dark state coincides with the initial state,  
 278  $|\Psi_0\rangle = |s\rangle$ . We then slowly switch off  $\Omega_r^{(k)}$  and switch on  $\Omega_s^{(k)}$ , which results in an adiabatic  
 279 rotation of the dark state  $|\Psi_0\rangle$  towards  $|r\rangle$ , and at the final time  $\tau$ , when  $|\Omega_r^{(k)}| \ll |\Omega_s^{(k)}|$ , we  
 280 obtain  $|\Psi_0\rangle \simeq |r\rangle$ . To realize this so-called counterintuitive pulse sequence, we use the time-  
 281 dependent boundary couplings

$$J_{s,r}(t) = \frac{J_{s,r}^{\max}}{2} \left( 1 \pm \tanh(\gamma t/\tau - \beta_{s,r}) \right), \quad (10)$$

282 where  $J_{s,r}^{\max} \simeq 0.5/\sqrt{N}$  as before, while the parameters  $\gamma = 6$ ,  $\beta_{s,r} = 2.3, 3.6$  and the process  
 283 duration  $\tau \propto N$  are chosen so as to optimize the overlap between the pulses and achieve  
 284 adiabaticity with sufficiently large effective pulse area  $\int_0^\tau dt \sqrt{|\Omega_s^{(k)}(t)|^2 + |\Omega_r^{(k)}(t)|^2} \gtrsim 10$  [27,  
 285 28]. We note that the adiabatic population transfer has been applied to multilevel systems  
 286 before [53, 54].

287 In Fig. 5 we illustrate the adiabatic transfer protocol for ordered chains of different length  
 288 and time-dependent couplings of Eq. (10) but otherwise the same parameters as in Fig. 4. We  
 289 achieve nearly perfect population transfer for all considered cases, see Fig. 5(a), at the expense  
 290 of longer duration of the process  $\tau$ , see Fig. 5(b). Note that during the transfer, as the system  
 291 adiabatically follows the coherent population trapping state  $|\Psi_0\rangle$ , the chain contains almost  
 292 no excitation at all times, Fig. 5(c).

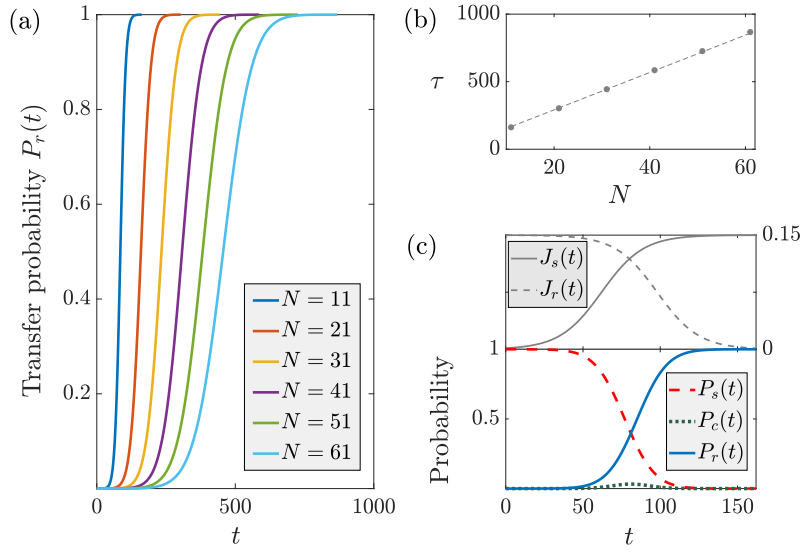


Figure 5: Stimulated adiabatic transfer of excitation between the sender and receiver spin using time-dependent couplings of Eq. (10), for chains with long-range exchange interactions and no disorder. (a) Transfer probability  $P_r(t)$  vs time  $t$  (in units of  $1/J$ ) for chains of different length. (b) Transfer time  $\tau$  (gray filled circles) as a function of  $N$ , and the linear fit  $\tau J = 14.1N + 6.9$  (dashed line). (c) Top panel shows the time-dependent coupling rates  $J_{s,r}(t)$  of Eq. (10), and the bottom panel shows the dynamics of excitation probabilities of the sender  $P_s(t)$ , receiver  $P_r(t)$  and intermediate chain  $P_c(t)$ , for  $N = 11$ .

## 293 5 Transfer probability in disordered chains

294 Having determined the localization lengths  $\xi$  in long disordered spin chains in Sec. 3 and po-  
 295 tentially suitable excitation transfer protocols in Sec. 4, we now analyze the mean probability  
 296  $\langle P_r \rangle$  of excitation transfer between the sender and receiver spins via disordered spin chains of  
 297 finite length  $N$  comparable to  $\xi$ .

298 **Static coupling to the chain.** We first consider the static transfer protocol of Fig. 4 with fixed  
 299 coupling rates  $J_{s,r} \simeq 0.5J/\sqrt{N}$  of the sender and receiver spins having energies  $\epsilon_{s,r} = -0.22J$ .  
 300 With the excitation initially localized at the sender spin, we terminate the evolution when the  
 301 excitation probability of the receiver spin attains its first maximum at  $t = \tau$  of Fig. 4(b). In  
 302 Fig. 6 we show the transfer probabilities  $\langle P_r \rangle$  averaged over many independent realizations of  
 303 disordered spin chains, involving spin-energy (diagonal) disorder, spin-position (off-diagonal)  
 304 disorder, and the combination of the two. As expected, increasing the chain length  $N$  de-  
 305 creases the transfer probability which is due to the stronger disorder-induced localization of  
 306 the eigenstates of the chain in the middle of the energy spectrum. We also observe that chains  
 307 with only the nearest-neighbor exchange interaction (with  $\epsilon_{s,r} = 0$ ) lead to better transfer  
 308 probability, especially for the case of off-diagonal disorder, Fig. 6(b), which is consistent with  
 309 their larger localization length under otherwise similar conditions, as discussed in Sec. 3 and  
 310 seen in Fig. 2(b).

311 **Time-dependent adiabatic couplings.** We finally consider the adiabatic transfer protocol of  
 312 Fig. 5 with the time-dependent coupling rates of Eq. (10) applied to the sender and receiver  
 313 spins in a counterintuitive order. In Fig. 7 we show the results of our numerical simulations  
 314 for the transfer probabilities  $\langle P_r \rangle$  averaged over many independent realizations of disordered

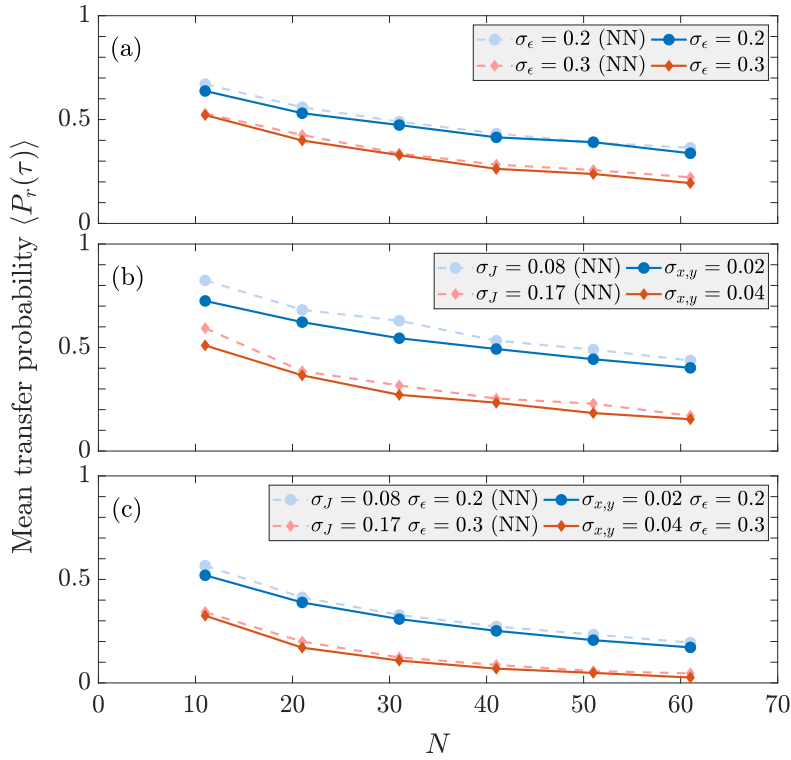


Figure 6: Mean excitation transfer probability  $\langle P_r \rangle$  vs chain length  $N$ , obtained upon averaging over 1000 independent realizations of disordered chains with long-range exchange interactions (solid lines with filled circles and diamonds) and nearest-neighbor interactions (dashed lines with light filled symbols), for (a) energy (diagonal) disorder with standard deviations  $\sigma_\epsilon$ , (b) position (off-diagonal) disorder with standard deviation  $\sigma_{x,y}$  or  $\sigma_J$ , and (c) combination of energy and position disorder. We use the static couplings of the sender and receiver spins  $J_{s,r} = 0.49J/\sqrt{N}$  having energies  $\epsilon_{s,r} = -0.22J$  ( $\epsilon_{s,r} = 0$  for the nearest-neighbor interacting chains), and the evolution is terminated at  $t = \tau$  of Fig. 4(b).

315 spin chains. Compared to the static transfer protocol, the performance of adiabatic transfer is  
 316 significantly better for all chain lengths and any kind of disorder, be it diagonal, off-diagonal, or  
 317 combination of both. We emphasize that in this study, we have focused on the spin excitation  
 318 or polarization transfer probability. In contrast, coherent quantum state transfer is much more  
 319 sensitive to diagonal disorder leading to larger dephasing during adiabatic transfer which is  
 320 necessarily slower than the static transfer [55].

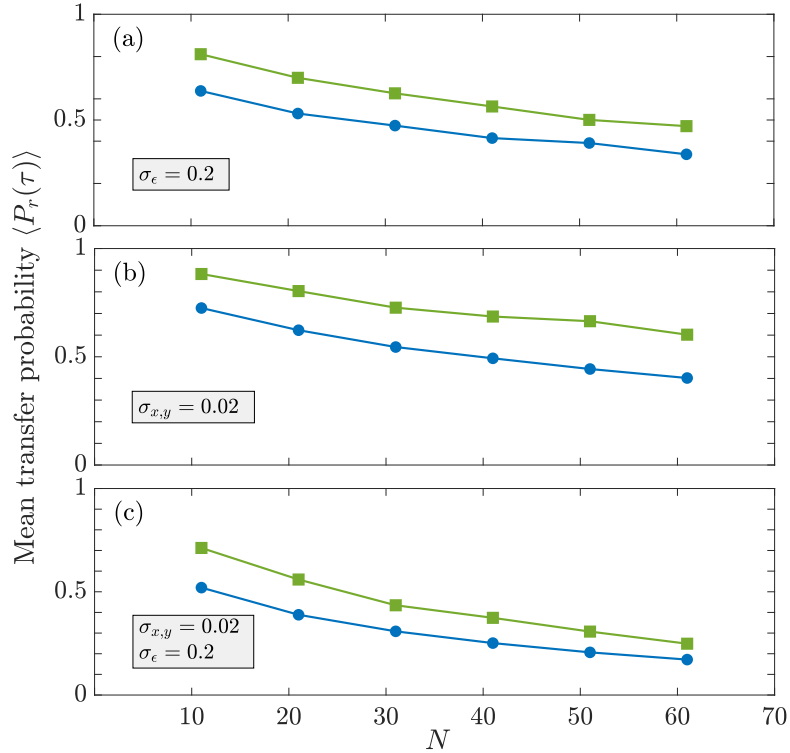


Figure 7: Mean excitation transfer probability  $\langle P_r \rangle$  vs chain length  $N$ , obtained upon averaging over 1000 independent realizations of disordered chains with long-range exchange interactions, for the stimulated adiabatic transfer (green solid lines with filled squares), compared to the static transfer of Fig. 6 (blue solid lines with filled circles), for (a) energy (diagonal) disorder with standard deviations  $\sigma_\epsilon$ , (b) position (off-diagonal) disorder with standard deviation  $\sigma_{x,y}$ , and (c) combination of energy and position disorder. We use the time-dependent couplings of Eq. (10) for the sender and receiver spins having energies  $\epsilon_{s,r} = -0.22J$ , with the transfer duration  $\tau$  of Fig. 5(b).

## 321 6 Conclusions

322 We have presented the results of our studies of disordered, one-dimensional spin-chains with  
 323 long-range exchange (resonant dipole-dipole) interactions and their ability to transfer spin  
 324 excitation or polarization over long distances. We have performed detailed numerical investi-  
 325 gations of the localization length in spin chains with either or both diagonal and off-diagonal  
 326 disorder. Many of our results concur with the previously known and well-understood prop-  
 327 erties of disordered spin chains, but we have also encountered interesting manifestations of  
 328 (de)localization of energy eigenstates that, to the best of our knowledge, have not been prop-  
 329 erly addressed before in the context of resonant dipole-dipole ( $1/r^3$ ) interactions, and thus  
 330 may warrant further investigation. These, in particular, include delocalization of the eigen-  
 331 states at the upper edge of the shifted energy band in spin chains with off-diagonal disorder,  
 332 and the modification of the shifted zero-energy Dyson peak of localization length, which we  
 333 found to be the most suitable eigenstate for the excitation transfer between the two ends of  
 334 the chain.

335 We have put forward two excitation transfer protocols: a) static protocol involving selective  
 336 coupling of the sender and receiver spins to the suitable eigenstate of the chain, and b) time-  
 337 dependent adiabatic protocol involving counter-intuitive sequence of couplings of the sender

338 and receiver spins to the chain, inspired by stimulated Raman adiabatic passage technique  
339 widely used in atomic and molecular physics. We have found that the adiabatic transfer of  
340 excitation via disordered spin chains has much better performance for all chain length and  
341 any kind of disorder, be it diagonal, off-diagonal, or combination of both. This attests, once  
342 again, the usefulness of this universal method.

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439 quantifies on how many lattice sites  $i$  the wavefunction has support, i.e., IPR is small  
440 for a uniformly delocalized wavefunction,  $|v_i|^2 \sim 1/N \forall i$ , and is large if many sites  
441 have vanishing populations. The latter, however, does not mean that the wavefunction is  
442 spatially localized, because a wavefunction having large populations on only a few lattice  
443 sites separated by large distance from each other would also have a large IPR. This is in  
444 fact what we observe for lattices with long-range exchange interactions and off-diagonal  
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487 the underlying lattice is not bipartite, i.e., in the presence of next-nearest neighbor inter-  
488 actions or diagonal disorder. In our case, the next-nearest neighbor interactions  $J/8$  make  
489 the underlying lattice only weakly non-bipartite, and the peak is shifted and suppressed,  
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