What is the Hamiltonian for parent high-temperature superconductors?

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Previous studies of the half-filled Hubbard model suggest that high-energy spin excitations in the high-temperture superconductor parent compoud La_2CuO_4 are well described when the interaction strength is in the weak to intermediate-coupling regime. Using the same methodology as a previous Quantum Monte Carlo study, it is shown in this paper that even weaker coupling is necessary to obtain agreement with experiment when realistic second-neighbor hopping is included. The value of the interaction strength obtained is too small to explain the Hubbard gap at half-filling, suggesting either that the single-mode approximation used in this work is inappropriate to describe high-energy spin excitations or that a more complicated Hamiltonian including either three bands or direct ferromagnetic Heisenberg exchange is necessary to describe the Physics.

Des études antérieures du modèle de Hubbard à demi rempli suggèrent que les excitations de spin à haute énergie du matériau La_2CuO_4 sont bien décrites quand la force de l'interaction est dans le régime de couplage faible à intermédiaire. Utilisant la même méthodologie qu'une étude antérieure basée sur le Monte-Carlo quantique, il est démontré ici qu'un couplage encore plus faible est nécessaire pour obtenir l'accord avec l'expérience lorsqu'un saut au deuxième voisin réaliste est inclus dans l'hamiltonien. La valeur de l'interaction ainsi obtenue est trop faible pour expliquer le gap de Hubbard à demi rempli. Ceci suggère soit que l'approximation à un mode utilisée dans ce travail n'est pas valable pour décrire les excitations de spin à haute énergie, ou qu'un hamiltonien plus compliqué, incluant trois bandes ou un échange ferromagnétique direct de type Heisenberg, est nécessaire pour décrire la physique.

1 Introduction

Electronic properties of a large fraction of solids can be predicted using band theory in its modern form, namely density functional theory combined with the so-called GW approach [1]. However, the understanding of materials with d and f electrons is most often beyond the capabilities of this approach. High temperature superconductors belong to this category. This is especially striking for the parent compounds, namely the undoped, non-superconducting versions of the high-temperature superconductors. Band theory predicts that they have a half-filled band and hence should be good metals, but experiment shows that they are antiferromagnetic insulators at low temperature, and that they remain insulators above their antiferromagnetic transition temperature. They are so-called Mott insulators. First-principle approaches combining density-functional theory and many-body theory are being developed right now [2] but still the most common approach in d and f electron systems is to work with phenomenological Hamiltonians that include band structure information in the form of hopping amplitudes that reproduce the calculated band structure, and residual interaction terms that have to be treated by many-body approaches. Experience indicates that at least the ratios of the hopping parameters obtained from band structure calculations are reliable. The value of the interaction strength and the absolute scale of hopping parameters can be better obtained by comparing the results of calculations with experiment.

For high-temperature superconductors, the Hamiltonian that is most commonly used is the two-dimensional Hubbard model on a square lattice with both first and second-neighbor hopping. It reads,

$$\begin{aligned} H &= -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle, \sigma} (c^\dagger_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma} + c^\dagger_{\mathbf{j},\sigma} c_{\mathbf{i},\sigma}) \\ &\quad -t' \sum_{\langle\langle \mathbf{i},\mathbf{j} \rangle\rangle, \sigma} (c^\dagger_{\mathbf{i},\sigma} c_{\mathbf{j},\sigma} + c^\dagger_{\mathbf{j},\sigma} c_{\mathbf{i},\sigma}) + U \sum_{\mathbf{i}} n_{\mathbf{i},\uparrow} n_{\mathbf{i},\downarrow} \end{aligned} \quad (1)$$

where $c^\dagger_{\mathbf{i},\sigma}(c_{\mathbf{i},\sigma})$ creates (annihilates) an electron of spin σ on site $\mathbf{i}$, $n_{\mathbf{i},\sigma}$ is the number of electrons of spin σ on site $\mathbf{i}$, t is the hopping amplitude over all nearest-neighbor bonds $\langle \mathbf{i},\mathbf{j} \rangle$, t' is the hopping amplitude over all next-nearest-neighbor bonds $\langle\langle \mathbf{i},\mathbf{j} \rangle\rangle$ and U is the on-site repulsion parameter. We work in units where hopping t, Boltzmann's constant k_B and Planck's constant $\hbar$ are all unity. Band structure calculations [3] reveal that a third neighbor hopping should also be included. Detailed comparisons with photoemission experiments [4][5][6], for example, confirm this result. Unless very detailed fits with experiment are required however, the third neighbor hopping can be neglected since it is generally smaller than the other two terms. Neglect of second-neighbor hopping t' however leads to qualitatively wrong results for the shape of the Fermi surface of both hole- and electron-doped high temperature superconductors. Also, $t' = 0$ would not lead to good fits to experimental photoemission or optical [7] data at half-filling.

In the present paper, we study the spin excitations of the above Hamiltonian in the insulating parent compound. This is motivated by recent neutron scattering experiments [8] on La_2CuO_4 that have, for the first time, allowed high resolution study of the high-energy dispersion of spin ex-

citations (or magnons). These are sensitive to details of the Hamiltonian, unlike the long-wavelength low-energy modes. By comparing the results of experiments with those of the effective spin Hamiltonian found in the large U limit of the above Hamiltonian, [9][10][11] the authors of Ref. [8] concluded that t' leads to effects that can be neglected since they are smaller than the ring-exchange contributions that are the first corrections to simple near-neighbor exchange. Given the nearest-neighbor exchange $J = 4t^2/U - 24t^4/U^3$, the ring-exchange $J_c = 80t^4/U^3$ and the second and third neighbor exhanges $J' = J'' = 4t^4/U^3$ (the latter are subdominant), they were able to find both U and t. At $10K$ for example, they found $t = 0.30 \pm 0.02eV, U = 2.2 \pm 0.4eV$. Unfortunately, this value of $U = 7.3t \pm 1.8t$ is at the limit of validity of the expansion in powers of $8t/U$ (where $W = 8t$ is the bandwidth). In addition, these authors [8] used only the leading order spin-wave analysis on the biquadratic part of the ring exchange Hamiltonian to obtain the theoretical predictions that they compare with experiment. It has been argued [12] that to the same order in (t/U), biquadratic and bilinear terms are in just the right ratio that linear spin wave analysis leads to a flat dispersion on the zone boundary, just like the Heisenberg model at the same level of approximation. Dispersion at high-frequency should be a purely quantum effect (higher order in $1/S$) when both biquadratic and bilinear terms are taken into account. So, Katanin and Kampf [13] found it appropriate to perform more sophisticated self-consistent spin-wave theory and they found a J that is a few percent larger than in Ref. [8], but their J_c is considerably smaller, namely about half the value found in Ref. [8]. If we use the same expression [9][10] as that used in Ref. [8] , $J_c/J = 20\,(t/U)^2 \left(1 - 6\,(t/U)^2\right)^{-1}$, the ratio $J_c/J = 0.24$ found by Katanin and Kampf [13] leads to $U = 9.5t$ that is more consistent with previous estimates, $U = 10t$, from photoemission [6]. It is noteworthy that the W/U expansion should be better justified for this value. Again, in this limit, the effect of t' would manifest itself through the second-neighbor hopping exchange integral, but its contribution should be more important since the ring-exchange term is smaller.

A lingering possibility is that the W/U expansion does not converge very well [11] and that, instead of effective spin models, one should really compare the full Hubbard Hamiltonian with experiments. This is what Sengupta, Scalettar and Singh [12] achieved by comparing Quantum Monte Carlo calculations with the experimental results of Ref. [8]. Using in addition the so-called single-mode approximation (SMA), they found that the frequency at $(\pi/2, \pi/2)$ is smaller by 12% than the frequency at the $(\pi, 0)$ wave-vector when $U/t = 6$ on an 8×8 lattice [12]. This corresponds well to the experimental value found in Ref. [8]. The value $U/t = 6$ found in that work confirmed an earlier independent result of Peres and Araujo[14] obtained using the Random Phase Approximation (RPA) for the Hubbard model. However, $U = 6t$ certainly corresponds to a regime where the W/U expansion breaks down so that it does not make sense to talk about direct and ring exchanges. Then, one cannot invoque the ring exchange contribution to neglect the second-neighbor hopping t'. In addition, the estimate $U = 6t$ is lower than that obtained by most other workers and is on the lower side of the critical value estimated necessary to obtain a finite-temperature Mott gap at half-filling [15][16].

The question of the effect of t' on the high-frequency spin excitations of the Hubbard model at half-filling is thus important. One would hope that comparison with experiment would lead us to a higher value of U, in better agreement with other estimates and more consistent with the large value of U necessary to obtain a Mott insulator at half-filling. Two studies based on the RPA have appeared for this problem.[17][18] The present paper addresses the same question using quantum Monte Carlo simulations.

In the following, the amplitude of the next-nearest neighbor hopping has been chosen such that as many wave vectors as possible cross the Fermi surface. For an 8×8 lattice, the optimal value is $t' = -0.35$ [19]. This is larger than $t' = -0.17$ obtained from band structure calculations [20][3] for La_2CuO_4 but comparable to values found in other high-temperature superconductors such as $YBa_2Cu_3O_7$ and $Bi_2Sr_2CaCu_2O_8$. Since our purpose is to answer whether in the presence of t' the value of U should be larger or smaller to obtain agreement with experiment, we find it preferable to work with a value of t' that is sufficiently large to clearly show the trend.

In the next section, we discuss several methodological aspects of this problem. First we describe details of the Quantum Monte Carlo calculations and then the single-mode approximation. We then present the results and conclude.

2 Methodological aspects

2.1 Quantum Monte Carlo simulations

In the context of this conference on high-performance computing, we find it appropriate to mention some technical details on the Quantum Monte Carlo simulations. We want to obtain thermal averages of operators in the grand-canonical ensemble. Direct calculation of the partition function $\mathrm{Tr}\left[e^{-\beta(H-\mu N)}\right]$ with $\beta = 1/T$ and μ the chemical potential, is basically impossible even on an 8×8 lattice. In that case, taking into account the fact that each site can be either empty, doubly occupied, or singly occupied with spin up or down, there are $4^{8\times 8} = 3.4 \times 10^{38}$ possible states. Monte Carlo methods with importance sampling are a method of choice in the case of statistical problems with huge state spaces. In the case of classical mechanics, it is quite simple to compute how $e^{-\beta(H-\mu N)}$ is modified when it is applied on two states that differ by a local change. That is all that is needed to perform Monte Carlo simulations. In the quantum case, the exponential of $\beta\,(H - \mu N)$ can be computed only if H can be diagonalized, which is the

problem we are faced with from the very beginning: H has a kinetic part K and a potential part V that are diagonal respectively in momentum and in coordinate space. The basis where $K+V$ is diagonal is unkown. To address this difficulty, the problem is first made to look more classical by using the so-called Trotter decomposition, $e^{-\beta(H-\mu N)} = e^{-\Delta\tau(H-\mu N)}e^{-\Delta\tau(H-\mu N)}\dots e^{-\Delta\tau(H-\mu N)}$ with the number of exponentials, or number of "time slices" N_τ given by $N_\tau = \beta/\Delta\tau$. In the limit $\Delta\tau \to 0$ one can write $e^{-\Delta\tau(H-\mu N)} = e^{-\Delta\tau K}e^{-\Delta\tau(V-\mu N)} + O\left(\Delta\tau^2\right)$ which means progress since we know the basis where either exponential is diagonal. However, the change of basis necessary to move from one operator to the next is still a formidable task for a many-body problem like the one we consider now, where the motion of electrons is not independent. To go around this, one performs a so-called Hubbard-Stratonovich transformation on $e^{-\Delta\tau(V-\mu N)}$. More specifically, one can use an identity [21] that is easily proven by recalling that $n_{\mathbf{i},\uparrow}$ and $n_{\mathbf{i},\downarrow}$ can take only the values 1 and 0 :

$$e^{-\Delta\tau U\left(n_{\mathbf{i},\uparrow}-\frac{1}{2}\right)\left(n_{\mathbf{i},\downarrow}-\frac{1}{2}\right)} = e^{-\Delta\tau U/4}\frac{1}{2}\sum_{x_i=\pm 1} e^{\lambda x_i\left(n_{\mathbf{i},\uparrow}-n_{\mathbf{i},\downarrow}\right)} \tag{2}$$

where $\cosh(\lambda) = e^{\Delta\tau U/2}$. There is now one Hubbard-Stratonovich variable x_i per site in space-time, in other words on a $L\times L$ lattice there are $2^{L^2N_\tau}$ possible values for the set of Hubbard-Stratonovich variables. At first it looks as if we have complicated the problem by increasing the number of variables to be traced over. However, at the end it is only the trace over Hubbard-Stratonovich variables that is finally sampled by Monte Carlo methods because the use of the above identity allows us to transform the problem into one where the electrons are independent but move in a space and time dependent potential (coming from the Hubbard-Stratonovich variables). This means that the quantum mechanical trace over fermions can now be performed exactly in algebraic time for any given configuration of the Hubbard-Stratonovich variables. The trace over fermions, however, is a determinant that can be either positive or negative, which means that to apply importance sampling, one must take the absolute value of the determinant and move the sign to the observable. That leads to the so-called sign problem: There are cases where the sign changes so often from one configuration to the next that importance sampling becomes exponentially inefficient. There are many other technical difficulties one must address, in particular the question of numerical stability at low temperature [22]. The reader is refered to a recent review [23] and to the original literature on this so-called Determinant Quantum Monte Carlo Method [24]. A review in French is also available [25].

For the simulations presented in this paper, we typically use 1.25×10^5 measurements, each measurement being performed after a full update of all the Hubbard-Stratonovich variables of the space-time lattice. The measurements are grouped in blocks of 250 measurements for estimation of the statistical error. The value of $\Delta\tau$ is $1/10$. We checked that, given the statistical uncertainties, larger $\Delta\tau = 1/8$ would not have changed our results. This is discussed further in the next section. The numerical stabilization at low temperature is performed by Gram-Schmidt decomposition every five time slices [22]. Also, averaging over independent simulations that each have their warmup cycles reduces ergodicity problems.

There are different possible estimators, namely $\langle S_zS_z\rangle$ and $\langle S_+S_-\rangle + \langle S_-S_+\rangle$, for the spin-spin correlation functions that we will need. We checked that $\langle S_zS_z\rangle$ had smaller statistical error at the temperatures of interest, so that is what we used. Since we do not have particle-hole symmetry, the average sign is different from unity and in addition the chemical potential corresponding to half-filling must be found by iteration. For example, at $\beta = 3$, $U = 6$ the average sign is 0.724 and the value $\mu = -.27995$ gives a filling of $0.99967\pm\ 0.4\times10^{-4}$. For such high temperature and high-energy properties, size 8×8 should be enough. A 6×6 lattice gives results for intermediate values of the wave vectors that are consistent interpolations between the wave vectors of the 8×8 lattice [12]. Further discussion of size effects is given in the section on results below.

The program is written in Fortran 90 with allocatable memory. It is compiled with the Intel Fortran Compiler, which is free for academia and performed faster than others we have tested. For an 8×8 lattice at these high temperatures, $\beta = 3$, the program typically takes $6.6\ MB$ of memory and 44 hours of computation time for 1.25×10^5 measurements and 1×10^4 warmups on a pentium IV processor running at $2.5GHz$. Computation time scales roughly like $\left(L^2\right)^3 N_\tau$. For example, 10^5 measurements and 2×10^4 warmups on a 12×12 system at the same temperature take 480 hours and $33\ MB$. Typically, 10 jobs with a thousand warmups and tens of thousands of measurements each are sent on the nodes of a Beowulf cluster and the results are averaged to obtain of order 10^5 measurements. In this way, one run at fixed U and temperature for an 8×8 system takes roughly a day for example on a cluster of $667MHz$ pentium III machines.

2.2 Single-mode approximation

Ideally, one should compute the imaginary part of the frequency and wave vector dependent spin susceptibility, which is accessible through neutron scattering. But this means that one should perform analytical continuation of the Quantum Monte Carlo calculations since these are performed in imaginary-time. This is usually achieved by using the so-called Maximum Entropy method [26]. For the problem at hand, in agreement with the authors of Ref. [12], we were unable to obtain reliable data using this approach. We thus followed the procedure of Ref. [12] and obtained the dispersion relation of the spin excitations from the so-called single-mode approximation (SMA)

$$\omega(\mathbf{q}) = 2S(\mathbf{q})/\chi(\mathbf{q}) \tag{3}$$

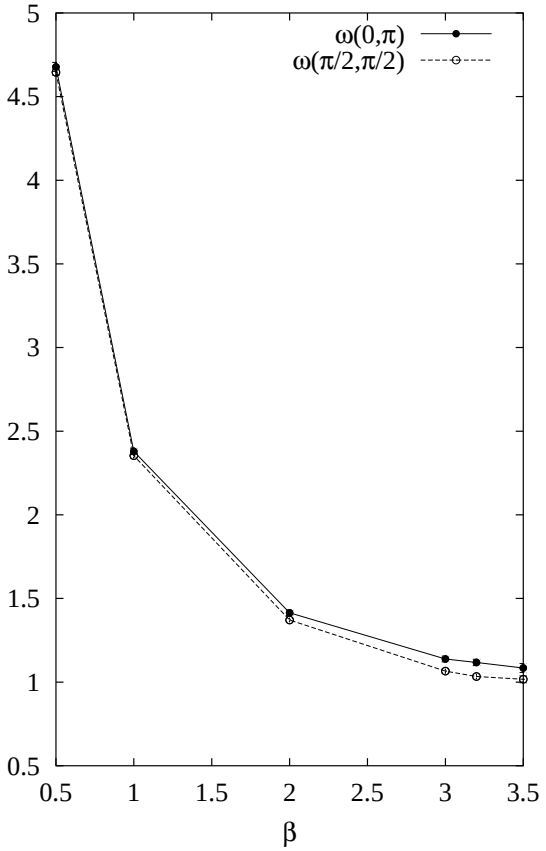

Figure 1. Frequency as a function of temperature for two wave vectors at $U = 6$ on an 8×8 lattice. The continuous line represents the energy at wave-vector $(0, \pi)$, and the dash-line the energy at wave-vector $(\pi/2, \pi/2)$. We observe that at low temperature (high β), the dispersion converges. Error bars are smaller than the symbols.

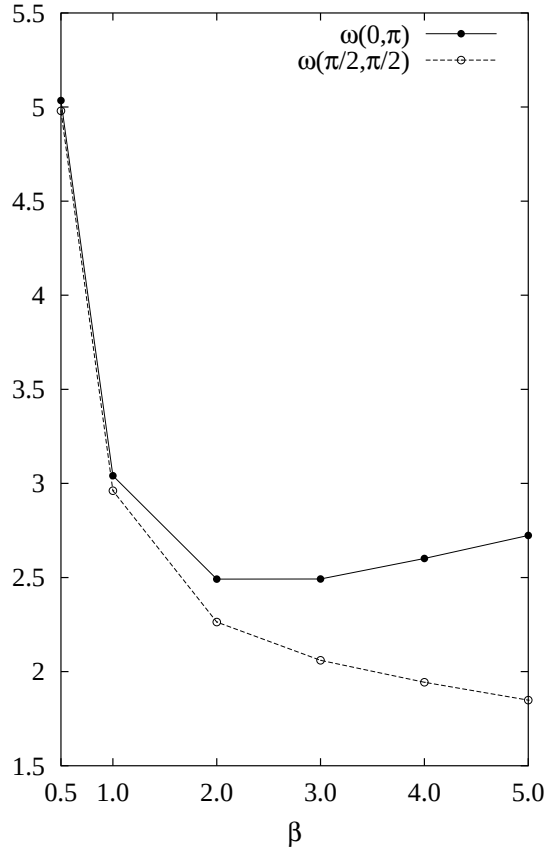

Figure 2. Frequency as a function of temperature for two wave vectors at $U = 0$ on an 8×8 lattice. This $U = 0$ case illustrates that when the SMA does not work, there is a strong temperature dependence. The symbols have the same meaning as in the previous figure.

where $S(\mathbf{q})$ is the spin structure factor and $\chi(\mathbf{q})$ is the zero-frequency spin susceptibility obtained simply from integration over imaginary time. This result becomes exact in the limit where the imaginary part of the spin susceptibility is peaked at only one frequency for any given wave vector. Indeed, using the fluctuation-dissipation theorem,

$$S(\mathbf{q}) = \int \frac{d\omega}{2\pi} \frac{2}{1 - e^{-\beta\omega}} \chi''(\mathbf{q},\omega) \tag{4}$$

and the spectral representation

$$\chi(\mathbf{q}) = \int \frac{d\omega}{\pi} \frac{\chi''(\mathbf{q},\omega)}{\omega}, \tag{5}$$

if the odd function $\chi''(\omega)$ is proportional to $\delta(\omega - \omega(\mathbf{q})) - \delta(\omega + \omega(\mathbf{q}))$ then the result Eq.(3) follows when $1 \gg e^{-\beta\omega(\mathbf{q})}$. As we shall see shortly, we work with $\beta = 3$ and $\omega(\mathbf{q}) \sim 1$ so the inequality is satisfied. It is known [27] however, that for $t' = 0$ and large U there is a broad multimagnon continuum above the single magnon mode. We expect an analogous continuum with finite t'. Sengupta *et al.* [12], based on the work of Ref. [27], argue that while the magnitude of the frequency found from the SMA is affected by the high frequency multimagnon continuum (the SMA in that case gives and upper bound for $\omega(\mathbf{q})$), nevertheless the overall shape of the dispersion relation is not affected by the continuum. Since we shall be using only information on ratio of frequencies, it is argued that this should be a sufficiently accurate approach.

We are interested in high-frequency modes hence the simulations, as in Ref. [12], can be performed at relatively high temperature. To prove this, Fig. (1) shows the value of the high-frequency modes at $(\pi, 0)$ and $(\pi/2, \pi/2)$ estimated from the SMA as a function of inverse temperature β for $U = 6$ and $t' = -0.35$. Although the estimated mode frequencies appear weakly temperature dependent at $\beta = 3$, their differences for $\beta = 3.0$, 3.2 and 3.5 are, respectively, 6.8%, 8.1% and 6.7%. There is no systematic drift in this difference. The fluctuation of about 13% seen between these last three numbers should be considered as coming from the error bars of the Quantum Monte Carlo.

With $t' = 0$ [12], the temperature dependence is weaker

beyond $\beta = 3$. The sign problem prevents us from doing simulations at $\beta = 4$, so we choose the same temperature as in Ref. [12], namely $\beta = 3$. Fig. (2) contrasts the same calculation in the case where the SMA does not work, namely at $U = 0$. Clearly, there is a strong temperature dependence, even at low temperature. In addition, a plot of the dispersion relation in the $U = 0$ case (not shown) reveals that the mode at (π, π) is not soft. The softening of the (π, π) point observed when $U = 6$ in Fig. (3) signals that antiferromagnetism is setting in. We checked that at $t' = 0$ we recover all the results of Ref. [12]

3 Results

3.1 No second-neighbor hopping

We first performed additional tests for dependence on size, temperature and impaginary time discretization. Size dependence was checked further by performing the simulations at $U = 6t$, $\beta = 3$ for a 12×12 lattice, which corresponds to the size where systematic convergence to the thermodynamic limit was better than about 3% percent in the work on the Heisenberg model of Ref.[27]. The values of $\omega(\pi, 0), \omega(\pi/2, \pi/2)$ that we found are identical to those for the 8×8 lattice to within the 0.5% statistical accuracy. Close to 10^6 samples were used for these tests. We also tried to check for size dependence at lower temperature on larger lattices, but results on 10^5 samples for $\beta = 5$ on a 12×12 lattice, for example, only give about 20% statistical accuracy, which is not enough. Simulations with better statistical accuracy for these parameters are prohibitive. Finally, as a further check of the systematic error introduced by the Trotter decomposition, we checked that for the 8×8 lattice, $\Delta\tau = 1/8$ and $\Delta\tau = 1/10$ give identical results for $\omega(\pi, 0), \omega(\pi/2, \pi/2)$ within 0.5% statistical accuracy.

Given that the work of Katanin and Kampf [13] suggests the value $U = 10t$ for a good fit to experiment, we performed simulations on 8×8 systems at $\beta = 3$. A large number of Monte Carlo samples $\left(10^6\right)$ is needed. We found that the dispersion between $\omega(\pi, 0)$ and $\omega(\pi/2, \pi/2)$ is flat to the 1.5% statistical accuracy. Not surprisingly, this interpolates between the results found in Ref. [12] for $U = 8t$ and for the Heisenberg model, which corresponds to the very large U limit. This disagreement with the results of Katanin and Kampf [13] may come from the fact that the SMA is not valid or from the fact that the self-consistent $1/S$ expansion is not justified in the presence of ring exchange.[28] Indeed, in that approach, the ring exchange contribution, which should be a correction to the direct exchange term, is in fact larger than direct exchange term by a factor S^2.

3.2 Finite second-neighbor hopping

We plot on Fig. (3) the magnon dispersion relation obtained for an 8×8 system at $U = 6$, $\beta = 3$ when $t' = 0$ and when $t' = -0.35$. In the latter case, the Quantum Monte Carlo error bars are much larger because of the sign problem. Let us focus on the dispersion on the line going between $(\pi/2, \pi/2)$ and $(\pi, 0)$. For this value of U, the case $t' = 0$ that was studied in Ref. [12] leads to $1 - \omega(\pi, 0)/\omega(\pi/2, \pi/2) = -12\%$ that corresponds to the experimental value of Ref. [8]. With $t' = -0.35$ the absolute value of this ratio is smaller.

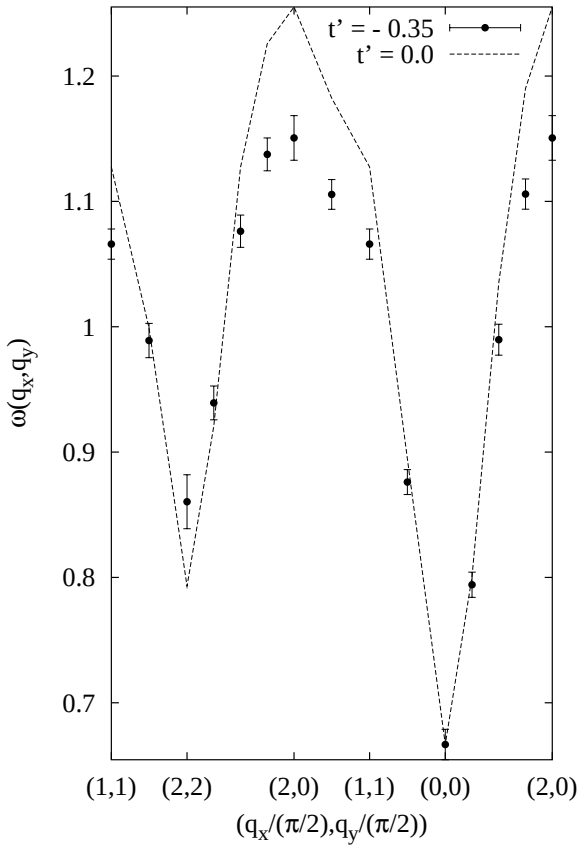

Figure 3. Energy dispersion relation in the SMA as a function of wave vector for $\beta = 3.0$ and $U = 6.0$ for an 8×8 lattice. The coordinates on the horizontal axis must be multiplied by $\pi/2$. The line corresponds to the case $t' = 0.0$, and the points correspond to the case $t' = -0.35$. Error bars represent the statistical Quantum Monte Carlo errors.

To fit the experimental value of the dispersion, we need a smaller value of U/t as demonstrated in Fig. 4 where we plot the dispersion relation along the $(0, \pi)$ to $(\pi/2, \pi/2)$ to $(\pi, 0)$ line. The data is normalized for each U such that, $\omega(\pi, 0) = 1$. Clearly, the dispersion increases with decreasing U and reaches the experimental value around $U = 5.0t \pm 0.5t$.

4 Discussion and conclusions

Previous QMC simulations [12] have suggested, in agreement with RPA calculations, [14][17] that the dispersion of high-frequency spin-wave excitations in the parent high-temperature superconductor La_2CuO_4 can be explained with the Hubbard model at $U = 6t$. We have

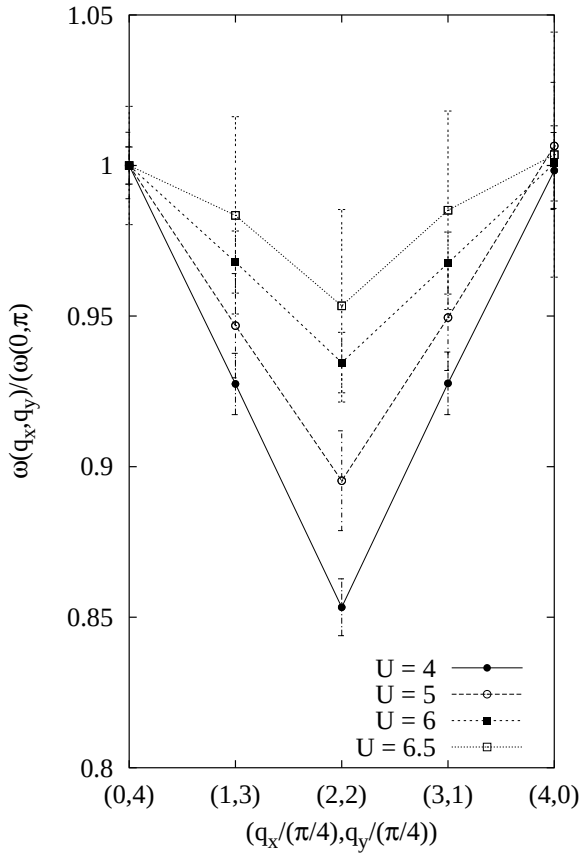

Figure 4. Energy dispersion relation along the $(0,\pi)$ to $(\pi/2,\pi/2)$ to $(\pi,0)$ line for $\beta = 3.0$ and $t' = -0.35$. The coordinates on the horizontal axis must be multiplied by $\pi/4$. Each line correspond to a fixed value of U. The dispersion increases with smaller U. Error bars represent the statistical quantum Monte Carlo error.

shown here that the addition of second-neighbor hopping $t' = -0.35t$ leads to an even smaller value of the interaction strength, namely $U = 5t \pm 0.5t$. This lowering of U is in agreement with RPA calculations [17][18] and is what would have been expected if we had been at strong coupling. Indeed, it is known that second-neighbor ferromagnetic exchange $(J_2 < 0)$ can explain the experimental dispersion [8] but second-neighbor hopping in a Hubbard model leads to an antiferromagnetic second-neighbor exchange $(J_2 > 0)$. This has to be compensated by a smaller U since lowering U tends to increase the dispersion in that weak coupling range of U values.

However, U of order $6t$ is too small to explain the Mott gap at half-filling. Comparisons of photoemission experiments with the results of exact diagonalization for example suggests $U = 10t$ [6].

One possibility is that the SMA is not accurate and that finite size effects are important so that the agreement with RPA calculations is fortuitous. Indeed, in the Heisenberg limit it is known [12] that the dispersion obtained with the QMC+SMA approach leads to a $(\pi/2,\pi/2)$ mode that is only 2% higher than the $(\pi,0)$ mode while more sophisticated calculations [27] suggest that this number should be 5% on an 8×8 system and 10% in the thermodynamic limit. The SMA in particular can be questioned since there is a multimagnon continuum at high frequency [27] that is different for the two wave vectors of interest. We however did several tests that did not invalidate the SMA nor suggested large size effects.

If the SMA is valid and size effects are not important, then the effective Hamiltonian obtained from the Hubbard model at $U = 10t$ is not sufficient to describe spin excitations. It is conceivable that direct ferromagnetic exchange between next-nearest neighbors J_2 has to be included explicitly in the effective Hamiltonian [8] but ab initio calculations [29] suggest antiferromagnetic J_2. Comparisons of exact diagonalizations with phonon assisted multimagnon infrared scattering also suggest antiferromagnetic J_2.[30] However, the convergence of the strong coupling expansion for mapping the three-band model onto an effective spin Hamiltonian is not so clear. In particular the sign of J_2 is ambiguous.[11] Another possibility is that in mapping the three-band model to a single-band model, the ring-exchange and direct-exchange contributions are not in the same proportion as those predicted from the simple one-band Hubbard model. [31] In other words, the mapping from a three-band model to a single-band model most probably leads to effective Hamiltonians in the spin and single-particle sectors whose relation is different from that expected from the simple Hubbard model.

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