Monte Carlo Methods in Theoretical Physics

Editors

Sergio Caracciolo
Scuola Normale Superiore, Pisa, Italy

Adelchi Fabrocini
Dipartimento di Fisica, Università di Pisa
Istituto Nazionale di Fisica Nucleare, Sezione di Pisa, Italy
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.

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Sergio Carninciolo and Adelchi Fabrocini
VARIATIONAL CALCULATIONS FOR STRONGLY CORRELATED ELECTRONS

Efstratios Manousakis

Department of Physics and
Center for Materials Research and Technology
Florida State University, Tallahassee, Florida 32306.

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 $^4$He and that of liquid $^3$He with $^3$He 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, 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:

$$
\hat{H} = -t \sum_{\langle ij \rangle \sigma} (\epsilon_{i \sigma} c_{i \sigma}^\dagger c_{j \sigma} + \epsilon_{j \sigma} c_{j \sigma}^\dagger c_{i \sigma}) + J \sum_{\langle ij \rangle} (\hat{S}_i \cdot \hat{S}_j - \frac{1}{4} \hat{n}_i \hat{n}_j).
$$

(1.1)

Here, the creation operator $c_{i \sigma}^\dagger$ creates an electron at the site $i$ with spin $\sigma$; the $\hat{S}_i$ is spin-$\frac{1}{2}$ operator which can be expressed in terms of the $c_{i \sigma}^\dagger$ 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 systems \( t > J \), 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 hole problem is equivalent to the spin-1/2 Heisenberg antiferromagnet on the square lattice and there is solid evidence 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. The problem of a finite density of holes has been studied by several mean field theories. 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, one needs to consider more than one complementary method and to compare the results. In this proceedings we shall discuss certain results obtained using a variational method which is based on a formal analogy of this problem to that of \( S = 1/2 \) Heisenberg and \( S = 3/2 \) Heisenberg models. This is an approximate method and can be improved by means of correlated basis perturbation theory, in 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 \( 4\text{He} \) and we discuss Jastrow-Marrow 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. We also discuss the case of a single hole in a quantum antiferromagnet and its analogy to the problem of a \( S = 1/2 \) impurity in liquid \( 4\text{He} \).

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, who have shown that liquid \( 4\text{He} \) when approximated as a quantum lattice gas model is equivalent to the ferrromagnetic spin-1/2 Heisenberg model. Using a unitary transformation of the basis, we make use of this analogy for quantum antiferromagnets. The eigenstates of the spin-1/2 Heisenberg antiferromagnet can be expressed as

\[
\psi > = \sum_{\ldots \psi (r_1, r_2, \ldots, r_N)} \psi (r_1, r_2, \ldots, r_N) \langle [-1]^{-\frac{1}{2}} (r_1, r_2, \ldots, r_N), \psi >, \tag{2.1}
\]

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 \( \psi (r_1, r_2, \ldots, r_N) \) gives the amplitude of that configuration in the state \( |\psi > \). \( L(c) \) is the number of spins pointing up in one sublattice. The phase \( (-1)^{\psi (c)} \) is separated from the amplitude \( \psi > \) in order to have a non-negative \( \psi > \) for any ground state configuration. It can be shown using this representation that the eigenvalue problem \( H |\psi > = E |\psi > \) reduces to a difference equation for \( \psi (r_1, r_2, \ldots, r_N) \) identical to the many-particle Schrödinger equation on a square lattice:

\[
-\frac{J}{4} \sum_{i \neq j} \left[ \psi (r_1, r_2, \ldots, r_i, \ldots, r_j, \ldots, r_N) - \psi (r_1, r_2, \ldots, r_j, \ldots, r_i, \ldots, r_N) \right] + \sum_{i \neq j} V_i \psi (r_1, r_2, \ldots, r_i, \ldots, r_j, \ldots, r_N) = \epsilon \psi (r_1, r_2, \ldots, r_N), \tag{2.2}
\]

where \( \epsilon \) is a vector of unit length that connects the site located at \( r_i \) with each of a given unit cell. Here \( \epsilon = \hat{E} \cdot \hat{d} + \mu_n J c_j + 2J \delta, \) 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 \( -\frac{\hbar^2}{2m} \) in the continuum limit) and the "particles" correspond to up spins and the with "mass" \( m = 2J \delta \) (we use units where \( \hbar = 1 \)); they interact via a pair potential \( V_i \), having an infinite on-site repulsion and \( V_\text{ij} = J (|\text{i} \neq \text{j}) \) are n.n. otherwise \( V_\text{ij} = 0 \). Since the energy functional 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 \( J > 0 \) and \( \epsilon \), (2.2) has different solutions depending on whether \( J < \epsilon \) or \( J > \epsilon \). The "potential" energy term dominates and the particles prefer to stay predominantly at the configuration that minimizes the interaction energy, thus creating a quantum solid which for "particle" density \( \rho (\epsilon) \) corresponds to an antiferromagnetically (AF) ordered state in the \( \epsilon \)-direction. In case \( J > \epsilon \), 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 (DLO) in the one-body density matrix and \( \psi (r_1, r_2, \ldots, r_N) = \psi (\epsilon) \) corresponds to an antiferromagnetically (AF) ordered state in the \( \epsilon \)-direction. In the isotropic case \( J = \epsilon \) 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:

\[
\psi (r_1, r_2, \ldots, r_N) = e^{-\sum_i \mu_i w_i}, \tag{2.3}
\]

where \( w_i = 0 \) for \( i = j \) and \( w_i \neq 0 \) 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 \( \mu_i = \frac{1}{2} \sum_j \mu_j s_{ij}^z \) (where \( \mu_i = 1 \) or 0 depending on whether there is a "particle" (up-spin) at site \( i \) or not), we obtain the Marshall state:

\[
\psi > = \sum_i e^{-\frac{1}{2} \sum_j \mu_j s_{ij}^z} \psi >, \tag{2.4}
\]
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:

\[
|\psi_0\rangle = \exp \left( -\frac{1}{2} \sum_{i<j} N_u(i,j) \right) |\psi\rangle, \tag{2.5}
\]

where \(|\psi\rangle\) is the Néel state with antiferromagnetic order in the \( z \) direction, i.e., a product over all sites of states \(|\pm \downarrow \rangle = \sqrt{2}(|+\uparrow \rangle + |\downarrow \uparrow \rangle)\) which are eigenstates of \( \hat{S}^z_i \) with eigenvalues +1/2 or -1/2 when the site \( i \) belongs to the A or B sublattice respectively. The variational state (2.4) is characterized by antiferromagnetic order with \( < \hat{S}_i^z > = < \hat{S}_i^x > = 0 \) and \( < \hat{S}_i^y > = \pm m \), where \( m \) is \( \frac{1}{2} \) and depends on the function \( u \). If we restrict the sum in (2.4) over configurations with zero \( z \)-component of the net spins we find that \( < \hat{S}_i^y > = < \hat{S}_i^x > = 0 \), 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 \( \frac{1}{2}(-1)^{r(i,j)}m^2 \) while \( < \hat{S}_i^x \hat{S}_j^y > \) 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 Hue 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 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

\[
|\psi\rangle = \frac{1}{N} \sum_k \left( \sqrt{\frac{1 + \gamma_k}{1 - \gamma_k}} - 1 \right) e^{i \gamma_k (\mathbf{q} \cdot \mathbf{r})}, \tag{2.6}
\]

where on the square lattice

\[
\gamma_k = \frac{1}{2} (\cos(k_x a) + \cos(k_y a)). \tag{2.7}
\]

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 \( \hat{\rho} = \sum_i \hat{S}_i^z \hat{S}_i^z \) acting on the interacting ground state; going back to the spin variables this operator is transformed to the operator \( \hat{S}_i^z = \sum_i \hat{S}_i^z \hat{S}_i^z \). Chester and Reatto\(^{44}\) 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

\[
u(r \to \infty) = \frac{mc}{4\pi \mu r^2}, \tag{3.1}
\]

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

Using the expression (2.6) for \( u_\psi \), we find

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

Comparing the tails (3.1) and (3.2) we obtain \( c = 2\sqrt{2} \) 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

\[
S(q,\omega) = \sum_{n \neq 0} < n | S(q) S(0) | n > \frac{1}{2} \delta(\omega - \omega_0). \tag{3.3}
\]

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

The structure factor is obtained as

\[
S(q) = < 0 | S(q) S(0) | 0 > = \int_0^\infty d\omega S(q,\omega). \tag{3.4}
\]

The \( \omega \)-moment of \( S(q,\omega) \) can be obtained as \( < 0 | [S(q) H, S(0)] | 0 > \) which gives

\[
\int_0^\infty d\omega S(q,\omega) = 4 f(1 - \eta_q), \tag{3.5a}
\]

where

\[
f = \frac{J}{4} < 0 | \sum_{i \neq f} S_i^- S_{i+f}^+, \sum_{i \neq f} S_i^+ S_{i+f}^- | 0 >. \tag{3.5b}
\]

A third sum-rule can be derived\(^{17}\) 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:

\[
\frac{1}{2\pi^2} = \lim_{q \to 0} \int dq S(q) \omega = \lim_{q \to 0} \sum_{n \neq 0} \frac{\text{int}(n | S(q) |)^2}{\omega_n - \omega_0}, \tag{3.6}
\]

where \( \omega_0 \) is the second derivative of the ground state energy per site \( (M) \) as a function of the magnetization \( M = \frac{1}{N} < 0 | \sum_i \hat{S}_i^z | 0 > \). The perpendicular susceptibility is given \( \chi = 1/\omega_0 \) in units of \( \mu_B = 1 \)(where \( \mu_B \) are the Bohr magneton and \( g \)-factor of the electron.

Fryman's assumption\(^{15}\) introduced for the elementary excitations of liquid \( ^3 \)He, 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 \( \hat{S}_i^z \) acting on the interacting ground state dominate in this limit. This leads to the following approximation for the spin-dynamical structure function\(^{16}\):

\[
\lim_{q \to 0} S(q,\omega) = 2 \pi \delta(\omega - \omega_0), \tag{3.7}
\]

and from the sum-rule (3.4) we find that \( \omega_0 = 4 f(1 - \eta_q) \frac{f}{S(q)} \). The combination of (3.5) and (3.7) gives

\[
\omega_0 = 4 f(1 - \eta_q) \frac{f}{S(q)}. \tag{3.8}
\]
Furthermore, $\lim_{q \to 0} \int_0^\infty \omega S(\omega, q) d\omega = \frac{1}{q}$, and $u(q \to 0) = c q$ and the spin-wave velocity is given by

$$c = \frac{1}{q},$$

(3.9)

where $q$ is the slope of $S(q)$ in the long-wavelength limit, i.e., $S(q \to 0) = a q$.

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

$$c = \sqrt{2f}\beta.$$  

(3.10)

This expression is equivalent to the following:

$$c^2 = \rho_s|x_1|,$$

(3.11)

which was derived by Halperin and Hohenberg\textsuperscript{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 $\mu_s = 2f$.

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

$$u(1) = u_{1,2}(2),$$

(3.12)

where $u_{1,2}(?)$ is that given by Eq. (2.6) (and can be approximated by 3.2) and $\sigma$ is a parameter of order 1. The tail $u(\sigma \to \infty)$ of (3.12) is given by the Chester and Reatto relation (3.1) with $c = \sigma q_0$, where $q_0 = 2.52$. This value of $c$ and that obtained from (3.10), by calculating $f$ and $\beta$ using the same variational wave function, must agree. Therefore $w_1$ and $u_{1,2}$ are determined by minimizing the ground state energy, while the parameter $\sigma$ can be determined self-consistently: given a value of $\sigma$ the spin-wave velocity $c$ is obtained by calculating $f$ and the curvature of $c(M)$. A new value of $\sigma$ is then obtained via $\sigma = \sigma(q)$. This is iterated until the input and output values of $\sigma$ 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 $u_{1,2}$ obtained by 

\[\text{Liu and Elser}\]

is shown by crosses, while that obtained using the paired-magnon analysis of Manousakis\textsuperscript{8} 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 $-0.0637 \pm 0.0002 F$, $-0.349 \pm 0.002, 1.22 \pm 0.02 G_0$ and $0.667 \pm 0.004 G_0$ respectively and they are in satisfactory agreement with Green's function Monte Carlo (GFMC) calculations\textsuperscript{14} and other calculations\textsuperscript{2}.

In Fig. 2 we give the results for $S(q)$ along the $(1,0)$ direction and it is compared to the GFMC calculation of Trivedi and Ceperley\textsuperscript{15}. In the inset we compare the $\omega(q)$ obtained from (3.8) along the same direction. More recently Liu and Manousakis\textsuperscript{11} 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.
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 \( |\vec{R}, r_1, r_2, \ldots, r_{N_u}, >\), with \( \vec{R} \neq r_1, r_2, \ldots, r_{N_u} \), where \( \vec{R} \) is the position of the hole and \( r_1, r_2, \ldots, r_{N_u} \) are the positions of the \( N_u \) up-spins. More precisely,
\[
|\vec{R}, r_1, r_2, \ldots, r_{N_u}, > = S_{r_1}^z S_{r_2}^z \ldots S_{r_{N_u}}^z |\vec{R}, >,
\]
where the reference state \( |\vec{R}, > \) 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
\[
|\psi(\vec{R}, r_1, r_2, \ldots, r_{N_u}, ) = \sum_{\vec{R}, r_1, r_2, \ldots, r_{N_u}} (\text{(-1)}^{(r_1 + r_2) + \cdots + r_{N_u}}) |\vec{R}, r_1, r_2, \ldots, r_{N_u}, >\]
where the sum runs over all possible positions of the hole and up-spins. The phase factor \( (\text{-1})^{(r_1 + r_2) + \cdots + r_{N_u}} \) is defined as before. In this representation we can write down the eigenvalue equation \( H|\psi(\vec{R}, r_1, r_2, \ldots, r_{N_u}, )\rangle = E|\psi(\vec{R}, r_1, r_2, \ldots, r_{N_u}, )\rangle \). We obtain:
\[
-\frac{J}{\hbar} \sum_{i=1}^{N_u} \left( \psi(\vec{r}_i - \vec{r}_j) - \psi(\vec{r}_i + \vec{r}_j) \right) - \frac{\lambda}{\hbar} \sum_{i=1}^{N_u} \left( \psi(\vec{r}_i) \right) - H_0 \psi(\vec{r}_i) + \text{h.c.}
\]
(4.3)
where \( \epsilon = E + J_3 N_u - 4t, E \) being the ground state energy eigenvalue of (1.1) and \( \delta \equiv \vec{r}_i - \vec{R} \) 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 (\( \nabla^2 \) in the continuum limit) with hole-"mass" \( \frac{\hbar}{2m} \) (we use units where \( \hbar = 1 \) and \( m = 1 \)), and the second has the form of an exchange between boson-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 \( \frac{\hbar}{2m} \). \( V_{ij} \) 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 \( 3^3 \) He atom in liquid \( 4^4 \) He, 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 \( 3^3 \) He impurity through liquid \( 4^4 \) He is:
\[
\psi(\vec{k}) = e^{i\vec{k}\cdot\vec{R}} \exp\left(-\frac{1}{2} \sum_{j} (\psi(\vec{r}_j - \vec{R}) + \lambda \psi(\vec{r}_j - \vec{R}))\right)
\]
(4.4)
where \( \psi \) is the wave function of the \( 3^3 \) He atom, \( \vec{r}_j \) are the coordinates of the \( 4^4 \) He atoms, \( \psi \) and \( \lambda \) accounts for the hard-core repulsion between pairs of \( 4^4 \) He atoms or between a \( 3^3 \) He atom and the \( 3^3 \) He impurity respectively. The term \( \exp\left(-\frac{1}{2} \sum_{j} (\psi(\vec{r}_j - \vec{R}) + \lambda \psi(\vec{r}_j - \vec{R}))\right) \) describes the collective motion of the \( 4^4 \) He 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 \( 3^3 \) He particle has an effective mass which is larger than its true mass. The form of the function \( \psi(\vec{r}) \) 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 the function \( \psi(\vec{r}) \) as:
\[
\psi(\vec{r}) = A \vec{r} \cdot \vec{F},
\]
(4.5)
in two dimensions.
We can now go back to spin variables using the identity \( \hat{u}(\vec{r}) = \frac{1}{2}(\vec{r} \cdot \vec{F} + 1) \) where \( \hat{u}(\vec{r}) \) is the boson number operator at lattice site \( \vec{r} \) (1 if there is an up-spin, zero otherwise); we obtain
\[
\sum_{\vec{R}, \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_u}} |\psi(\vec{R}, \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_u}, )\rangle \langle \psi(\vec{R}, \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_u}, )| = \sum_{\vec{R}, \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_u}} \langle \psi(\vec{R}, \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_u}, )| \psi(\vec{R}, \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_u}, )\rangle
\]
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
\[
\sum_{\vec{R}, \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_u}} |\psi(\vec{R}, \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_u}, )\rangle \langle \psi(\vec{R}, \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_u}, )| = \sum_{\vec{R}, \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_u}} \langle \psi(\vec{R}, \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_u}, )| \psi(\vec{R}, \vec{r}_1, \vec{r}_2, \ldots, \vec{r}_{N_u}, )\rangle
\]
(4.7)
where the state \( |\psi, \vec{R}, > \) is the Niel state with staggered magnetization in the \( x \) direction and a hole at \( \vec{R} \). Therefore, the spin-backflow correlation operator \( e^{i\vec{A} \cdot \vec{F}} \) rotates the local spin by an angle \( \vec{A} \) which behaves, at large distances, as in (4.5) whereas \( e^{-i\vec{A} \cdot \vec{F}} \) generates a magnetization along the \( x \)-direction.
Boninsegna and Manousakis's (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 \( u_j \) was chosen to be the same with that determined by Liu and Manousakis. BM found the following simple parameterization for the short-range part of the functions \( \phi_j(\vec{r}) = A_j \sin(\kappa \cdot \vec{r}) \) and \( \lambda_j(\vec{r}) = A_j \cos(\kappa \cdot \vec{r}) \).
For distances larger than one lattice spacing away from the hole, BM took the form (4.9) and treated \( A_j \) as variational parameter. They found that \( \lambda \) 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 \( \Delta E(\vec{R}) = E(\vec{R}) - E(\vec{R}) \) in the total energy with one-hole (no-hole), to those obtained by exact numerical diagonalisation on a \( 4 \times 4 \) lattice for several values of \( \kappa/J \) and at \( \kappa = \frac{1}{2}, \frac{3}{2} \), where the dispersion curve has its minimum. \( \Delta E \) is given in units of \( t \).
The difference between the exact ground state energy and the variational state at small values of \( \kappa/J \) can be attributed to an incomplete description of spin-background fluctuations given by the factor \( \exp\left(-\frac{1}{2} \sum_{i<j} u_{ij} \psi^* \psi \right) \). For \( \kappa/J \geq 0.5 \) the variational and exact results begin to differ.

A typical result for the hole-band \( \Delta E(\vec{R}) \) is shown in Fig. 4 calculated for \( \kappa/J = 0.5 \) 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 $\Delta E(\tilde{k}) = E(\tilde{k}) - E_0$ (Ref. 8), shown as circles joined by a solid line, are compared to those obtained by exact numerical diagonalization on a $4 \times 4$ lattice (dashed line).

$\tilde{k} = \left( \frac{\pi}{4}, \frac{\pi}{4} \right)$, and attains its maximum value at $\tilde{k} = (\pi, \pi)$. Notice that the effective mass of the hole is smaller in the direction $(0, 0)$ to $(\pi, \pi)$ than in the direction $(0, 0)$ to $(\pi, 0)$. Most of these features of the hole band have been revealed by other approaches and in particular they were discussed in Ref. 20 where the authors were studying the problem from the itinerant limit.

The bandwidth $W = E(\frac{\pi}{4}, \frac{\pi}{4}) - E(\pi, \pi)$ is found to grow as $t^2J$ at small $t$. At large values of $t/J$ the bandwidth is expected to be proportional to $J$ because of processes which relax the turnover spin 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 of the antiferromagnetic moment of the background $d\mathbf{m}(r \rightarrow \infty) \sim \frac{\mathbf{k}_F}{3}$ 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 $\Delta E(\tilde{k})$, calculated in Ref. 8 for $t/J = 0.5$ along the paths $\Gamma M X T$ and $M M'$ of the Brillouin zone (shown in the inset).

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ABOUT LONG RANGE P,-U+/-U' MODELS

A. Moreo
Department of Physics, University of California, Santa Barbara,

ABSTRACT

Using a quantum Monte Carlo approach with different symmetries as a new U-+U' model. For the first time, the bandwidth is smaller than the bandwidth of the system, where the correlations are enhanced. The model is reversed when the filling decreases, so that we studied increases as a function of the long range superconducting order parameter.

Since the discovery of high-$T_c$ superconductivity, many new materials have been discovered. We explain how the superconducting state is formed by quantum Monte Carlo simulations using the model proposed by U+U'. The model is reversed when the filling decreases, so that we studied increases as a function of the long range superconducting order parameter.

Experimental measurements have been done on materials with very precise numerical information. Away from half-filling, less data is needed. This information increases the computer time needed to reach the correct results.

The Hubbard model is defined as

$$H = -t \sum_{<ij>,\sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow},$$

where $t$ is the hopping parameter, $U$ is the on-site repulsion, and $n_{i\sigma}$ is the occupation number of the $\sigma$th electron at site $i$. The model describes the electronic structure of transition metal oxides and high-$T_c$ superconductors.