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LETTER TO THE EDITOR

Possibility of quasiparticle behaviour in the strongly correlated Hubbard model

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Abstract. I calculate an exact expression for the Green function of a single hole in a Néel background, for *finite* Ising interaction $J_z \equiv 4t^2/U$ where t is the hopping (overlap) integral in the Hubbard model and U the usual on-site interaction. In 1D for fixed boundary conditions, loops are absent and thus the expression is exact and independent of the retraceable path approximation, while in 2D the expression is exact to within the exclusion of loops. The spectral function $A(\omega)$ shows delta-function peaks at well defined energy spacings, with damping only at frequencies $\omega > 5/2J_z$ different from earlier results. These peaks are necessary for the existence of quasiparticles. I present an argument that, for sufficiently large U, the discrete spectrum in $A(\omega)$ merges to a continuous 'band' as the weight $\propto J_z$ of the poles vanishes in the $U = \infty$ limit and hence that use of the latter does not necessarily imply incoherent behaviour in the system.

With the idea that the new high-T_c superconductivity may be associated with the copper oxide layers in these compounds, and the similarity of various physical properties [1] with the predictions of theories based on Mott-charge-transfer insulators, a first-principles investigation of the properties of the large-U Hubbard model is of great importance. One class of theories and investigations is based on the possibility of superconductivity in the single-band large-U 2D Hubbard model [2, 3]. The starting Hamiltonian in these theories is the usual one for no double occupancy namely,

$$H = t \sum_{\langle i,j\rangle,\sigma} (1 - n_{i,-\sigma}) c^\dagger_{i,\sigma} c_{j,\sigma} (1 - n_{j,-\sigma}) + J \sum_{\langle i,j\rangle} (S_i S_j - \tfrac{1}{4} n_i n_j) \tag{1}$$

where t is the overlap integral between nearest neighbour sites i and j, U is the on-site Coulomb repulsion, $S_i(S_j)$ the spin on the ith (jth) site, $n_i \equiv c_i^\dagger c_i$ and $J \equiv 4t^2/U$ is the usual superexchange interaction.

A question of great interest is the possibility of quasiparticle behaviour of a single hole in an antiferromagnetic background. In the weakly doped limit, where hole–hole scattering can be neglected, the single-hole problem is of relevance to the copper oxide high-T_c superconductors in which the antiferromagnetism of equation (1) in the half-filled band case has been experimentally observed. In an early paper, Brinkman and Rice [4] considered this question in the $U = \infty$ limit ($J_z = 0$) using the retraceable path approximation. More recently, approximate diagrammatic approaches based on Green

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function decoupling schemes [5–7] reconsidered the problem justifying the validity of their approximations by comparison with the $U = \infty$ limit of [4].

It is the purpose of this paper to re-examine the issue of quasiparticle behaviour by a systematic introduction of finite J_z into the retraceable path approximation. I derive an exact expression for the Green function (propagator) for a single hole in a Neél background (half-filled band) and evaluate the spectral function. The delta-function peaks which I obtain are necessary for quasiparticle behaviour. Bloch-type quasiparticle behaviour conclusively emerges when the wave function is written as a *superposition* of all possible states.

In the Ising limit $J_\perp \to 0$, the motion of the hole changes the Néel background, generating a succession of 'string' states in which the spins appear 'overturned' with respect to the Néel background [2, 8]. Within this basis, the properties of the 2D spectral function which I present are necessary for quasiparticle behaviour. However, it is generally supposed that the continuous spectrum in the infinite U limit [4] is associated with incoherent behaviour of the hole. On sufficiently short time scales $\tau \ll J_\perp^{-1}$ such that the background remains unchanged as the hole hops, quasi-particle behaviour may not be incompatible with a 'continuous' spectrum as is commonly thought [4–6, 8]. Thus theories based on the limit $U \to \infty$ may actually be applied to quite realistic situations.

In 1D, the string can be at most of length one. Taking the Néel state as the zero of energy, the state derived from this state by addition of a vacancy has energy $J_z/2$ in 1D, J_z in 2D. For fixed boundary conditions there are no loops [4]. Thus the Green function in 1D is given in a single calculation exactly by

$$G_{i,j}^{1D}(\omega) = G_{i,i}^{1D}(\omega)\delta_{i,j} \equiv G^{1D}(\omega) = \frac{1}{\frac{1}{2}J_z + \{(\omega - J_z)^2 - 4t^2\}^{1/2}} \tag{2}$$

independent of the retraceable path approximation. In the $U \to \infty$ limit $J_z \to 0$, equation (2) reduces to the two square root singularities at $\pm 2t$ of [4]. With the change of variable $u \equiv -\{1 - 4[\omega/w - (t/U)]^2\}^{1/2}$ where $w \equiv 4t$ is the bandwidth in 1D, we have for $-1 \leqslant u \leqslant 0$,

$$\mathrm{Im}\, G^{1D}(\omega) = \frac{1}{2t}\frac{u}{[u^2 + (t/U)^2]} \underset{U\to\infty}{\longrightarrow} -\frac{1}{(4t^2 - \omega^2)^{1/2}}. \tag{3}$$

This function is peaked at $|u| = (t/U)$ or equivalently at $\omega \simeq \pm 2t + J_z \mp \frac{1}{16}J_z^2$. The absence of off-diagonal terms in (2) implies that the 'equilibrium' $G_k(\omega) = 0$ unless $k = 0, \pm\pi n, n = 0, 1 \ldots$ in units of the lattice spacing. It is evident from figure 1 that Im G has no peak at $\omega = 0$. From (3) we see that the lineshape differs from a Lorentzian. These differences from [6] could originate from the $J_\perp$ terms neglected here. Such terms, which include spin waves, become least important for $k = \pm\pi/2$ or frequencies large compared with a spin wave frequency [1]. Thus for this choice of wave number, and for frequencies away from the origin, the lineshapes of [6] should be most similar to (3). Figure 1 shows the peaks and shift in the spectrum introduced by making t/U finite. Perhaps worth pointing out is that [9] calculates an expression, which is similar in principle, with Bloch states introduced at the outset, generated from the initial Néel state producing a 'string' through the action of a sequence of raising and lowering operators $S^\pm$ which does not explicitly include more important $S_i^z S_j^z$ terms in the Hamiltonian. This results in equation (15) of [9] being very similar to, but not exactly the same as, (2) above, in which the string of overturned spins generates interactions

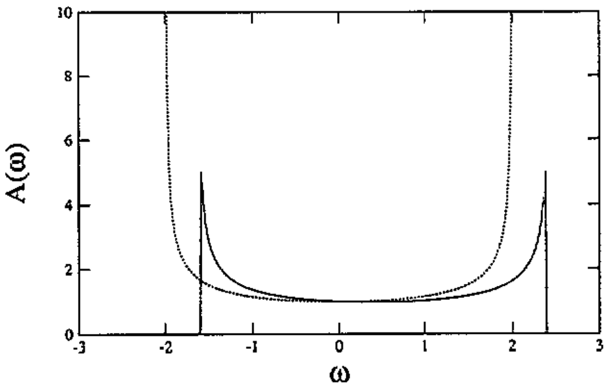

Figure 1. $A(\omega)$ versus ω/t for $t = 1$ and $J_z = 0$ (dotted curve), $J_z = 0.4$ (full curve).

$\propto S_i^z S_j^z$ neglected in [9], though it does not include $J_\perp$ for the reasons mentioned in the introduction.

Using the 'string' states of length l as approximate eigenstates [8] the Green function in 2D is given by

$$G_{i,j}(\omega) = G_{i,i}(\omega)\delta_{i,j} \equiv G(\omega) = \frac{1}{\omega - J_z + (4/\sqrt{3})[J_\nu(z)/J_{\nu-1}(z)]} \tag{4}$$

which is exact within the zero-loop retraceable path approximation. Here $\nu \equiv \gamma z$, $\gamma \equiv -[\omega - \frac{5}{2}J_z]/(2t\sqrt{3})$, $z \equiv \sqrt{3}U/(2t)$ and $J_\nu(z)$ is the cylindrical Bessel function of order ν [11]. $G_{i,j}$ is diagonal owing to the neglect of loops and the restriction to nearest neighbour hopping processes in (1). These, together with random spin flips, relax the condition that the hole must return to its original position in order to leave the antiferromagnetic background unchanged. However, inclusion of loops is believed to introduce only a weak [6, 9, 10] k-dependence into the dispersion relation for quasi-particles while random spin flips are not expected to be more important.

We can write (4) in the form

$$G(\omega) \equiv \frac{1}{\omega - \Sigma(\omega)}$$

where

$$\Sigma(\omega) \equiv J_z - \frac{4}{\sqrt{3}}\frac{J_\nu(z)}{J_{\nu-1}(z)} \tag{5}$$

and for $\nu \neq -n$ [11],

$$f(z) \equiv \lim_{\nu\to\gamma z} \frac{J_\nu(z)}{J_{\nu-1}(z)} = \lim_{\nu\to\gamma z} -\sum_{n=1}^{\infty}\left\{\frac{1}{z - j_{\nu-1,n}} + \frac{1}{z + j_{\nu-1,n}}\right\}. \tag{6}$$

The zeros $j_{\nu-1,n}$ of the Bessel function $z^{\nu-1}J_{\nu-1}(z)$ are purely real for $\nu > 0$, hence $\Sigma(\omega)$ is purely real for $\omega < \frac{5}{2}J_z$. In this region, therefore, there is no damping to the poles of $G(\omega)$ (mathematically this corresponds to no branch line in $\Sigma(\omega)$, i.e. no discontinuity

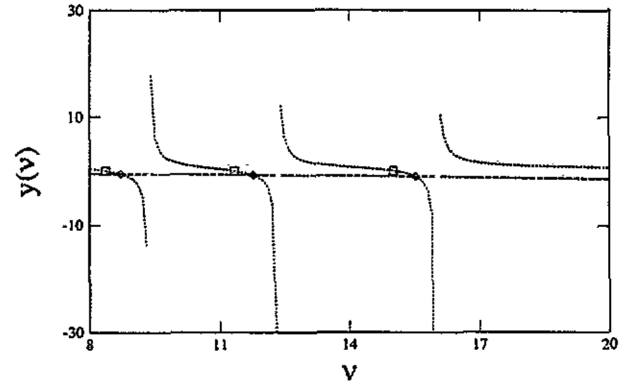

Figure 2. Graphical solution of equation (9) for $t = 1$, $z = 20$ ($J_z \simeq 0.17$). The dotted curve shows $y = f(\nu)$, the broken curve shows $y = g(\nu)$, almost parallel to the line $y = 0$. The first three poles in $A(\omega)$, which are graphical solutions to (9), are marked by diamonds (exact) and squares (to order $\nu^{-2/3}$) at $\nu = 8.69, 11.76, 15.52$ and $8.35, 11.33, 15.01$, respectively.

in $\Sigma(\omega)$ across the real ω axis). Hence, quasiparticle behaviour corresponding to excitations with well defined energy is predicted at frequencies given by the delta-function peaks in the spectral function [12]

$$A(\omega) \equiv -2\mathrm{Im}\, G(\omega) = 2\pi\delta[\omega - \mathrm{Re}\,\Sigma(\omega)] \qquad \omega < \tfrac{5}{2}J_z. \tag{7}$$

Physically these peaks correspond to the allowed energies of the hole in the system and are necessary for quasiparticles. The peaks occur at frequencies ω_n such that

$$\omega_n - \mathrm{Re}\,\Sigma(\omega_n) = 0 \tag{8}$$

i.e. at the solutions to the equation

$$g(\nu) = f(\nu) \tag{9}$$

where $g(\nu) \equiv 9/4z - 3\nu/2z$ and $f(\nu) \equiv J_\nu(z)/J_{\nu-1}(z)$. The peaks have no damping in this range which implies that the original basis states are good approximations to the true eigenstates, and that the hole makes no 'transitions' into different states by scattering with the background. However, for $\omega > \tfrac{5}{2}J_z$, equations (5) and (6) imply that $\mathrm{Im}\,\Sigma \neq 0$ and hence that peaks in $A(\omega)$ will have some width, contrary to [5].

If we suppose that the $U = \infty$ limit of (4) gives the same result as [4] then from (6) we have the exact equality,

$$\lim_{\nu \to \gamma z} \frac{J_\nu(z)}{J_{\nu-1}(z)} \underset{U\to\infty}{\longrightarrow} -\gamma[1 \pm (1/\gamma)\sqrt{\gamma^2 - 1}] \qquad \nu - 1 \neq -n \tag{10}$$

i.e. that the discrete spectrum of zeros and poles of the function $f(\nu)$ merges to a branchline on the real ω axis. For $U < \infty$ the zeros and poles of $f(\nu)$ are separated by a narrow region of order $(1/\nu)$ whereas the first few zeros (poles) of $f(\nu)$ are separated by order $(1/\nu)^{2/3}$ (see figure 2). In this limit, the poles of $f(\nu)$ merges into the branch cut along the real ω axis, coincident with the appearance of the 'incoherent' continuous spectrum of Brinkman and Rice [4]. This $U \to \infty$ limit ensures that $\Delta\varepsilon$, the spacing of adjacent energy levels, is small compared with the time for hopping of the hole from one site to the next, so that the hole can hop over many sites in time τ, i.e. $\Delta\varepsilon \sim J_z^{2/3} \ll \tau^{-1}$ (thus $J_\perp \ll \tau^{-1}$). Since as $J_z \to 0$ this condition becomes more easily satisfied, one important consequence is that the absence of discrete poles in the Brinkman–Rice continuous density of states does not necessarily imply lack of quasi-particle behaviour in the large-U limit of the Hubbard model; the shape of $A(\omega)$ in the $U \to \infty$ limit may be regarded as an approximate 'envelope' of the delta-function peaks in the finite U limit. Thus at least in the limit $\Delta\varepsilon \ll \tau^{-1}$, the $U \to \infty$ limit may prove a realistic approximation even in the presence of finite J_z [1].

We now proceed to solve (9) approximately. Neglecting terms of order $1/\nu$ compared with 1, the solutions of (9) near the lower band edge are given by the solutions of $f(\nu) = 0$, or equivalently by

$$z - j_{\nu,n} = 0. \tag{11}$$

An expansion about the nth pole in (6), accurate to order $1/\nu$, gives

$$(z - j_{\nu_n - 1,n})g(\nu_n) + 1 = 0. \tag{12}$$

The first three solutions of (12) are

$$\omega_n \simeq -2\sqrt{3}(1 - a_n/z^{2/3} + 1/3z) \tag{13}$$

where [13] $a_1 = 1.856$, $a_2 = 3.245$ and $a_3 = 4.382$. In particular, the lowest pole occurs at a value of

$$\omega \simeq -2\sqrt{3}(1 - 0.81 J_z^{2/3} - 0.63 J_z). \tag{14}$$

From (14) we see the original 2D bandwidth $W/2 = 4$ is narrowed by $\sim J_z$ for $J_z > 0.4$. This result (14) is valid only for frequencies very near the lower band edge located at $-2\sqrt{3}$ [4, 5]. The lowest peak occurs for $J_z \sim 0.2$ at $\omega \sim 0.6\,(2\sqrt{3}) \sim -2.1$ very near the result ~ -2 obtained in figure (10) of [9] using the Heisenberg model for $k = (\pi/2, \pi/2)$ when spin waves in the retraceable path approximation are least important, and for $J_z \sim 0.05$ at $\omega \sim -0.86(2\sqrt{3} \sim -2.98$ very near -2.8 in the integrated spectral function $A(\omega)$ of figure 9 of [9] for calculations done on the Néel state. Surprisingly, figure 14 of [9] showing $J_z = 0.2$ in the *pure* Ising limit, exhibits a peak at a much higher value ($\omega \sim -0.4$) than predicted in this pure Ising calculation. Although their calculation is done on finite systems, properties of these systems should already begin to approach those of infinite systems at least in functional dependence on J_z^{14}.

Close to the poles one can write to order $1/\nu$

$$\begin{aligned} A(\omega) &= 2\pi\delta[g(\nu) + (z - j_{\nu-1,n})^{-1}] \\ &= 2\pi\delta(\omega - \omega_n)Z(\omega_n) \end{aligned} \tag{15}$$

where $Z(\omega_n)$ is the weight of each of these poles, given by

$$Z(\omega_n) \equiv \left| \frac{\mathrm{d}}{\mathrm{d}\omega} \frac{3\nu}{2z} z - j_{\nu-1,n}^{-1} \right|^{-1}_{\omega=\omega_n} = \tfrac{4}{9} J_z(1 + \mathrm{O}(J_z^{1/3})) \tag{16}$$

which is similar to [5].

In a continuum (in frequency space) approximation, in which we replace the continuous index ν for $\nu \gg 1$ by the integral index n with $n \gg 1$, $f_\nu(z) \simeq f_n(z) = J_n(z)/J_{n-1}(z)$. Neglecting terms of order $(1/n)$ the solutions of (9) are the zeros of the Airy functions $\mathrm{Ai}(-\psi)$ where $\psi \equiv (z-n)/(2z)^{1/3}$. Since, however, $J_{-n}(z) = (-1)^n J_n(z)$, to order $J_z^{2/3}$, the spectrum of excitations of the hole is symmetric in $\pm\omega$ in contrast to the result for ν continuous.

To summarize, by examining the properties of an exact Green function calculated systematically in the Ising limit, several new results have emerged for a single hole in an antiferromagnetic background. I argue that the 'continuous band' of infinite-U theories does not necessarily exclude quasiparticle behaviour, as is generally supposed. In 1D, the $U = \infty$ square root singularities at the upper and lower band edges are replaced by finite peaks in an exact calculation. In 2D, I give analytic expressions for the first three peaks in the density of states, which is shown to have damping of its delta-function peaks only at frequencies $\omega > +5/2J_z$. In a continuum (in frequency space) approximation, the (undamped) spectrum is symmetric with respect to $\pm\omega$ in the distribution of its peaks up to $\sim J_z^{2/3}$ and in the weight of the peaks at least to order J_z.

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