Hopping disorder, magnon-energy renormalization, and two-magnon Raman scattering in an antiferromagnet

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Effects of hopping disorder in the Mott-Hubbard antiferromagnet are studied, both perturbatively and also using the exact-eigenstate method, in the strong correlation limit. It is shown that while the low-energy, long-wavelength magnon modes are only weakly affected, the high-energy modes are strongly affected because of a cooperative effect arising from local correlations in hopping disorder. Implications of this highly asymmetric magnon-energy renormalization for two-magnon Raman scattering in cuprate antiferromagnets are also discussed. [S0163-1829(97)04718-8]

I. INTRODUCTION

Recently there has been renewed interest in the two-magnon Raman scattering in cuprate antiferromagnets such as La_2CuO_4, $YBa_2Cu_3O_6$, etc.[1] It had been suggested earlier that strong quantum fluctuations in these low-spin ($S=1/2$) systems were responsible for the anomalously large Raman linewidth,[2–5] which could not be quantitatively understood within the simple Fleury-Loudon theory involving nearest-neighbor magnon interaction.[6,7] Several new ideas have been advanced recently which suggest that the anomalous features such as the large linewidth, significant asymmetry in line shape, and substantial intensity seen in the classically forbidden A_{1g} symmetry have to be understood within new frameworks. These include the exchange disorder caused by zero-point lattice vibration,[1] and resonant Raman scattering in which the incident photon energy is comparable to the charge gap in cuprates.[8]

When lattice distortions, caused by quantum and thermal fluctuations, are taken into account in the adiabatic or Born-Oppenheimer approximation, the hopping terms t_{ij}, and hence the exchange couplings J_{ij}, which depend upon the instantaneous position of ions, must therefore include random terms. This approximation should be valid for high-energy magnon excitations in cuprates where the magnon energies of order $2J\sim 2000\ \mathrm{cm}^{-1}$ are much greater than the Debye energy $\hbar\omega_D\sim 340\ \mathrm{cm}^{-1}$. The exchange disorder caused by zero-point lattice vibration was recently taken into account within a nearest-neighbor (NN) Heisenberg model where the exchange energy $J+\delta J_{ij}$ at each bond includes random terms.[1] For a Gaussian distribution of the random terms, this model was studied using the quantum Monte Carlo (QMC) technique and Raman intensities were obtained numerically in different scattering symmetries. Satisfactory fitting was obtained with the experimental Raman intensity line shape for a Gaussian variance of $\sigma\sim 0.4$. However, no clear insight emerges from this QMC calculation regarding the explicit effects of exchange disorder on (i) low-energy, long-wavelength magnon modes, (ii) the magnon velocity, and (iii) the high-energy magnon modes with energy $\sim 2J$ which are mainly responsible for the Raman scattering. Ascertaining the exchange-disorder-induced renormalization of the magnon energy scale is of vital importance, however, as it is from comparison of this scale with experiments (such as neutron scattering, Raman scattering, magnetization versus temperature, etc.) that a reliable value of J for the cuprates is extracted.

In this paper we therefore examine these questions in the context of the Mott-Hubbard antiferromagnet (AF) with off-diagonal disorder. We consider the following Hubbard Hamiltonian on a square lattice, with randomness in the hopping terms, and with a filling of one fermion per site, so that an antiferromagnetic insulating state is obtained. Generalization to three dimensions and to other bipartite lattices is straightforward. Random terms δt_{ij} are included in NN hopping terms, and are chosen independently for each NN pair of sites from a Gaussian distribution,

$$\hat{H}=-\sum_{\langle ij\rangle,\sigma}(t+\delta t_{ij})(\hat{a}^{\dagger}_{i\sigma}\hat{a}_{j\sigma}+\mathrm{H.c.})+U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, \quad (1)$$

$$P(\delta t_{ij}/t)=\frac{1}{\sqrt{2\pi\sigma}}\exp\left[-\frac{(\delta t_{ij}/t)^2}{2\sigma}\right]. \quad (2)$$

The distribution width $\sqrt{\sigma}$ measures the disorder in hopping. Since for weak disorder $\delta J_{ij}/J\sim 2\delta t_{ij}/t$, therefore the distribution widths $\sqrt{\sigma_J}$ and $\sqrt{\sigma_t}$ for random exchange-energy terms and hopping terms should be related via $\sigma_J=4\sigma_t$. An estimate for σ_J has been obtained[1] using $\sigma_J=\alpha\cdot\langle\delta r\rangle/r$, where the relative amplitude of the zero-point motion $\langle\delta r\rangle/r$ was estimated as about 5%. The dependence of the exchange energy J on the in-plane Cu-Cu distance r is taken to be of the form $J\sim r^{-\alpha}$. The exponent α for cuprates has been obtained using high-pressure studies[9] in the range $\alpha=4\pm 2$, whereas a stronger dependence ($\alpha=6.8\pm 0.8$) has been reported by others.[10] In their QMC calculations Nori *et al.* have considered the cases $\sigma_J=0.3$, 0.4, and 0.5.

We have examined—both perturbatively and using the exact-eigenstate method—effects of hopping disorder on magnon energies, their wave functions, and on the density of states (DOS). In both schemes the magnon modes are obtained at the level of random phase approximation (RPA). At this level the magnon propagator has the form $[\chi^{-+}(\omega)]=[\chi^0(\omega)]/\mathbf{1}-U[\chi^0(\omega)]$, where $[\chi^0(\omega)]$ is the

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zeroth-order antiparallel-spin particle-hole propagator evaluated in the broken-symmetry AF state. Eigensolutions of the $[\chi^0(\omega)]$ matrix yield the magnon energies and wave functions. In the perturbative analysis we obtain the disorder-induced perturbation to $[\chi^0(\omega)]$, and obtain resulting corrections to its eigenvalues, which then yield the renormalized magnon energies. For analytical convenience we have considered the strong correlation limit as the perturbative analysis is particularly simple in this limit. We have also numerically obtained $[\chi^0(\omega)]$ using the self-consistent exact eigenstates of the HF Hamiltonian in the AF state with the random hopping terms included from the beginning. This method can be applied for arbitrary interaction strength U/t.

We find that there is strong renormalization in the energy of high-energy magnon modes due to a cooperative effect arising from local correlations in hopping disorder, which results in appreciable magnon DOS well above the maximum energy $2J$ for the pure system, even for σ as small as 0.1. This result is significant because it not only clearly shows how the two-magnon Raman scattering intensity, which involves the one-magnon DOS, can extend well beyond the energy $4J$ when hopping disorder is present, but it also yields an insight into why Raman scattering is so sensitive to the tiny zero-point fluctuations. We also show that these high-energy magnon modes at the upper end of the spectrum are strongly localized in regions of the lattice where the locally averaged hopping strength is maximum, i.e., at sites where all δt_{ij}'s connecting to the site have maximum average. We have also obtained the energy renormalization of the low-energy, long-wavelength modes, both to first order and second order in $\delta t_{ij}/t$. We find that the first-order correction to magnon energies are of the random-walk type, which decrease like $1/\sqrt{N}$ with increasing system size, but can be significant for finite-size lattices. The second-order correction, on configuration averaging, yields a momentum-independent multiplicative renormalization of the magnon energy by a factor $1+\sigma$, i.e., $\omega_q = 2J(1+\sigma)\sqrt{1-\gamma_q^2}$. Thus the Goldstone mode is preserved, and the low-energy, long-wavelength magnons are weakly perturbed by off-diagonal, hopping disorder. This is in contrast to the case of potential scattering (diagonal disorder) where in two dimensions singular corrections to low-energy magnon modes were obtained.[11]

II. PERTURBATIVE ANALYSIS

To obtain the magnon energies and wave functions, we evaluate the transverse spin fluctuation (magnon) propagator $\chi^{-+}(rt,r't') \equiv \langle \mathrm{AF}|S^-(rt)S^+(r't')|\mathrm{AF}\rangle$ which, at the RPA level, is given by $[\chi^0(\omega)]/\mathbf{1}-U[\chi^0(\omega)]$ after Fourier transformation to frequency space. Here $[\chi^0(\omega)]$ is the antiparallel-spin particle-hole propagator evaluated in the broken-symmetry, self-consistent state, with matrix elements given by $[\chi^0(\omega)]_{ij} = i\int (d\omega'/2\pi) G_{ij}^{\uparrow}(\omega') G_{ji}^{\downarrow}(\omega'-\omega)$. The magnon energies are then given by the poles in the magnon propagator, $1-U\lambda(\omega)=0$, where $\lambda(\omega)$ is the eigenvalue of the $[\chi^0(\omega)]$ matrix.

In the perturbative technique, the disorder-induced perturbation $[\delta\chi^0]$ to the $[\chi^0(\omega)]$ matrix is obtained diagrammatically in powers of $\delta t_{ij}/t$. Resulting corrections to the eigenvalues of $[\chi^0(\omega)]$ then yield the renormalization in magnon energies. Diagrams which contribute to $[\delta\chi^0]$ to first order in δt_{ij} are shown in Fig. 1(a). The upper and lower lines are, respectively, the $\uparrow$-spin and $\downarrow$-spin propagators with frequencies ω' and $\omega'-\omega$. In the diagonal matrix element $[\delta\chi^0]_{ii}$, k is summed over all NN sites of i. Other diagrams are obtained by exchanging the i and k vertices of the dashed line and by putting the dashed line in the lower ($\downarrow$-spin) propagator, etc. In the strong correlation limit we obtain

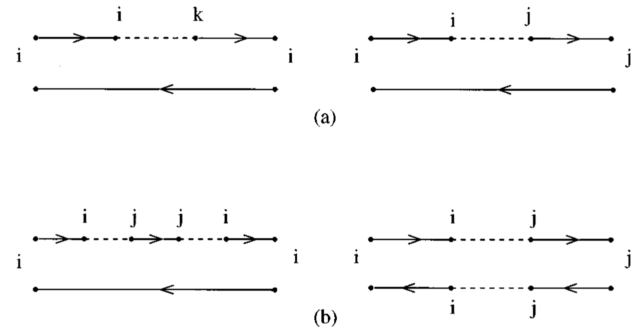

FIG. 1. Diagrams contributing at the (a) first-order level in δt (dashed lines) and (b) second-order level to the diagonal matrix element $[\delta\chi^0]_{ii}$ and the nearest-neighbor matrix element $[\delta\chi^0]_{ij}$.

$$[\delta\chi^0]_{ii} = -\frac{t^2}{2\Delta^3}\sum_k \delta t_{ik}/t, \quad [\delta\chi^0]_{ij} = -\frac{t^2}{2\Delta^3}\,\delta t_{ij}/t, \tag{3}$$

where $2\Delta = mU$ is the Hubbard gap characterizing the AF insulating state, and only terms up to order (t^2/Δ^3) have been retained, appropriate to the strong correlation limit. We notice that the sum of all the NN matrix elements $[\delta\chi^0]_{ij}$ is precisely the diagonal matrix element $[\delta\chi^0]_{ii}$. An immediate consequence of this correlation is that the Goldstone mode is preserved and that generally the effective scattering of low-energy, long-wavelength modes is weak. To begin with we consider the first-order correction to the eigenvalue $\lambda(\omega)$ due to the perturbation $[\delta\chi^0]$. For this we require the eigensolutions of $[\chi^0(\omega)]$ in the pure AF state, which can be labeled by momentum due to translational symmetry within the two-sublattice basis. We first consider the case of low-energy, long-wavelength modes for which $q \ll 1$ and $\omega/2J \ll 1$. Up to order q^2, $(\omega/2J)^2$ and in the strong-correlation limit, the eigenvector and eigenvalue of $[\chi^0(\omega)]$ for the pure AF are given by[12]

$$\phi_q^{(0)}(r) = \frac{1}{\sqrt{N}} \begin{pmatrix} \sqrt{1+\omega/2J} \\ -\sqrt{1-\omega/2J} \end{pmatrix} e^{iq\cdot r}, \tag{4}$$

$$\lambda_q^{(0)} = \frac{1}{U} - \frac{t^2}{\Delta^3}\left[\frac{q^2}{4} - \frac{1}{2}\left(\frac{\omega}{2J}\right)^2\right]. \tag{5}$$

Therefore for the first-order correction we obtain

$$\delta\lambda_q^{(1)} = \langle \phi_q^{(0)} | [\delta\chi^0] | \phi_q^{(0)} \rangle = -\frac{1}{2}\frac{t^2}{\Delta^3}\left[(r_x+r_y)\left(\frac{\omega}{2J}\right)^2 + r_x q_x^2 + r_y q_y^2\right], \tag{6}$$

where

$$r_x \equiv \frac{1}{N} \sum_i \delta t_{ij}/t \quad (\vec{r}_j = \vec{r}_i + a\hat{x})$$

and

$$r_y \equiv \frac{1}{N} \sum_i \delta t_{ij}/t \quad (\vec{r}_j = \vec{r}_i + a\hat{y}) \tag{7}$$

are the lattice averages of the random hopping terms δt_{ij} taken in the x and y directions, respectively. Significantly the order ω terms cancel exactly for arbitrary distribution of δt_{ij}, and their cancellation follows from the fact that the A- and B-sublattice sums of the diagonal terms $[\delta\chi^0]_{ii}$ are identical, i.e., $\Sigma_{i\in A}[\delta\chi^0]_{ii} = \Sigma_{i\in B}[\delta\chi^0]_{ii}$.

Now, r_x and r_y will vanish for an infinite system if the random hopping terms δt_{ij} are distributed symmetrically about zero, and therefore in the infinite-size limit, there will be no first-order correction to long-wavelength magnon energies. However, for a finite-size system the averages r_x and r_y are like random-walk averages and will scale like $1/\sqrt{N}$. This is because the terms $\Sigma_i \delta t_{ij}/t$ in r_x and r_y are sums of N Gaussian random variables, and therefore will themselves have a Gaussian distribution of width $\sqrt{N\sigma}$.

Solving for ω from the equation, $1 - U(\lambda_q^{(0)} + \delta\lambda_q^{(1)}) = 0$ yields the renormalized magnon energies for long-wavelength modes:

$$\omega_q = \sqrt{2}J[q_x^2(1+3r_x+r_y) + q_y^2(1+3r_y+r_x)]^{1/2}. \tag{8}$$

We therefore expect strong but nonsingular corrections due to this finite-size effect to the magnon (spin-wave) velocity. We have confirmed this finite-size effect through the exact-eigenstates method and indeed find, for system sizes in the range 10×10 to 18×18, a $1/\sqrt{N}$ scaling in the correction to the magnon velocity.

We now examine the effects of hopping disorder to first order on the high-energy magnon modes with energy $\approx 2J$. In the pure AF the maximum magnon energy is $2J$ and these magnon modes have nonzero amplitudes only on sites of one sublattice, corresponding to creating spin deviation on these sites. The energy cost due to a spin deviation of this kind is therefore $4(J/2) = 2J$, where $J/2$ is the bond strength and 4 is the number of broken bonds. Now, when hopping disorder is present the highest-energy magnon mode will correspond to creating a spin deviation on that site where the sum of the NN bonds is maximum. This will clearly occur in a region of the lattice where the hopping disorder terms δt_{ij} neighboring a site have the maximum average. In fact, generally the high-energy magnon modes with energy $\geqslant 2J$ will be localized around such sites across the lattice.

Interestingly, in such regions where the locally averaged hopping is significantly higher than the bulk average t, the diminished U/t ratio leads to a lowering of the local staggered magnetization $m(r)$, and hence of the local charge gap $2\Delta(r) \equiv m(r)U$. Thus the localization of the high-energy magnon modes in such regions is suggestive of the high-energy magnons acquiring a charge due to hopping disorder and getting trapped in the local depressions of the charge gap. This can be seen formally by examining the self-energy correction, $\Sigma_{ij} = U^2 \delta\chi_{ij}^0$, to the magnon modes due to hopping disorder, particularly the diagonal terms which will act like potential terms for the magnons. From Eq. (3) we obtain

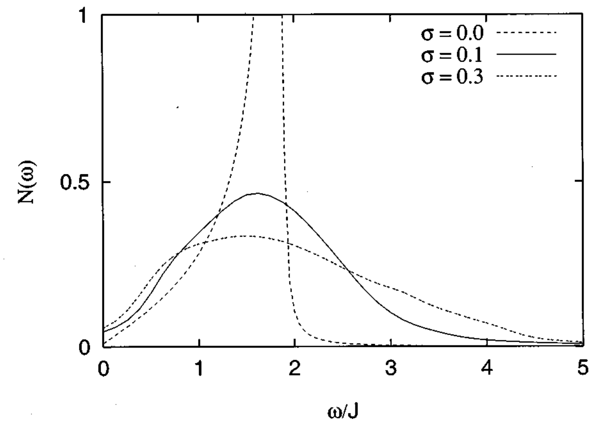

FIG. 2. The configuration-averaged magnon density of states obtained numerically from the exact-eigenstate analysis for a 10×10 hopping disordered system with $\sigma = 0.1$ and 0.3, in the strong correlation limit ($U/t = 10$).

$$\Sigma_{ii} = -J \sum_\delta \frac{\delta t_{i,i+\delta}}{t}. \tag{9}$$

Now $\Sigma_\delta \delta t_{i,i+\delta}/t$ is the sum of z (coordination number) Gaussian variables and will therefore itself have a Gaussian distribution with an effective second moment of $z\sigma$. Thus the local self-energy Σ_{ii} has a scale of J and is randomly distributed according to a Gaussian distribution with a much bigger width $\sqrt{z\sigma}$. The high-energy magnons thus effectively experience a random potential and therefore get trapped in the local potential depressions. In fact, Σ_{ii} precisely yields the extra magnon energy for the localized high-energy modes, and therefore we can conclude that these modes will extend well beyond $2J$ in energy, and that the excess in energy will have a Gaussian distribution of width $\sqrt{z\sigma}$. This result has a significant impact on the one-magnon density of states, indicating that there will be a Gaussian tail in the DOS extending well beyond energy $2J$. Indeed, this is evident from Fig. 2 showing the magnon DOS obtained via the exact-eigenstate analysis which is discussed in the following section.

We have thus shown that while the low-energy, long-wavelength magnon modes are very weakly affected by hopping disorder, on the other hand the high-energy magnon modes are strongly affected because of a cooperative effect due to local correlations in hopping disorder. There is therefore a strong asymmetry in the energy shifts of low-energy and high-energy magnon modes, which is also evident from the magnon DOS shown in Fig. 2. Now the asymmetric line shape in the two-magnon Raman scattering in cuprate antiferromagnets has been a puzzling feature. If indeed it is the randomness in hopping due to zero-point motion which is responsible for this feature, then we have shown that this asymmetry is basically arising from the asymmetric energy renormalization of high-energy and low-energy magnons due to hopping disorder. Also, the strong energy renormalization of high-energy magnons due to this cooperative effect of hopping disorder leads to an insight into the extraordinary sensitivity of the Raman scattering process on zero-point motion of the lattice. This is the central result of this paper.

We have seen that the first-order correction to $[\chi^0(\omega)]$ yields a vanishing contribution to the low-energy, long-wavelength magnon energies in the limit of infinite system size. Therefore it is necessary to consider second-order correction to $[\chi^0(\omega)]$, for which the relevant diagrams are shown in Fig. 1(b). Summing all the processes, we obtain, after configuration averaging,

$$\langle \delta\chi^0_{ii}\rangle = -\frac{2t^2}{U^3}\sum_k \left\langle\left(\frac{\delta t_{ik}}{t}\right)^2\right\rangle = -\frac{2zt^2}{U^3}\;\sigma,$$

$$\langle \delta\chi^0_{ij}\rangle = -\frac{2t^2}{U^3}\left\langle\left(\frac{\delta t_{ij}}{t}\right)^2\right\rangle = -\frac{2t^2}{U^3}\;\sigma. \tag{10}$$

After adding to $[\chi^0(\omega)]$, and Fourier transforming within the two-sublattice basis, we obtain

$$[\chi^0(q,\omega)] = \frac{1}{U}\;\mathbf{1} - (1+\sigma)\;\frac{t^2}{\Delta^3}\begin{bmatrix} 1+\dfrac{\omega}{2J'} & \gamma_q \\ \gamma_q & 1-\dfrac{\omega}{2J'}\end{bmatrix}, \tag{11}$$

where $2J' \equiv 2J(1+\sigma)$ is the renormalized magnon-energy scale. Therefore, all magnon energies are simply renormalized by a momentum-independent multiplicative factor $(1+\sigma)$, and we have

$$\omega_q = 2J(1+\sigma)(1-\gamma_q^2)^{1/2}. \tag{12}$$

III. EXACT-EIGENSTATE ANALYSIS

We now briefly describe the exact-eigenstate method for obtaining the magnon energies and wave functions. Details of this method have been given earlier for the impurity-doped Mott-Hubbard AF with on-site potential disorder.[13] The idea is to self-consistently obtain the AF state for the hopping-disordered system within the Hartree-Fock approximation, and then determine the magnon eigensolutions from the transverse spin propagator, evaluated in the broken-symmetry state. Since we are concerned here with an AF insulating state for the one-fermion-per-site system, the HF-plus-fluctuations approach is expected to be quantitatively accurate even in the strong correlation limit, as has been shown to be the case for the pure system.[14]

Within the HF approximation we construct the Hamiltonian matrix on a two-dimensional square lattice with periodic boundary conditions. The random hopping terms δt_{ij} are obtained for each pair of NN sites using a Gaussian random number generator. In the site basis matrix elements of the Hamiltonian for spin σ are given by $\langle i|\hat{H}_\sigma|i\rangle = U\langle n_{i\bar{\sigma}}\rangle$ and $\langle i|\hat{H}_\sigma|j\rangle = -(t+\delta t_{ij})$ if i and j are nearest neighbors. Starting with some initial configuration for the spin densities, the Hamiltonian matrix is constructed and diagonalized to yield the eigensolutions $\{E_{l\sigma},\phi_{l\sigma}\}$. From these the spin densities are reevaluated, the H matrix is updated, and the procedure iterated until self-consistency is achieved. These exact eigenstates of the self-consistent AF state are used to construct the $[\chi^0(\omega)]$ matrix as described earlier.[13]

TABLE I. Variation of the configuration-averaged maximum magnon energy $\overline{\omega_m}$ with hopping disorder strength σ. Also shown are the configuration-averaged increase in magnon energy $\overline{\omega_m} - \omega_m^0$ for the highest magnon mode relative to the pure-case energy ω_m^0, and comparison with the configuration-averaged maximum self-energy correction $\overline{\Sigma}_m$ evaluated from Eq. (9).

σ	$\overline{\omega_m}/J$	$(\overline{\omega_m}-\omega_m^0)/J$	$\overline{\Sigma}_m/J$
0.0	1.89	0	0
0.1	3.05	1.16	1.12
0.2	3.44	1.55	1.58
0.3	3.95	2.06	1.93

It is convenient to express the transverse spin fluctuation propagator at RPA level in terms of the eigensolutions $\{\phi_\lambda(\omega),\lambda(\omega)\}$, of the $[\chi_0(\omega)]$ matrix:

$$[\chi^{-+}(\omega)] = \sum_\lambda \frac{|\phi_\lambda(\omega)\rangle\langle\phi_\lambda(\omega)|}{1-U\lambda(\omega)}. \tag{13}$$

In this form we have a propagator representation for the magnon, with the magnon wave function given by the eigenvector $|\phi_\lambda(\omega)\rangle$ and magnon energies obtained from the pole, $1-U\lambda(\omega)=0$. The energy ω_n of the nth magnon mode is obtained by solving, $1-U\lambda_n(\omega_n)=0$ for the appropriate (nth from the top) eigenvalue $\lambda_n(\omega)$. The root of the equation, $\lambda_n(\omega_n)=1/U$ is determined by obtaining $\lambda_n(\omega)$ for closely spaced values of ω on both sides of the root, and finally linearly extrapolating between them. Suppose (λ_n^1,ω_n^1) and (λ_n^2,ω_n^2) are two sets of values for two energies very close to, and on either side of the root, then the root ω_n is determined from

$$\lambda(\omega_n) = \frac{1}{U} = \lambda_n^1 + \frac{\lambda_n^2-\lambda_n^1}{\omega_n^2-\omega_n^1}\;(\omega_n-\omega_1). \tag{14}$$

The whole procedure therefore involves obtaining the self-consistent state for a given realization of the hopping-disordered system, followed by constructing and diagonalizing the $[\chi^0)(\omega)]$ matrix, and finally from the set of eigenvalues $\lambda_n(\omega)$ the magnon energies are obtained by interpolation as described above. This scheme for obtaining the magnon energies is then repeated for several configurations.

We find that the highest magnon energies always extend well beyond the maximum energy $2J$ for the pure case. Even for σ as low as 0.1, the highest magnon energy obtained is about $3.4J$. This is in agreement with the perturbative analysis finding that the high-energy magnon modes are strongly renormalized due to the correlated effect of hopping disorder.

In Table I we show the variation with σ of this hopping-disorder-induced increase in the magnon energy for the highest magnon mode, and compare with the perturbative result derived earlier [Eq. (9)]. For a given σ the highest magnon mode energy is configuration-averaged over 25 configurations of the hopping-disordered system to yield $\overline{\omega_m}$. The difference with the maximum magnon energy ω_m^0 for the pure case yields the excess due to hopping disorder. This difference is compared with the perturbative result for the magnon self-energy given in Eq. (9) for high-energy magnon modes with energy near $2J$. For a given realization of the random hopping terms, the nearest-neighbor sum $\Sigma_\delta \delta t_{i,i+\delta}/t$ is performed for all lattice sites, yielding the local self-energies Σ_{ii}. From this the maximum is picked out, and this is averaged over 25 different configurations, yielding the configuration-averaged maximum self-energy correction, $\overline{\Sigma_m}$. That the excess in magnon energy for the highest mode matches well with the maximum of the local self-energy correction strongly supports the idea that high-energy magnon modes involve spin deviations at those sites where the locally averaged hopping terms are maximum. This implies that the upper end of the magnon-energy spectrum is entirely determined by local correlations in the random hopping terms. In as much as this part of the magnon spectrum is most important in the two-magnon Raman scattering, features such as the strong asymmetry can thus be traced to these local correlations in hopping disorder.

A convenient way to exhibit the strong renormalization of high-energy magnons is via the magnon density of states:

$$N(\omega) = \lim_{\eta\to 0} \frac{1}{\pi}\frac{1}{N_n}\sum_n \frac{\eta}{(\omega-\omega_n)^2+\eta^2}, \tag{15}$$

where ω_n's denote the magnon energies and η is chosen to be of the order of average level spacing. N_n represents the total number of modes obtained from the 50 different configurations considered. The results for the magnon DOS are plotted in Fig. 2 for different values of σ. Also shown for comparison is the DOS for the pure system which extends up to energy $\sim 2J$. It is observed that the DOS for the hopping-disordered system extends well beyond the maximum energy $2J$, though the position of the peak remains roughly the same.

We have also examined the magnon wave function for modes at the high-energy end of the spectrum, and find that indeed these modes are strongly localized in certain regions of the lattice, as expected from the analysis discussed earlier. The magnon amplitudes are contained in the eigenvectors $|\phi_\lambda(\omega)\rangle$ of the $[\chi^0(\omega)]$ matrix evaluated at the magnon energies. A useful way to exhibit the magnon modes on the lattice is via arrows with size proportional to the local magnon amplitude ϕ_λ^i, and orientation proportional to the rotation angle $\theta_i = \sin^{-1}(\phi_\lambda^i/S_z^i)$, where S_z^i is the local magnetization.[15] The zero-energy (Goldstone) mode in this representation is characterized by identical rotation angles, despite the local magnetization and magnon amplitudes having different magnitudes on the lattice sites due to disorder. We have also confirmed that this localization of high-energy magnon modes occurs in those regions of the lattice where the locally averaged hopping is significantly higher than the bulk average, so that the locally averaged U/t ratio and the local magnetization are low.

In conclusion, we have studied the Mott-Hubbard antiferromagnet with hopping disorder, both perturbatively and also using the exact-eigenstate method, in the strong correlation limit. We have shown that while the low-energy, long-wavelength magnon modes are only weakly affected, the high-energy modes on the other hand are strongly affected because of a cooperative effect arising from local correlations in hopping disorder that is possible. There is therefore a strong asymmetry in the energy shifts of the low-energy and high-energy magnon modes. If indeed zero-point motion leads to hopping disorder in cuprates, then this work provides a qualitative understanding of the anomalous linewidth and asymmetric line shape seen in the two-magnon Raman scattering in cuprate antiferromagnets. Also, the strong energy renormalization of high-energy magnons due to the cooperative effect of hopping disorder leads to an insight into the extraordinary sensitivity of the Raman scattering process on the zero-point motion of the lattice.

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