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HOLE EXCITATIONS IN QUANTUM ANTIFERROMAGNETS

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We explore certain aspects of the problem of a quantum antiferromagnet (QAF) with and without holes using an interesting analogy with the problem of helium liquids. Density fluctuations in liquid ^4He correspond to spin-waves in the QAF; holes introduced in the QAF couple to the spin-fluctuations in a similar way that ^3He impurities introduced in liquid ^4He couple to the density fluctuations of the liquid. We generalize the ideas of Feynman-Cohen introduced for the problem of Helium liquids to the case of holes in a QAF. We find that the mobile-hole creates a long-range dipolar spin-backflow which has interesting consequences for the hole-band and the hole-hole interaction.

There are arguments suggesting that the copper oxygen based high temperature superconductors are systems involving strongly correlated electrons. In the simplest case, certain aspects of the behavior of correlated electrons could be described by the $t-J$ model[1] given by

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

and its generalizations. Here $c_{i,\sigma}$ is a hole creation operator, $\vec{s}_i$ is the spin-$\frac{1}{2}$ operator and t the electron hopping matrix element. The notation $j(i)$ means that the summation is over all four nearest neighbors (n.n) j of the site i. The strong on-site Coulomb repulsion is taken into account by restricting the action of the Hamiltonian operator in a subspace of the Hilbert space having states with singly occupied sites. The $t-J$ model can be supplied with a next-nearest hopping term as well as other additional terms in order to more realistically represent both the strong-coupling limit of the Hubbard model and the physics of strongly correlated electrons. Our point here, however, can be made with the aid cf the above simpler model and our conclusions should be appropriately modified when such terms are taken into account.

At half-filling the model reduces to the spin-$\frac{1}{2}$ Heisenberg antiferromagnet, which has significant phenomenological success with respect to certain magnetic properties of the undoped materials.[2] A series of techniques and ideas have been applied to study the motion of a hole and the possibility of pairing between holes in the $t-J$ model. In particular, we wish to mention the work of Shraiman and Siggia[3] who have pointed out that a mobile-hole in a QAF causes a coherent rearrangement of the spin-background around the hole creating a coherent long-range dipolar distortion of the staggered magnetization field. Such distortion has been thought to cause a transition to a spiral phase at any finite hole concentration in a quantum antiferromagnet.[4]

Here, we shall discuss an interesting analogy of the problem of holes in a QAF to that of ^3He impurities in liquid ^4He and explore certain ideas which had been applied to study the latter problem. We generalize the ideas of Feynman-Cohen[5] for the motion of an impurity in a dense quantum Bose liquid to the problem of a hole excitation in the $t-J$ model. It is known that a mobile impurity, introduced in such a liquid, strongly couples to the density fluctuations of the system in a way that a coherent distortion of the density field at long-distances occurs to accommodate the impurity motion. This distortion has a classical analogy in hydrodymamics where it is known as backflow current. The same phenomenon occurs in the case of a hole in a quantum antiferromagnet, where its motion is hindered by the antiferromagnetic alignment and thus the hole strongly couples to the spin-fluctuations of the antiferromagnet. This results to a coherent rearrangement of the spincorresponding to a coherent long-range dipolar spin rotation. We also find that as a result of this long-range distortion, holes with opposite momenta, in a certain range of the angle θ between the vectors $\vec{k}$ and $\vec{r}$, feel an effective attraction.

The analogy of hard-core Bose fluids with spin systems was first pointed out by Matsubara and Matsuda[6] 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. Here, using a unitary transformation of the basis[7], we make use of this analogy for quantum antiferromagnets (AF).

Let us consider the case of no-hole, where the eigenstates of this model can be expressed as $|\Psi>= \sum_{\{\vec{r}_i\}}\psi(\{\vec{r}_i\})(-1)^{L(c)}|\{\vec{r}_i\}>$, where the configuration $|c>$ is labeled by the location of the up-spins, i.e., $|c>=|\vec{r}_1,\vec{r}_2...\vec{r}_{N_u}>=s^+_{\vec{r}_1}s^+_{\vec{r}_2}...s^+_{\vec{r}_{N_u}}|F>$; $|F>$ is the ferromagnetic state with all spins pointing down and N_u is the number of spins pointing up. The amplitude $\psi(\{\vec{r}_i\})$ is symmetric under exchange of any two coordinates $\vec{r}_i,\vec{r}_j$, and $\psi(\{\vec{r}_i\})=0$, if $\vec{r}_i=\vec{r}_j$ for any pair i,j. Thus, in this formulation, spins pointing up can be regarded as "hard-core" bosons. The phase $(-1)^{L(c)}$ ($L(c)$ is the number of up-spins in one sublattice) is separated from the amplitude ψ in order to have a non-negative ψ for any ground state configuration[7]. In this representation, it can be shown that the eigenvalue problem, $H|\Psi>=E|\Psi>$, reduces to a difference equation, for $\psi(\{\vec{r}_i\})$, identical to the many-particle Schrödinger equation on a square lattice. It describes a quantum lattice-gas of bosons with "mass" $m=2/J$ (we use units where the lattice constant $a=1$ and $\hbar=1$) interacting via a pair potential V_{ij} having an infinite on-site repulsion ($V(\vec{r}=0)=\infty$), $V_{ij}=J$ if ij are n.n; otherwise $V_{ij}=0$.

The ground state of a Bose-fluid has a broken symmetry, the Bose-condensate, which in the magnetic language corresponds to AF long-range order. A simple and non-trivial ground state wave function which takes into account short-range correlations due to the existence of the hard-core is the Jastrow wave function $\psi_0(\{\vec{r}_i\})=\prod_{i<j}f_{ij}$, where $f_{ij}=0$ for $i=j$ and $f_{ij}>0$ for $i\neq j$ and it is number operator counting the "particles" (up-spins) by $s^z_i+\frac{1}{2}$ we can go back to the spin variables. We obtain the Marshall[7] state

$$|\psi_0>=\sum_c(-1)^{L(c)}exp\Big(-\frac{1}{2}\sum_{i<j}u_{ij}s^z_is^z_j\Big)|c>, \quad (2)$$

where the sum over i,j now runs over all pairs of sites. The summation over c is over spin configurations having N_u spins pointing in the positive z direction. If we extend the sum over all possible configurations, then the state (2) takes the following form

$$|\psi_0>=exp\Big(-\frac{1}{2}\sum_{i<j}u_{ij}\hat{s}^z_i\hat{s}^z_j\Big)|\phi>. \quad (3)$$

Here $|\phi>$ 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 $\hat{s}^x_i$ with eigenvalues $+1/2$ or $-1/2$ when the site i belongs to the A or B sublattice respectively. The variational state (3) is characterized by antiferromagnetic order with $<\hat{s}^y_i>=<\hat{s}^z_i>=0$ and $<\hat{s}^x_i>=\pm m^\dagger$, where the value of the staggered magnetization $m^\dagger$ depends on the function u. If we restrict the sum in (2) over configurations with zero z-component of the net spin (i.e. $N_u=N/2$), we find that $<\hat{s}^x_i>=<\hat{s}^y_i>=<\hat{s}^z_i>=0$; however each of the two correlation functions $<\hat{s}^x_i\hat{s}^x_j>$ and $<\hat{s}^y_i\hat{s}^y_j>$ at large distances approaches the value $\frac{1}{2}(-1)^{i+j}m^{\dagger 2}$ while $<\hat{s}^z_i\hat{s}^z_j>$ approaches zero.

The elementary excitations in the Bose-system are density fluctuations which in the magnetic system correspond to spin-waves. 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 square lattice spin-$\frac{1}{2}$ quantum antiferromagnet we obtain[8] $u(r\to\infty)=\frac{c}{J\pi r}$, c being the spin-wave velocity. The optimization of the Jastrow wave function (u_{ij}) has been carried out by Liu and Manousakis [8] who used the variational Monte Carlo (VMC) technique by both minimizing the ground state energy and by satisfying sum-rules in a self-consistent way. Their wave function gives $-0.6639J$ for the ground state energy per bond which compares well with the presumably exact

The same wave function gives accurate values for the spin-wave velocity ($c = 1.22 \pm 0.02\sqrt{2}Ja$) and the moments of the Raman scattering intensity (M_1 and M_2), as compared with other techniques.[8] Using the same value for the AF coupling $J = 1500^\circ K$ found in Ref. 2 by fitting the temperature dependent correlation length in pure La_2CuO_4 (a system presumably without holes), they obtain quite satisfactory agreement with the observed values of c, M_1 and M_2 for the same material.

In the Hilbert space with N_u up-spins and one hole a basis vector can be written as $|\vec{R}, \{\vec{r}_i\}>$, where $\vec{R} \neq \vec{r}_i$ is the hole position and $\vec{r}_i$ the positions of the up-spins. The most general eigenstate of (1) having N_u up-spins can be written as $|\Psi >= \sum_{\vec{R},\{\vec{r}_i\}}(-1)^{L(c)}\Psi(\vec{R},\{\vec{r}_i\})|\vec{R},\{\vec{r}_i\}>$. In this representation, the Hamiltonian includes the same boson kinetic energy and boson-boson interaction terms as in the no-hole case and three additional terms. The first two additional terms are the hole kinetic energy whose "mass" is $m_h = 1/2t$, and an interaction potential between the hole and the boson featuring an infinite on-site repulsion, and it is equal to $J/2$ for nearest-neighbors and zero otherwise. This describes the lattice Hamiltonian of an interacting boson gas with an impurity and is analogous to the problem of a ^3He atom in liquid ^4He. Lastly, there is a term which involves a two-"particle" exchange operator, and represents the exchange taking place between the hole and a nearest-neighboring boson. A variational ansatz for the wave function is obtained by multiplying the Jastrow wave function for spins by a correlation operator of the form $e^{-i\vec{k}\cdot\vec{R}}exp\{-\sum_j\Big(i\phi_{\vec{k}}(\vec{r}_j-\vec{R})+\lambda_{\vec{k}}(\vec{r}_j-\vec{R})\Big)\}$ which takes into account boson-impurity correlations. The imaginary part can describe "backflow" effects, as in the Feynman-Cohen treatment of the problem of a ^3He impurity in liquid ^4He;[5] there, $\phi_{\vec{k}}$ describes the collective motion of ^4He atoms which move out of the way in order to make room for a ^3He impurity to pass through, filling the empty space it leaves behind. Due to this effect, the ^3He atom inside liquid ^4He 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 the long-distance behavior of $\phi_{\vec{k}}(\vec{r})$ for two-dimensions, is obtained as

$$\phi(\vec{r} \to \infty) = A(\vec{k})\frac{\vec{k}\cdot\vec{r}}{r^2}. \qquad (4)$$

If we go back to spin variables, the hole wave function, within a multiplicative constant, is given by

$$|\Psi_{\vec{k}}>=\sum_{\vec{R}} e^{-i\vec{k}\cdot\vec{R}}e^{-\sum_i(\lambda_i+i\phi_i)\hat{s}_i^z}|\psi_{\vec{R}}>, \qquad (5)$$

where $|\psi_{\vec{R}}>$ is given by (2) with the difference that there is no spin at site $\vec{R}$. The functions λ_i and ϕ_i are abbreviations for $\lambda_{\vec{k}}(\vec{r}_i-\vec{R})$ and $\phi_{\vec{k}}(\vec{r}_i-\vec{R})$ respectively and we should keep in mind that they are functions of both the vector joining the hole with the spin at i and of the momentum $\vec{k}$. If we allow the sum over configurations in the expression for $|\psi_{\vec{R}}>$ to run over all possible configurations rather than just those with fixed number of bosons, we should use (3) for $|\psi_{\vec{R}}>$ with a hole at $\vec{R}$. This state has a well defined direction of the staggered magnetization (x direction).

Next, we show that the $\lambda_{\vec{k}}$ and $\phi_{\vec{k}}$ correlations can also be interpreted as local spin rotations and are necessary in order to relieve the local spin environment from the incoherence created by the hole motion. First, we set $u = 0$ in the state (5) which can be written as

$$|\Psi^0_{\vec{k}}>=\frac{1}{\sqrt{M}}\sum_{\vec{R}\epsilon\pm} e^{-i\vec{k}\cdot\vec{R}}|\vec{R}>\prod_{\vec{r}_i\neq\vec{R}}|\chi(\vec{r}_i)>_\pm, \qquad (6)$$

where

$$|\chi(\vec{r}_i)>_\pm= e^{-(\lambda_i+i\phi_i)\hat{s}_i^z}|\pm\hat{x}>_i, \qquad (7)$$

and $|\pm\hat{x}>_i$ are eigenstates of $\hat{s}_i^x$. The state $\chi(\vec{r}_i)$ after normalization can be expressed as $|\chi(\vec{r}_i)>_\pm= exp(-\frac{i}{2}\theta_i^\pm\hat{n}_i\cdot\vec{\sigma}-i\phi_i\hat{s}^z_{\vec{r}_i})|\pm\hat{x}>_i$, where $\vec{\sigma}$ are the Pauli matrices and $\hat{n}_i=(-sin(\phi_i),cos(\phi_i),0)$. This state can be interpreted as a local rotation of the spin vector which points in the $\pm\hat{x}$ direction by an angle ϕ_i around the positive z axis and subsequently by an angle θ_i around the vector $\hat{n}_i$ out of the $x-y$ plane towards the positive direction. The angle $\theta_i^\pm$ is related to the parameter λ_i as follows $\theta_i^+ = 2tan^{-1}\Big(tanh(\frac{\lambda_i}{2})\Big)$ and $\theta_i^- = -2tan^{-1}\Big(coth(\frac{\lambda_i}{2})\Big)$.

the problem can be solved analytically. The wave function (7) can be parametrized as follows

$$|\chi(\vec{r}_i)>_\pm = \rho_i|\pm\hat{x}>_i + \sqrt{1-\rho_i^2}e^{i\omega_i}|\mp\hat{x}>_i . \quad (8)$$

The states (7) and (8) apart from a multiplicative constant can be made identical provided that the functions λ_i, ϕ_i, ρ_i, ω_i are related in the following way $\phi_i = -tan^{-1}\left(\frac{2\rho_i\sqrt{1-\rho_i^2}}{2\rho_i^2-1}sin\omega_i\right)$, and $\lambda_i = -\frac{1}{2}ln\left(\frac{1+2\rho_i\sqrt{1-\rho_i^2}cos\omega_i}{1-2\rho_i\sqrt{1-\rho_i^2}cos\omega_i}\right)$. In this form, the expectation value of the J-term of (1) apart from a constant is given by $< V >= -\frac{3J}{2}\sum_i \rho_i^2$ and is independent of ω_i. Therefore, the relative phase ω_i can be found by minimizing the hopping energy only. In an antiferromagnetically aligned spin system, when a hole moves to a nearest-neighboring site it creates a state which is orthogonal to the original state. In order to minimize the hopping energy, one has to allow for maximum overlap between the initial and the final state, and this can be achieved if the spins around the hole are in a non-pure spin state. The overlap between the state obtained by acting with H on (6) and the state (6) itself attains its maximum magnitude by choosing $\omega_{\vec{\delta}} = -\vec{k}\cdot\vec{\delta}$. Choosing $\rho_{\vec{\delta}} = \rho$, the expectation value of the Hamiltonian (1), within a constant, is obtained as $< H_{t-J} >= -8t\rho^7\sqrt{1-\rho^2} - 6J\rho^2$ and the optimal value of the parameter ρ lies in the interval $\rho_c \leq \rho \leq 1$ and depends monotonically on t/J with $\rho(t/J=0)=1$ and $\rho(t/J\to\infty)\equiv\rho_c=\sqrt{\frac{7}{8}}$. The expectation values of the n.n. spin operators is obtained as $< s^x_{\vec{\delta}} >_\pm = \pm\frac{1}{2}(2\rho^2-1)$, $< s^y_{\vec{\delta}} >_\pm = \rho\sqrt{1-\rho^2}sin(\vec{k}\cdot\vec{\delta})$, $< s^z_{\vec{\delta}} >_\pm = \rho\sqrt{1-\rho^2}cos(\vec{k}\cdot\vec{\delta})$.

Far away from the hole, the problem can be solved by expanding the energy expectation value and keeping up to terms quadratic in λ, ϕ and $\nabla\lambda$ and $\nabla\phi$. Minimizing the resulting expression we find that the function λ should decay within a few lattice spacings from the hole, whereas the function ϕ has the behavior given by Eq. (4). The planar distortion a $1/r$ power-law at long distances from the hole. There is a magnetization along the direction orthogonal to plane which decays exponentially with the distance from the hole and thus it is confined

In summary, the operator, $e^{-i\phi_i \hat{s}_i^z}$ rotates the spin, which points in the x direction in the uncorrelated state, by an angle ϕ_i which behaves, at large distances, as in (4), whereas $e^{-\lambda_i \hat{s}_i^z}$ generates the magnetization along the z-direction.

The minimization of the hole energy with the full wave function (5) which includes background fluctuations has been carried out by Boninsegni and Manousakis[10] who used the VMC technique. Their results have been compared with exact diagonalization results available only on small size lattices and they are in reasonable agreement; the VMC calculation, however, has been carried out on much larger size lattices also. They find that the minimum of the hole energy-band is at $(\frac{\pi}{2},\frac{\pi}{2})$ and the effective mass of the hole for the perpendicular directions around the minimum is different. In fact, the hole effective masses in the direction $(\pi,0)$ to $(0,\pi)$ is much larger than that in the perpendicular direction $(0,0)$ to (π,π). Similar band-structure has been revealed by a number of other approaches.[3, 11, 12] In addition, the long-range distortion of the staggered magnetization, given by (4), remains after the inclusion of the quantum fluctuations by allowing u_{ij} to be different from zero. The ferromagnetic moment which is perpendicular to the direction of the staggered magnetization also remains and is localized in the immediate neighborhood of the hole. However, the ferromagnetic moment depends on $\vec{k}$ and it is zero at the minimum of the band.

This type of distortion of the spin background has been thought to cause a spiral phase[4] at any finite fraction of holes. The order parameter in such phase is proportional to $\vec{Q}_\alpha = \hat{m}^\dagger \times \partial_\alpha \hat{m}^\dagger$. Using our wave function for the case of a single-hole, we find that at distances far away from the hole $\vec{Q}_\alpha \sim \frac{\hat{z}}{r^2}[(\vec{k} - 2\frac{(\vec{k}\cdot\vec{r})\vec{r}}{r^2})\cdot\hat{\alpha}]$ where $\alpha = \hat{x},\hat{y}$.

Our qualitative picture of a single-hole excitation in a quantum antiferromagnet is the following: We separate the region around the hole into two parts, the "core" region of approximate radius r_c and the region outside the core. The length scale r_c is of the order of the average length of the path of the hole in the "string"-like picture of the Brinkman-Rice approach and is an increasing function of t/J. This energy excitations in the hole spectrum. For $r > r_c$, the spin background is coherently distorted from the antiferromagnetic alignment by an angle given be Eq. (4). The region of the "core" is characterized by a ferromagnetic moment perpendicular to the plane of the staggered magnetization which vanishes at the minima of the hole band. If there is only a hopping matrix element t' between different sublattices and $t = 0$, there is no need for the creation of such long-range distortion. However, when the hole is delocalized and $t \neq 0$, the presence of the long-range distortion is necessary in order for the overlap between two displaced hole states to be non-zero.

Within this picture of the quasihole, we find that there is an effective long-range dipolar attraction between two holes. The origin of the attraction between holes with opposite momenta is the fact that the least amount of damage due to the long-range dipolar distortion of the staggered magnetization is caused when the holes stay at opposite valleys of the reduced Brillouin-Zone and close to each other. The long-range part of the effective interaction can be estimated by using the non-linear σ model to describe the long wavelength limit of the Heisenberg antiferromagnet. From a semiclassical point of view, we can estimate the long-distance part of the effective interaction by calculating the difference between the energy cost to create two quasiholes with opposite momenta at infinite distance and at finite distance $r >> r_c$. We find

$$V_{eff}(r >> r_c, \theta) = -c(\vec{k})J\frac{cos(2\theta)}{r^2}, \qquad (9)$$

where θ is the angle between the vectors $\vec{k}$ and $\vec{r}$. Here, $c(\vec{k})$ is a constant of order 1 which depends on $\vec{k}$. Hence, there is a $1/r^2$ attraction for $-\frac{\pi}{4} \leq \theta \leq \frac{\pi}{4}$ and $\frac{3\pi}{4} \leq \theta \leq \frac{5\pi}{4}$. This attraction is caused by the dipolar distortion and as argued previously, is expected to exist on more general grounds when a hole is delocalized in an AF background. In addition, the interaction given by (9) between a pair of holes and other holes is weak once the holes in the pair come sufficiently close to each other because the distortion of the background is repaired. Thus, this part of the interaction favors pairing and not phase separation.

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REFERENCES

1. P.W. Anderson, Science **235**, 1196 (1987).
2. E. Manousakis, Rev. of Mod. Phys. to be published (January 1991 issue). See references therein.
3. B. Shraiman and E. Siggia, Phys. Rev. Lett. **60**, 740 (1988) and *ibid*, **61**, 467 (1988).
4. B. Shraiman and E. Siggia, Phys. Rev. Lett. **62**, 1564(1989). B. Chakraborty et al., Phys. Rev. **B42**, 4819 (1990).
5. R.P. Feynman, Phys. Rev. **94**, 262 (1954); R.P. Feynman and M. Cohen, Phys. Rev. **102**, 1189 (1956).
6. T. Matsubara and H. Matsuda, Prog. Theor. Phys. **16**, 569 (1956).
7. W. Marshall, Proc. R. Soc. London Ser. A **232**, 48 (1955).
8. E. Manousakis, Phys. Rev. B **40**,4904(1989); Z. Liu and E. Manousakis, Phys. Rev. B **40**, 11437 (1989).
9. J. Carlson, Phys. Rev. **B40**, 846 (1989). N. Trivedi and D. M. Ceperley, Phys. Rev. **B40**, 2747 (1989).
10. M. Boninsegni and E. Manousakis, Technical report FSU-SCRI-90-147.
11. J. R. Schrieffer, X. G. Wen and S. C. Zhang, Phys. Rev. B **39**, 11663 (1989).
12. S. A. Trugman, LA-UR-90-1299, 1990.