Proceedings of the Elba International Physics Center (EIPC)

Monte Carlo Methods in Theoretical Physics

Editors

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FOREWORD

The *Workshop on Monte Carlo Methods in Theoretical Physics* was held at the Elba International Physics Center (EIPC) in Marciana Marina, Italy, from June 27 to July 6, 1990 and this volume summarizes most of the contributions presented in the Workshop.

The topics dealt with have been Lattice Methods in QCD, Variational Monte Carlo, Green Functions Monte Carlo, Path Integral Monte Carlo and Diffusion Monte Carlo in Atoms&Molecules, Condensed Matter, Electronic Systems and Nuclear Physics.

The first days of the Workshop have been devoted to tutorial lectures, while the actual Workshop has taken place in the subsequent days .

One of the aims of the meeting was to bring together researchers from different fields to discuss the applications of Monte Carlo methods to rather different problems and thus to stimulate a cross-disciplinary interaction.

The Workshop was also intended to introduce young researchers to the Monte Carlo techniques and, in this respect, the organizers wish to thank D.Ceperley, M.Kalos, E.Marinari, P.Menotti and V.R.Pandharipande for their efforts in preparing and delivering the tutorial lectures.

We owe all participants and lecturers our sincere thanks for making the meeting interesting and fruitful.

The financial support of the Italian Consiglio Nazionale delle Ricerche (CNR), Istituto Nazionale di Fisica Nucleare (INFN), Scuola Normale Superiore di Pisa, Universita' di Lecce, the Marciana Marina's local government and the Azienda Autonoma di Turismo dell'Isola d'Elba is gratefully aknowledged.

We also want to warmly thank Bruna Ceccarelli, Carla Gentile, Antonella Sapere and Giacomo Monteleone for their unvaluable help in the organization of the workshop.

Finally, we wish to thank the Director of EIPC, Stefano Fantoni, for his constant assistance in the organization of the meeting.

Sergio Caracciolo and Adelchi Fabrocini

MONTE CARLO METHODS IN THEORETICAL PHYSICS
eds. S. Caracciolo, A. Fabrocini, 1992. ETS Editrice, Pisa

VARIATIONAL CALCULATIONS FOR STRONGLY CORRELATED ELECTRONS

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ABSTRACT

We develop variational wave functions for the ground state as well as spin and hole excitations in a quantum antiferromagnet. The wave functions are introduced by means of an analogy of this problem to that of pure liquid ^4He and that of liquid ^4He with ^3He impurities. The wave functions are used to study the excitations in the case of the antiferromagnetic Heisenberg model and the $t-J$ model on the square lattice.

1. INTRODUCTION

The $t-J$ model is under intense theoretical investigation because it may be relevant to the physics of the copper-oxide superconductors;[1] in addition, it is one of the simplest models to describe strong electron correlations arising from the on-site Coulomb repulsion present in certain materials where their valence electrons are almost localized. It describes a mixture of interacting spin and charge degrees of freedom which are associated with the electron coordinates only. It contains a Heisenberg antiferromagnetic exchange which allows for quantum spin fluctuations and a hole hopping term. The electronic motion is subject to constraints in which configurations with double occupancy of the same Wannier state are only allowed as virtual processes due to their high energy cost; the restriction of the available Hilbert space introduces the coupling between spin and charge degrees of freedom. These effects can be realized in condensed matter and can be described in a minimal way by the $t-J$ model:

$$\hat{H} = -t \sum_{<i,j>,\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma}) + J \sum_{<ij>} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} \hat{n}_i \hat{n}_j). \qquad (1.1)$$

Here, the creation operator $c^{\dagger}_{i,\sigma}$ creates electrons at the site i with spin σ; the $\vec{S}_i$ is spin-$\frac{1}{2}$ operator which can be expressed in terms of the $c^{\dagger}_{i,\sigma}$ and $c_{i,\sigma}$ operators. J is the antiferromagnetic coupling and t is the hopping matrix element that describes hole hopping. Because of the strong two-dimensional features of the copper-oxide based

superconductors we are interested in the model (1.1) on the square lattice. Generalizations of the $t-J$ model, in order to describe certain features of the materials more realistically, have been also discussed in the recent literature.

Perturbative methods are probably applicable in certain range of the ratio t/J. Since, in the copper-oxide materials $t > J$, we are also interested in the regime of large t and therefore, nonperturbative methods are necessary to study this regime. Several features of the problem with and without holes have been understood in terms of a combination of methods. For example, the no-hole problem is equivalent to the spin-$\frac{1}{2}$ Heisenberg antiferromagnet on the square lattice and there is solid evidence[2] based on analytical, semianalytical and purely numerical techniques that the ground state of this model is ordered and its low-lying excitation spectrum is qualitatively described within spin-wave theory. The motion of a hole in a quantum antiferromagnet has also been studied by a number of methods.[3] The problem of a finite density of holes has been studied by several mean field theories.[4]

Due to the fact that there is no exact solution beyond one dimension and exact numerical diagonalization methods and quantum Monte Carlo methods for fermions are restricted to very small size lattices[5] one needs to consider more than one complementary method and to compare the results. In these proceedings we shall discuss certain results[6,7,8] obtained using a variational method which is based on a formal analogy of this problem to that of ^3He-^4He mixtures. We shall study the ground state and spin-wave excitations in the undoped $t-J$ model as well as hole excitations. We use a known analogy of the problem of spin systems to that of a Boson fluid. In order to construct variational wave functions, we shall use this analogy and ideas used in the case of other strongly correlated systems such as liquid ^4He and ^3He-^4He mixtures. This is an approximate method and can be improved by means of correlated basis perturbation theory;[9] the latter scheme consists of a rather involved calculation but, in principle, it can become the framework of calculating the corrections to the variational calculation systematically.

In the next section, we introduce the analogy of the undoped antiferromagnet to that of pure liquid ^4He and we discuss Jastrow-Marshall type of ground state wave functions. In section 3, we discuss spin excitations and how to obtain an optimized Jastrow ground state wave function for the ground state which is consistent with the existence of zero point motion of spin-waves. In section 4, we discuss the case of a single hole in a quantum antiferromagnet and its analogy to the problem of a ^3He impurity in liquid ^4He.

2. ANALOGY WITH BOSE FLUIDS

We shall outline the analogy of hard-core Bose fluids with spin-systems, which was first pointed out by Matsubara and Matsuda[10] who have shown that liquid ^4He when approximated as a quantum lattice-gas model is equivalent to the ferromagnetic spin-$\frac{1}{2}$ Heisenberg model. Using a unitary transformation of the basis[11], we make use of this analogy for quantum antiferromagnets. The eigenstates of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet can be expressed as

$$|\psi>=\sum_{\vec{r}_1,\vec{r}_2,...,\vec{r}_{N_u}} \psi(\vec{r}_1,\vec{r}_2,...,\vec{r}_{N_u})(-1)^{L(c)}|\vec{r}_1,\vec{r}_2,...,\vec{r}_{N_u}>, \tag{2.1}$$

where the configuration $|c>$ is labeled by the location on the lattice of the spins pointing up (N_u is the number of up-spins) and the function $\psi(\vec{r}_1,\vec{r}_2,...,\vec{r}_{N_u})$ gives the amplitude of that configuration in the state $|\psi>$. $L(c)$ is the number of spins pointing up in one sublattice. The phase $(-1)^{L(c)}$ is separated from the amplitude ψ in order to have a non-negative ψ for any ground state configuration.[11] It can be shown using this representation that the eigenvalue problem $H|\psi>=E|\psi>$ reduces to a difference equation for $\psi(\vec{r}_1,\vec{r}_2,...,\vec{r}_{N_u})$ identical to the many-particle Schrödinger equation on a square lattice:

$$-\frac{J_{xy}}{4}\sum_{i=1}^{N_u}\sum_{\vec{\delta}}\Big(\psi(\vec{r}_1,...,\vec{r}_i+\vec{\delta},...,\vec{r}_{N_u})-\psi(\vec{r}_1,...,\vec{r}_i,...,\vec{r}_{N_u})\Big)+\sum_{i<j}V_{ij}\psi(\vec{r}_1,\vec{r}_2,...,\vec{r}_{N_u})$$
$$=\epsilon\psi(\vec{r}_1,\vec{r}_2,...,\vec{r}_{N_u}), \tag{2.2}$$

where $\vec{\delta}$ is a vector of unit length that connects the site located at $\vec{r}_i$ with each of the four n.n. Here $\epsilon = E - \frac{NJ}{2} + N_u(J_{xy}+2J)$, where N is the total number of sites on the square lattice. The first term has the form of the kinetic energy operator (it becomes $-t\nabla^2$ is the continuum limit) and the "particles" correspond to up spins and the with "mass" $m = 2/J_{xy}$ (we use units where $a = 1$ and $\hbar = 1$); they interact via a pair potential V_{ij} having an infinite on-site repulsion and $V_{ij} = J$ if ij are n.n; otherwise $V_{ij} = 0$. Since the wave function ψ is symmetric with respect to "particle" permutations, this represents a quantum lattice-gas of bosons.

This is a useful representation because our knowledge about the system of Bose-particles can be used for the magnetic system also. Depending on the relative magnitude of J_{xy} and J, (2.2) has different solutions. For $J_{xy} << J$, the "potential" energy term dominates and the particles prefer to stay predominantly at the configuration that minimizes the Ising interaction, thus creating a quantum solid which for "particle" density $\rho = \frac{1}{2}$ ($S^z_{tot} = 0$) corresponds to an antiferromagnetically (AF) ordered state in the z-direction. In case $J_{xy} >> J$, the "kinetic" energy dominates and the system behaves as a quantum liquid. The ground state of the system, in this case, has a condensate which corresponds to off-diagonal long-range-order (LRO) in the one-body density matrix and $<\psi|b_0^\dagger|\psi>=n_c\neq 0$ where $b_0^\dagger$ creates a "particle" at the zero-momentum state and n_c is the condensate fraction. Going back to the spin-variables this means that $<\psi|m_x^\dagger|\psi>=<\psi|m_y^\dagger|\psi>=n_c$, where $m^\dagger_{x,y}$ are the components of the staggered magnetization. Therefore, in this case the magnetic system is characterized by AF LRO in the $x-y$ plane. In the isotropic case $J_{xy} = J$ there is spherical symmetry and hence by a rotation in the spin-space the "potential" and the "kinetic" energy terms can be interchanged. The ground state, however, can spontaneously break such symmetry by choosing a given direction to develop staggered magnetization aided by the presence of an external staggered field which shall be removed after taking the thermodynamic limit.

The simplest non-trivial ground state wave function of a Bose-fluid which takes into account short-range correlations due to the existence of the hard-core is the Jastrow wave function:

$$\psi_0(\vec{r}_1,\vec{r}_2,...,\vec{r}_{N_u})=e^{-\frac{1}{2}\sum_{i<j}u_{ij}}, \tag{2.3}$$

where $u_{ij}=\infty$ for $i=j$ and $u_{ij}\neq 0$ for $i\neq j$. The state (2.3) has a broken symmetry associated with the Bose condensate. Inserting (2.3) in (2.1) and going back to the spin variables by replacing $\rho_i=\frac{1}{2}(\sigma_i^z+\frac{1}{2})$ (where $\rho_i=1$ or 0 depending on whether there is a "particle" (up-spin) at site i or not), we obtain the Marshall[11] state

$$|\psi_0>=\sum_c(-1)^{L(c)}exp\Big(-\frac{1}{2}\sum_{i<j}u_{ij}\sigma_i^z\sigma_j^z\Big)|c>. \tag{2.4}$$

Here the sum runs over all lattice sites and if we extend it not only over those configurations with N_u up-spins but over all possible configurations this state takes the following form:

$$|\psi_0 >= exp\Big(-\frac{1}{2}\sum_{i<j} u_{ij}\hat{\sigma}_i^z\hat{\sigma}_j^z\Big)|\phi >, \tag{2.5}$$

where $|\phi >$ is the Nèel state with antiferromagnetic order in the x direction, i.e., a product over all sites of states $|\pm\hat{x}>_i \equiv \frac{1}{\sqrt{2}}(|+>_i \pm|->_i)$ which are eigenstates of $\hat{S}_i^x$ with eigenvalues $+1/2$ or $-1/2$ when the site i belongs to the A or B sublattice respectively. The variational state (2.5) is characterized by antiferromagnetic order with $< \hat{S}_i^y >=< \hat{S}_i^z >= 0$ and $< \hat{S}_i^x >= \pm m^\dagger$, where $m^\dagger$ is $\leq \frac{1}{2}$ and depends on the function u. If we restrict the sum in (2.4) over configurations with zero z-component of the net spin we find that $< \hat{S}_i^x >=< \hat{S}_i^y >=< \hat{S}_i^z >= 0$, however each of the two correlation functions $< \hat{S}_i^x\hat{S}_j^x >$ and $< \hat{S}_i^y\hat{S}_j^y >$ at large distances approach the value $\frac{1}{2}(-1)^{i+j}m^{\dagger 2}$ while $< \hat{S}_i^z\hat{S}_j^z >$ approaches zero.

Wave functions of the form (2.4) have been used in the past to study the ground state of the spin-$\frac{1}{2}$ Heisenberg antiferromagnet by several authors, including Marshall[11] and more recently by Huse and Elser and by Horsch and Linden.[12]

The paired-phonon analysis known from the theory of quantum fluids[13] has been used by the author[6] to find an analytic form for the Jastrow correlation factor. Including the contribution of paired-magnon states in the ground state, the Jastrow factor is obtained as

$$u_{ij} \equiv \frac{1}{N}\sum_{\vec{k}}\Big(\sqrt{\frac{1+\gamma_{\vec{k}}}{1-\gamma_{\vec{k}}}}-1\Big)e^{i\vec{k}.(\vec{r}_i-\vec{r}_j)}, \tag{2.6}$$

where on the square lattice

$$\gamma_{\vec{k}} = \frac{1}{2}(cos(k_x a)+cos(k_y a)). \tag{2.7}$$

The ground state energy obtained in this approach is the same as the result of spin-wave theory.

3. SPIN EXCITATIONS

The elementary excitations in the Bose-fluid are density fluctuations (phonons in the long-wavelength limit) which in the magnetic system correspond to spin-waves. In the Bose-system they are created by the density operator $\rho_{\vec{q}} = \sum_{i=1}^{N_u} e^{i\vec{q}\cdot\vec{r}_i}$ acting on the interacting ground state; going back to the spin variables this operator is transformed to the operator $S_{\vec{q}}^z = \sum_{i=1}^{N} S_i^z e^{i\vec{q}\cdot\vec{r}_i}$. Chester and Reatto[14] have shown that the zero-point motion of the long-wavelength modes of the Bose-system (zero-sound) gives rise to a long-range tail in the Jastrow wave function. For a 2D spin-$\frac{1}{2}$ system we obtain

$$u(r\to\infty) = \frac{mc}{4\rho_0\pi r}, \tag{3.1}$$

where c is the spin-wave velocity and $m = 2/J$ (when $J_{xy} = J$). The ground state of the Heisenberg antiferromagnet has zero total S_z and the number of up spins is $N_u = \frac{N}{2}$, giving $\rho_0 = 1/2$.

Using the expression (2.6) for u_{ij}, we find

$$u(r\to\infty) = \frac{\sqrt{2}}{\pi r}. \tag{3.2}$$

Comparing the tails (3.1) and (3.2) we obtain $c = c_0 = \sqrt{2}Ja$ which is the value found by linear SWT.

The Jastrow wave function (2.6) possesses AF LRO with the staggered magnetization in the $x-y$ plane and therefore the dynamic structure function corresponds to

$$S(\vec{q},\omega) \equiv \sum_{n\neq 0} |< n|S_{\vec{q}}^z|0 >|^2\delta(\omega-\omega_{n0}). \tag{3.3}$$

Notice that $S(\vec{q},\omega)$ defined by this equation in the equivalent hard-core Bose representation corresponds to the density-density correlation function.

The structure factor is obtained as

$$S(\vec{q}) \equiv< 0|S_{-\vec{q}}^z S_{\vec{q}}^z|0 >= \int_0^\infty d\omega S(\vec{q},\omega). \tag{3.4}$$

The ω-moment of $S(\vec{q},\omega)$ can be obtained as $< 0|[S_{-\vec{q}}^z,[H,S_{\vec{q}}^z]]|0 >$ which gives

$$\int_0^\infty d\omega\omega S(\vec{q},\omega) = 4f(1-\gamma_{\vec{q}}), \tag{3.5.a}$$

where

$$f \equiv \frac{J}{4} < 0|S_i^+S_{i+\vec{\delta}}^- + S_i^-S_{i+\vec{\delta}}^+|0 > . \tag{3.5.b}$$

A third sum-rule can be derived[7] by studying the response of the spin-system to an external magnetic field in the z-direction. This is analogous to the compressibility sum-rule known in the theory of quantum fluids and in this case is translated to the "magnetic susceptibility sum-rule". We obtain:

$$\frac{1}{2\epsilon''} = \lim_{q\to 0}\int_0^\infty \frac{S(\vec{q},\omega)}{\omega}d\omega = \lim_{q\to 0}\sum_{n\neq 0}\frac{|\langle n|S_q^z|0\rangle|^2}{E_n-E_0}, \tag{3.6}$$

where ϵ'' is the second derivative of the ground state energy per site $\epsilon(M)$ as a function of the magnetization $M = \frac{1}{N} < 0|\sum_i S_i^z|0 >$. The perpendicular susceptibility is given by $\chi_\perp = 1/\epsilon''$ in units of $g\mu_B = 1$, where μ_B and g are the Bohr magneton and g-factor of the electron.

Feynman's assumption[15] introduced for the elementary excitations of liquid ^4He, states that in the long-wavelength limit a single-phonon (in this case: single-magnon) excitation dominates the dynamical structure function. This is equivalent to the statement that only excitations created by the $S_{\vec{q}}^z$ acting on the interacting ground state dominate in this limit. This leads to the following approximation for the spin-dynamical structure function[16]:

$$\lim_{q\to 0} S(\vec{q},\omega) = Z_{\vec{q}}\delta(\omega-\omega_{\vec{q}}), \tag{3.7}$$

and from the sum-rule (3.4) we find that $Z_{\vec{q}} = S(\vec{q})$. The combination of (3.5) and (3.7) gives

$$\omega_{\vec{q}} = \frac{4f(1-\gamma_{\vec{q}})}{S(\vec{q})}. \tag{3.8}$$

Furthermore, $\lim_{q\to 0}\int_0^\infty \omega\, S(\vec{q},\omega)\, d\omega = fq^2$, and $\omega(q\to 0) = cq$ and the spin-wave velocity is given by

$$c = \frac{f}{s}, \tag{3.9}$$

where s is the slope of $S(\vec{q})$ in the long-wavelength limit, i.e., $S(q\to 0) = sq$.

Using the sum-rule (3.6) and Eq. (3.7), we obtain

$$c = \sqrt{2f\epsilon''}. \tag{3.10}$$

This expression is equivalent to the following:

$$c^2 = \rho_s/\chi_\perp, \tag{3.11}$$

which was derived by Halperin and Hohenberg[17] looking at the problem from a somewhat different angle. Halperin and Hohenberg used the analogy between the spin-system and liquid helium and the hydrodynamics of the two-fluid model. The present derivation allows identification of the phenomenological parameters and furthermore their evaluation from the microscopic Hamiltonian. The spin-stiffness constant in the approach explained above can be identified as $\rho_s = 2f$.

Liu and Manousakis[7] (LM) have optimized the Jastrow wave function by minimizing the ground state energy and requiring it to satisfy sum rules for $S(\vec{q},\omega)$ in a self-consistent way. They used the Jastrow-Marshall form (2.4), including in the sum only configurations with zero magnetization, and took $u_1 \equiv u(1,0) = u(0,1)$ and $u_{\sqrt{2}} \equiv u(1,1)$ as variational parameters and

$$u(\vec{r}) = \alpha u_{LR}(\vec{r}), \quad for \quad \sqrt{x^2+y^2} \geq 2, \tag{3.12}$$

where $u_{LR}(\vec{r})$ is that given by Eq. (2.6) (and can be approximated by 3.2) and α is a parameter of order 1. The tail $u(r\to\infty)$ of (3.12) is given by the Chester and Reatto relation (3.1) with $c = \alpha c_0$, where $c_0 = \sqrt{2}Ja$. This value of c and that obtained from (3.10), by calculating f and ϵ'' using the same variational wave function, must agree. Therefore u_1 and $u_{\sqrt{2}}$ are determined by minimizing the ground state energy, while the parameter α can be determined self-consistently: given a value of α the spin-wave velocity c is obtained by calculating f and the curvature of $\epsilon(M)$. A new value of α is then obtained via $\alpha = c/c_0$. This is iterated until the input and the output value of α are the same.

The wave function obtained with this approach is shown in Fig. 1 by open-squares and the solid-line is used as a guide to the eye. The function u_{ij} obtained by Huse and Elser is shown by crosses, while that obtained using the paired-magnon analysis of Manousakis[6] and is given by Eq. (2.6) is shown by open circles. The extrapolated values to the infinite system for the ground state energy per site, the staggered magnetization, spin-wave velocity and perpendicular susceptibility are $-0.6637 \pm 0.0002J$, -0.349 ± 0.002, $1.22 \pm 0.02c_0$ and $0.667 \pm 0.004\chi_{\perp,0}$ (where $\chi_{\perp,0} \equiv \frac{1}{8J}$) respectively and they are in satisfactory agreement with Green's function Monte Carlo (GFMC) calculations[18] and other calculations.[2]

In Fig. 2 we give the results for $S(\vec{q})$ along the $(1,0)$ direction and it is compared to the GFMC calculation of Trivedi and Ceperley[18]. In the inset we compare the $\omega_{\vec{q}}$ obtained from (3.8) along the same direction. More recently Liu and Manousakis[19] have calculated moments of the Raman scattering intensity using the variational wave function and their results are in good agreement with those obtained by series expansion and exact diagonalization techniques.

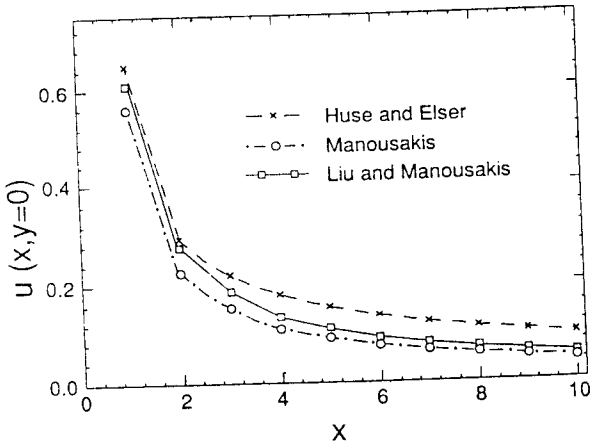

Figure 1. The function u_{ij}, as obtained with different approaches explained in the text, is shown. The lines are guides to the eye.

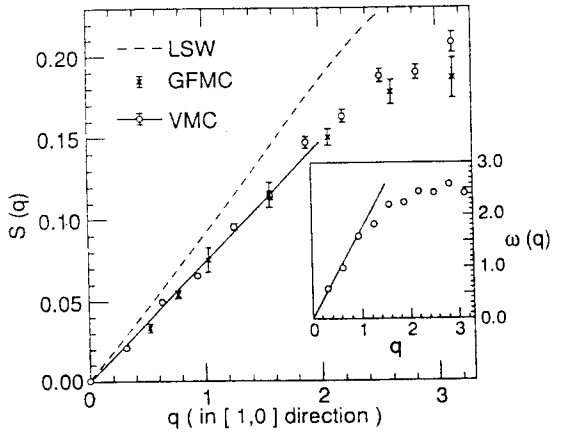

Figure 2. The $S(\vec{q})$ along the $(1,0)$ direction, as calculated in Ref. 7 with the VMC method, is compared to that obtained by the GFMC calculation of Ref. 18. The dashed-line is the result of linear spin-wave theory. In the inset we compare the $\omega_{\vec{q}}$ obtained from (3.8).

4. HOLE EXCITATIONS

Let us consider the Hilbert space of all possible states of the system, with N_u up-spins and one hole. A basis vector can be written as $|\vec{R},\vec{r}_1,\vec{r}_2...\vec{r}_{N_u}>$, with $\vec{R}\neq\vec{r}_1,\vec{r}_2,...\vec{r}_{N_u}$, where $\vec{R}$ is the position of the hole and $\vec{r}_1,\vec{r}_2,...,\vec{r}_{N_u}$ are the positions of the N_u up-spins. More precisely,

$$|\vec{R},\vec{r}_1,\vec{r}_2...\vec{r}_{N_u}>=S^+_{\vec{r}_1}S^+_{\vec{r}_2}...S^+_{\vec{r}_{N_u}}|\vec{R},F>, \tag{4.1}$$

where the reference state $|\vec{R},F>$ is the "down" ferromagnetic state with the hole at $\vec{R}$. The most general eigenstate of (1.1) having N_u up-spins can be written as

$$|\psi>=\sum_{\vec{R},\vec{r}_1,\vec{r}_2,...,\vec{r}_{N_u}}(-1)^{L(c)}\psi(\vec{R},\vec{r}_1,\vec{r}_2,...,\vec{r}_{N_u})|\vec{R},\vec{r}_1,\vec{r}_2,...,\vec{r}_{N_u}>, \tag{4.2}$$

where the sum runs over all possible positions of the hole and up-spins. The phase factor $(-1)^{L(c)}$ is defined as before. In this representation we can write down the eigenvalue equation $\hat{H}|\psi>=E|\psi>$ for the function $\psi(\vec{R},\vec{r}_1,\vec{r}_2,...,\vec{r}_{N_u})$. We obtain:

$$\begin{aligned}&-t\sum_{\vec{\delta}}(\psi(\vec{R}+\vec{\delta},\vec{r}_1,...,\vec{r}_{N_u})-\psi(\vec{R},\vec{r}_1,...,\vec{r}_{N_u}))-t\sum_i\psi(\vec{r}_i,\vec{r}_1,...,\vec{R},...,\vec{r}_{N_u})\delta_{<\vec{r}_i\vec{R}>}\\&-\frac{J}{4}\sum_{i=1}^{N_u}\sum_{\vec{\delta}}(\psi(\vec{R},\vec{r}_1,...,\vec{r}_i+\vec{\delta},...,\vec{r}_{N_u})-\psi(\vec{R},\vec{r}_1,...,\vec{r}_i,...,\vec{r}_{N_u}))\\&+\sum_{i<j}(V_{ij}+U(\vec{r}_i-\vec{R}))\psi(\vec{R},\vec{r}_1,\vec{r}_2,...,\vec{r}_{N_u})=\epsilon\psi(\vec{r}_1,\vec{r}_2,...,\vec{r}_{N_u})\end{aligned} \tag{4.3}$$

where $\epsilon=E+3JN_u-4t$, E being the ground state energy eigenvalue of (1.1) and $\delta_{<\vec{r}_i\vec{R}>}$ is equal to one for nearest-neighbors and zero otherwise. The first and the second term come from the hole hopping term and they describe exchanges between the hole and the down-spins and up-spins respectively. The first, therefore, has the standard kinetic energy form (∇^2 in the continuum limit) with hole-"mass" $\frac{1}{2t}$(we use units where $a=1$ and $\hbar=1$), and the second has the form of an exchange between bose-particles and hole when they are nearest neighbors. The third term is the same as in (2.2) and has the form of the kinetic energy operator for the bosons introduced above whose "mass" is $\frac{2}{J}$. V_{ij} has been defined before and U is the interaction potential between a hole and a boson, featuring an infinite on-site repulsion and it is equal to $J/2$ for nearest-neighbor sites and zero otherwise. Apart from the second term, (4.3) is the lattice version of the Hamiltonian for an interacting boson gas in which a foreign particle is moving. This is analogous to the problem of a moving ^3He atom in liquid ^4He; we may therefore extend the variational approach to this problem, as outlined in Ref. 15 to our case. A variational ansatz for the wave function describing the motion of a ^3He impurity through liquid ^4He is[15,9]

$$\psi(\vec{k})=e^{-i\vec{k}\cdot\vec{R}}exp\Big(-\sum_j\Big(i\phi_{\vec{k}}(\vec{r}_j-\vec{R})+\lambda_{\vec{k}}(\vec{r}_j-\vec{R})\Big)-\frac{1}{2}\sum_{i<j}u(\vec{r}_i-\vec{r}_j)\Big) \tag{4.4}$$

where $\vec{R}$ is the coordinate of the ^3He atom, $\vec{r}_i,\vec{r}_j,...$ are the coordinates of the ^4He atoms. u_{ij} and λ accounts for the hard-core repulsion between pairs of ^4He atoms or between a ^4He atom and the ^3He impurity respectively. The term $exp[-i\sum_i\phi_{\vec{k}}(\vec{r}_i-\vec{R})]$ describes the collective motion of the ^4He atoms which move out of the way, in order to make room for the impurity to pass through, filling the empty space it leaves behind. Due to this effect, the ^3He particle has an effective mass which is larger than its true mass. The form of the function $\phi_{\vec{k}}(\vec{r}_i-\vec{R})$ can be determined by imposing on the wave function (4.4) the condition that it gives a divergence-free current. Following Ref. 15, we can obtain the large-distance long-wavelength behavior of $\phi_{\vec{k}}(\vec{r})$ as

$$\phi_{\vec{k}}(\vec{r})=A_k\frac{\vec{k}\cdot\vec{r}}{r^2}, \tag{4.5}$$

in two-dimensions.

We can now go back to spin variables using the identity $\hat{n}(\vec{r})=\frac{1}{2}(\sigma^z_{\vec{r}}+1)$ where $\hat{n}(\vec{r})$ is the boson number operator at lattice site $\vec{r}$ (1 if there is an up-spin, zero otherwise); we obtain

$$|\psi(\vec{k})>=\sum_{\vec{R},c}(-1)^{L(c)}e^{-i\vec{k}\cdot\vec{R}}exp\Big(-\sum_i(\lambda^i_{\vec{k}}+i\phi^i_{\vec{k}})\sigma^z_i-\frac{1}{2}\sum_{i<j}u_{ij}\sigma^z_i\sigma^z_j\Big)|\vec{R},c>, \tag{4.6}$$

where the sum over i and j now runs over all lattice sites. If we allow the sum to run over all configurations (4.6) becomes

$$|\psi(\vec{k})>=\sum Re^{-i\vec{k}\cdot\vec{R}}exp\Big(-\frac{1}{2}\sum_i(\lambda^i_{\vec{k}}+i\phi^i_{\vec{k}})\hat{\sigma}^z_i-\frac{1}{2}\sum_{i<j}u_{ij}\hat{\sigma}^z_i\hat{\sigma}^z_j\Big)|\phi,\vec{R}>, \tag{4.7}$$

where the state $|\phi,\vec{R}>$ is the Nèel state with staggered magnetization in the x direction and a hole at $\vec{R}$. Therefore, the spin-backflow correlation operator $e^{-\frac{1}{2}\phi_i\hat{\sigma}^x_i}$ rotates the local spin by an angle ϕ^i which behaves, at large distances, as in (4.5) whereas $e^{-\frac{1}{2}\lambda_i\hat{\sigma}^z_i}$ generates a magnetization along the z-direction.

Boninsegni and Manousakis[8] (BM) have used (4.6) and the VMC technique with and without restricting the sum over configurations having total $S^z=0$ to compute the hole energy. The VMC calculation was carried out on several lattices with periodic boundary conditions and the function u_{ij} was chosen to be the same with that determined by Liu and Manousakis[7]. BM found the following simple parameterization for the short-range part of the functions $\phi_{\vec{k}}(\vec{\delta})=A_o sin(\vec{k}\cdot\vec{\delta})$ and $\lambda_{\vec{k}}(\delta)=A_o cos(\vec{k}\cdot\vec{\delta})$. For distances larger than one lattice spacing away from the hole, BM took the form (4.5) and treated $A_{\vec{k}}$ as variational parameter. They found that λ is very small beyond nearest-neighbors. Details and justification of the choice of the variational parameters and the minimization are given in Ref. 8.

Fig. 3 compares the results of the VMC calculation for $\Delta E(\vec{k})=E(\vec{k})-E_0$, where $E(\vec{k})$ (E_0) is the total energy with one-hole (no-hole), to those obtained by exact numerical diagonalization on a 4×4 lattice[5] for several values of t/J and at $\vec{k}=(\frac{\pi}{2},\frac{\pi}{2})$, where the dispersion curve has its minimum. ΔE is given in units of t. The difference between the exact ground state energy and the variational energy at small values of t/J can be attributed to an incomplete description of spin-background fluctuations given by the factor $exp[-\frac{1}{2}\sum u_{ij}\sigma^z_i\sigma^z_j]$. For $t/J\geq0.5$ the variational and exact results begin to differ.

A typical result for the hole-band $\Delta E(\vec{k})$ is shown in Fig. 4 calculated for $t/J=0.5$ and without the restriction on the total S^z. The curve features a minimum at

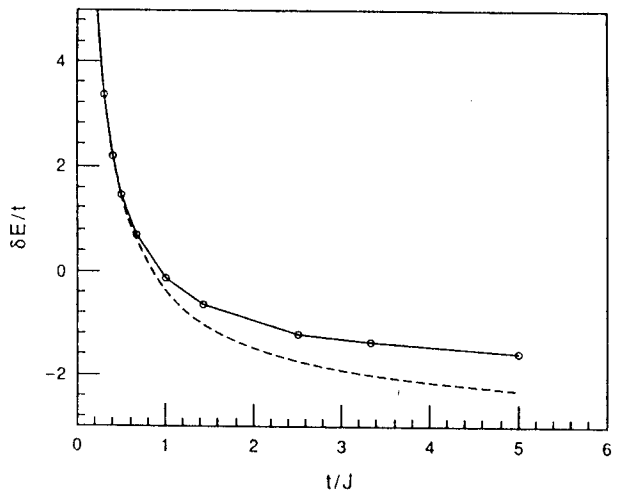

Figure 3. The results of the VMC calculation for the hole energy $\Delta E(\vec{k}) = E(\vec{k}) - E_0$ (Ref. 8), shown as circles joined by a solid line, are compared to those obtained by exact numerical diagonalization on a 4×4 lattice[5] (dashed line).

$\vec{k} = (\frac{\pi}{2}, \frac{\pi}{2})$, and attains its maximum value at $\vec{k} = (\pi, \pi)$. Notice that the effective mass of the hole is smaller in the direction $(0,0)$ to (π,π) than in the direction $(0,\pi)$ to $(\pi,0)$. Most of these features of the hole-band have been revealed by other approaches[3] and in particular they were discussed in Ref. 20 where the authors were studying the problem from the itinerant limit.

The bandwidth $W = E(\frac{\pi}{2},\frac{\pi}{2}) - E(\pi,\pi)$, is found to grow as t^2/J at small t. At large values of t/J the bandwidth is expected to be proportional to J because of processes which relax the overturn spins due to the hole motion. Our wave function needs to be improved in that range by including hole-boson exchange correlations. The large value of the hopping matrix element t (small "bare" hole mass) increases the probability of such processes.

BM found that the quasihole excitation creates both a planar long-range distortion[3] of the antiferromagnetic moment of the background $\delta m^{\dagger}(r \to \infty) \sim \frac{\vec{k}\cdot\vec{r}}{r^2}$ and a ferromagnetic moment localized in the immediate neighborhood of the hole, pointing in the perpendicular direction. The magnitude of the ferromagnetic moment depends on the momentum of the excitation, and at the minimum of the hole band only the long-range AF planar distortion is present.

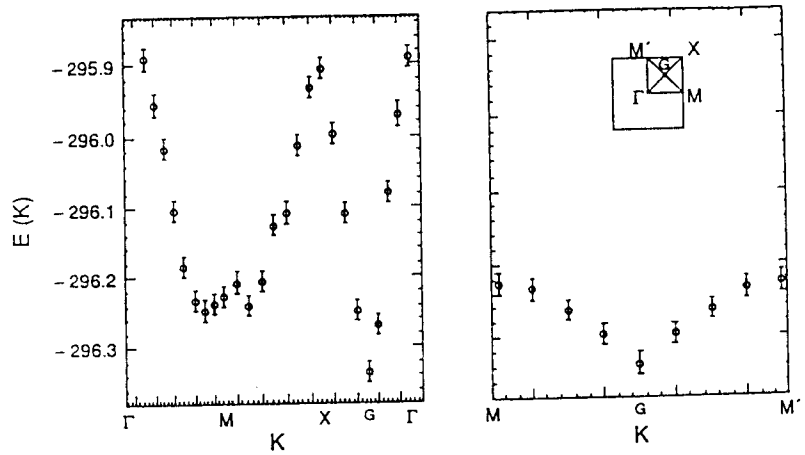

Figure 4. The hole-band $\Delta E(\vec{k})$, calculated in Ref. 8 for $t/J = 0.5$ along the paths $\Gamma M X \Gamma$ and $M M'$ of the Brillouin zone (shown in the inset).

ACKNOWLEDGEMENTS

This work is supported in part by the Supercomputer Computations Research Institute which is partially supported by the U.S. Department of Energy through contract No. DE-FC05-85ER250000. This work was suppor

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