Excitations in a nearly half-filled Hubbard model with $U=\infty$

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It is shown that, even near half filling, the elementary excitations of the large-U Hubbard model form wide bands of width $\sim t$, the intersite hopping integral, and that the slave-boson-based mean-field approximation is qualitatively wrong in the relevant limit. This large $-U$ limit has no Kondo-type divergences.

In the context of high-temperature superconductors, there is considerable interest in the elementary excitations associated with the Hubbard model.[1-3] The fact that, e.g., $YBa_2Cu_3O_6$ is an antiferromagnetic insulator suggests that an appropriate beginning model for these materials might be a half-filled Hubbard Hamiltonian with a large Coulomb U and doped by a small concentration n_0 of holes. It is important to understand under what circumstances these excitations correspond to a Fermi liquid.

Many years ago Brinkman and Rice[4] considered the problem of a *single* hole in an otherwise half-filled, large-U, Hubbard model and showed that, depending on the nature of the spin-wave function, the hole has a mass equal to or $\sim$20–25% less than the electron mass. However, except for the ferromagnetic case, the spin-wave functions considered cannot be stationary states in the presence of a finite concentration of holes. In general, the kinetic (spatial) and spin-wave functions are interdependent in a fashion which is not well understood, and for this reason these pioneering results cannot be trivially extended to the present problem. In one dimension, for $U=\infty$, a *finite* concentration of holes, and independent of the spin-wave function, the exact solution[5] corresponds to quasiparticles which occupy a broadband with a width $2t$, where t is the hopping integral. In this case there is no coupling between the kinetic and spin degrees of freedom, e.g., there is a Curie rather than Pauli susceptibility. In contrast, Nagaoga's theorem shows, again for a small but finite concentration of holes, two or more dimensions, and strictly the $U\rightarrow\infty$ limit, that such a coupling *does* exist and implies a "ferromagnetic" ground state. For large but finite U there will be a competition between this "ferromagnetic" tendency and the antiferromagnetic exchange interaction and the nature of the spin-wave function becomes less clear.

Perhaps the best understood example in which a coupling of this type leads to a Fermi-liquid theory is the single-ion Kondo effect. It is *possible* that, with a finite concentration of holes, the present problem might be equivalent to a periodic Kondo problem. For the *single-ion* Kondo problem, Coleman[6] has proposed a method of performing an expansion in $1/N$, where N is the orbital degeneracy. In the large N limit the partition function is dominated by a saddle point which corresponds to a mean-field theory. The expansion in $1/N$ then yields an approximate solution for finite N. A well-defined large-N limit requires that the slave-boson constraint $Q_i=1$ be modified to $Q_i=qN>1$. Kotlair and Ruckenstein[3] argue that the large-N saddle point is not unique, but that one choice corresponds to the popular Gutzwiller approximation, and that, at least for the Anderson-lattice model, the Kondo effect is already "built in." Recently, Kotlair and Liu[2] have shown, for large U, the large-N limit results in a simple Fermi liquid with a Pauli susceptibility and a band of width, n_0zt, i.e., proportional to n_0. Usually it is suggested that this band narrowing reflects the "block off" of hopping by other particles. Such calculations suggest that the Kondo effect is *not* involved. Apparently, there is not the usual energy scale $T_K\sim D\exp[-(1/|\rho J|)]$ where $D=n_0zt$, $\rho\sim 1/D$, and J is the effective exchange constant. However, this is not clear, since writing $J\sim V^2/\epsilon_d$, here both V and $\epsilon_d\sim n_0t$ so that $J\sim n_0t$ while $\rho\sim(1/D)\sim(1/n_0t)$ so that $T_K\sim D\sim n_0t$, i.e., the exponential factor is of order unity. It *is* possible to interpret the narrow band as being equivalent to the single-ion Kondo resonance.

The purpose of the work described here was to help resolve these issues. The problem is formulated using slave bosons and the equation-of-motion method. A new type of time-ordered Green's function will be introduced. It is well known that the limit of large but finite U is equivalent to $U=\infty$ plus a local antiferromagnetic interaction $+|J_0|\mathbf{S}_i\cdot\mathbf{S}_j$ where this $|J_0|\sim t^2/U$. It is clear that this exchange only affects the spin-wave function and so formally it will be assumed that $U=\infty$, *but* no initial assumption will be made about the spin-wave function. Three possible lattice structures will be considered, a one-dimensional chain, the Bethe lattice, and the two-dimensional square lattice. Three variants of the model will also be considered. Of principal interest is the regular Hubbard model as described above; however, for comparison a one-dimensional Anderson model, obtained by setting $U=\infty$ for site $n=0$ and $U=0$ for all the other N_s sites, is considered (n_0 is now measured relative to the state with $2N_s+1$ electrons). The third model is the extended Hubbard model of Kotlair and Liu with $Q_i=qN>1$.

It is found that interchanging particles *of different spin,* leads to the coupling between the kinetic and spin degrees of freedom and therefore that the three different lattice

types and three variants of the model represent different cases. For the Hubbard model in one-dimension, particles cannot be interchanged while, for the Bethe lattice, such interchanges involve $O(t^6)$ and $(n_0)^2$, and are negligibly small in the $n_0 \to 0$ limit. For a square lattice, interchanges occur when a hole passes around a loop and involve only $O(t^4)$ and n_0. For both the Anderson and Kotlair-Liu, $qN > 1$, models it becomes possible to interchange particles in a process which involves $O(t^2)$, n_0, and which occurs even in one dimension. Certainly, in the absence of this process, and for one dimension, only a broadband exists and the inevitable conclusion is that the narrow band, or Kondo resonance, according to the model, arises from the $O(t^2)$ process. For the Hubbard model, this process and the associated narrow band are unphysical. It follows, for one dimension, or for the small n_0 and the Bethe lattice, that the renormalization represented by expansion in $1/N$ should completely remove the narrow band and replace it with a broad one for $N=2$. (As it should at $N=1$ for the Anderson model.) Even for a square lattice, the expansion in $1/N$ with $N=2$ must also represent a large renormalization since, even if such a narrow band exists, it would reflect a process involving loops, i.e., quite different physics from the $O(t^2)$ process.

The Hubbard Hamiltonian is

$$\mathcal{H} = t \sum_{\substack{nm,\sigma \\ st}}{}' c^\dagger_{nm\sigma} c_{st\sigma} + U \sum_{nm} c^\dagger_{nm\uparrow} c_{nm\uparrow} c^\dagger_{nm\downarrow} c_{nm\downarrow} ,$$

where $c^\dagger_{nm\sigma}$ creates an electron, with spin σ, at the site with index nm, and where the prime on the sum indicates that the sum on st is over z near neighbors only.

It does not seem to be widely realized that there is a mechanical way in which to replace physical operators with their slave-boson equivalent.[7] If $\hat{O}$ is such a *physical* operator

$$\hat{O} \to \sum_{\alpha,\beta} e^{i(\phi_\alpha - \phi_\beta)} s^\dagger_\alpha \langle \alpha | \hat{O} | \beta \rangle s_\beta ,$$

where α,β identify a given state and where $s^\dagger_\alpha$ is the auxilliary fermion or boson, depending upon whether $|\alpha\rangle$ corresponds to an odd or even number of electrons. The total number of these auxilliary particles is constrained, i.e., $Q = \sum_\alpha s^\dagger_\alpha s_\alpha = 1$. Here the usual gauge, $\phi_\gamma = 0$ for all γ, will be used. A convention is required in order to specify the exact meaning of the state $|\uparrow\downarrow\rangle = c^\dagger_{nm\uparrow} c^\dagger_{nm\downarrow} |\rangle = -c^\dagger_{nm\downarrow} c^\dagger_{nm\uparrow} |\rangle$. Because of this convention there is an asymmetric spin dependence in the slave-boson replacement of the operators $c^\dagger_{nm\sigma} = f^\dagger_{nm\sigma} b_{nm0} + \sigma b^\dagger_{nm\uparrow} f_{nm-\sigma}$, in an obvious notation. Here, since $U=\infty$, $c^\dagger_{nm\sigma} = f^\dagger_{nm\sigma} b_{nm0}$ and the Hamiltonian reduces to

$$\mathcal{H} = t \sum_{\substack{n,m,\sigma \\ s,t}}{}' f^\dagger_{nm\sigma} b_{nm0} b^\dagger_{st0} f_{st\sigma} . \tag{1}$$

In the equation of motion method a simple inhomogeneous term results if a new time-ordered Green's function

$$g_{nm}(t) = \langle T_t' [c^\dagger_{nm\sigma}(t) c_{nm\sigma}(0)] \rangle$$

is defined, where

$$T_t' [c^\dagger_{nm\sigma}(t) c_{nm\sigma}(0)] = \begin{cases} \sum_\sigma c^\dagger_{nm\sigma}(t) c_{nm\sigma}(0), & \text{if } t > 0 , \\ -c_{nm\sigma}(0) c^\dagger_{nm\sigma}(t), & \text{if } t < 0 . \end{cases}$$

Since no site is doubly occupied, the number of holes $n_{nm0} = c_{nm\uparrow} c^\dagger_{nm\uparrow} = c_{nm\downarrow} c^\dagger_{nm\downarrow}$. *By design,* it follows that the inhomogeneous term in the equation of motion for $g_{nm}(t)$ is unity. The equation of motion for $c^\dagger_{nm\sigma} = f^\dagger_{nm\sigma} b_{nm0}$,

$$(\epsilon + \mu) f^\dagger_{nm\sigma} b_{nm0} = -t \sum_{st} \left(\sum_{\sigma'} f^\dagger_{nm\sigma} f_{nm\sigma'} f^\dagger_{st\sigma'} b_{st0} + b^\dagger_{nm0} b_{nm0} f^\dagger_{st\sigma} b_{st0} \right) , \tag{2}$$

where μ is the chemical potential. This equation is exact but not useful. A hierarchy of equations is developed until a point is reached where they can be simplified.

Initially, only a certain subclass of terms is retained. Quite generally, sites on the lattice can be designated as being *number* diagonal or not. At a number diagonal site there is a $b^\dagger_{nm0}$ for every b_{nm0} and a $f^\dagger_{nm\sigma}$ for each $f_{nm\sigma'}$. The site is *spin* diagonal if it is number diagonal *and* if it is possible to have $\sigma = \sigma'$ for each $f^\dagger, f$ pair. Because the Hamiltonian conserves particle number, there can only be an odd number of number off-diagonal sites. Retained are terms which have the minimum, i.e., a single, number off-diagonal site. Ignored are the commutators with diagonal sites, i.e., $[f^\dagger_{nm\sigma} f_{nm\sigma} f^\dagger_{st\sigma} b_{st0}, \mathcal{H}] \to f^\dagger_{nm\sigma} f_{nm\sigma} [f^\dagger_{st\sigma} b_{st0}, \mathcal{H}]$. The effect of this latter commutator is to shift the number off-diagonal site from st to one of its neighbors. It follows that such "single-particle" terms can be put in correspondence with walks of a particle on the lattice. It is easy to show that each site on the walk is associated with a matrix,

$$A^{nm}_{\sigma\sigma'} = (f^\dagger_{nm\sigma} f_{nm\sigma'} + \delta_{\sigma\sigma'} b^\dagger_{nm0} b_{nm0}) .$$

Consider first a walk with M steps, *with no back steps;* the corresponding term on the left of the equation of motion, Eq. (2), is

$$t \left(\frac{t}{\epsilon + \mu} \right)^{M-1} (A^{nm} A^{st} \cdots A^{ab} C^{cd})_\sigma ,$$

where the terminating matrix

$$C^{uv}_\sigma = f^\dagger_{uv\sigma} b_{uv0} .$$

Specializing to a Bethe lattice, in order to return to nm, a particle must retrace its original path, i.e., must make back steps. Any walk with a *single* back step, must contain an initial $M+1$ steps which do *not* repeat. The next step returns to the previous site and requires the evaluation of the commutator

$$[A^{ab}_{\sigma\sigma'} C^{cd}_{\sigma'}, \mathcal{H}_{abcd}] = Q_{cd} f^\dagger_{ab\sigma} b_{ab0} = f^\dagger_{ab\sigma} b_{ab0} , \tag{3}$$

where, for the last equality, the constraint, $Q_{cd} = 1$, has been used. This equation represents the crucial step which distinguishes the three different models. For the $qN > 1$ model evaluating the commutator leads to extra terms. For the Anderson model, the commutator is the

same *but* the equivalent of

$$Q_{cd}=\left(\sum_{\sigma} c^{\dagger}_{cd\sigma}c_{cd\sigma}\right)+c_{cd\sigma}c^{\dagger}_{cd\sigma}=1\,,$$

unless the site $cd=0$, is simply the fermion commutation rule $c^{\dagger}_{cd\sigma}c_{cd\sigma}+c_{cd\sigma}c^{\dagger}_{cd\sigma}=1$. Using this in place of the constraint $Q_{cd}=1$ gives an extra term which eventually leads to the usual Kondo divergences. The net result for this walk, for the Hubbard model, is

$$t\left(\frac{t}{\epsilon+\mu}\right)^{M+1}(A^{nm}A^{st}\cdots C^{ab})_{\sigma}\,,$$

which contains the appropriate prefactor for a walk of $M+2$ steps but has *lost* the A matrices for the last two steps. As such a walk continues, each back step can be contracted in this fashion until eventually the walk returns to the beginning site *nm* whence the result for a walk of M *total* steps is simply

$$[t/(\epsilon+\mu)]^{M-1}(C^{ab})_{\sigma}=[t/(\epsilon+\mu)]^{M-1}f^{\dagger}_{nm\sigma}b_{nm0}\,,$$

and so the single-particle result is

$$(\epsilon+\mu)g_{nm}(\epsilon)=1+t\sum_{\text{walks}}\left(\frac{t}{\epsilon+\mu}\right)^{M-1}g_{nm}(\epsilon)\,, \quad (4)$$

where all walks start and end at *nm*. (It is easy to show that there are no additional inhomogeneous terms in this system of equations for the Green's functions.) This is the principal result but is perhaps deceptively simple. It coincides with[4] a certain approximation for the single-hole problem, but represents an extension of those results to the problem with many holes. The significance is essentially negative, i.e., for an approximation which gives Kondo divergences for the Anderson model, there are none for the Hubbard model.

Most of the omitted terms in the equations of motion are zero. A given *step* on the lattice is associated with a hopping term $\mathcal{H}_{nmst\sigma}=tf^{\dagger}_{nm\sigma}b_{nm0}b^{\dagger}_{st0}f_{st\sigma}+\text{H.c.}$ On a Bethe lattice, each $\mathcal{H}_{abcd\sigma}$ must occur in the equations of motion in a different sense an even number of times, and at a given stage a certain $\mathcal{H}_{abcd\sigma}$ can lead to a finite commutator only if at least one of the two site labels has appeared in an earlier commutator (or is *nm*). Taking such a commutator in an order different from that involved in the single-particle term should produce an extra number of off-diagonal sites, in pairs. However, when *both* sites have appeared previously, the relevant commutator is

$$[A^{ab}A^{cd},\mathcal{H}_{abcd\sigma}]=0\,.$$

Finite terms involve commutators in which only *one* of the sites involved has occurred in a previous commutator. The first such term involves n_0 and appears in $O(t^4)$ which is unexpected since, if it were not for the external vertices, on a Bethe lattice, terms which involve the interchange of electrons correspond to "shunting" particles at a node, they require $z\geq 3$ and involve $(n_0)^2$ and $O(t^6)$ (see below). In fact, the $O(t^4)$ term also occurs for $z=2$, i.e., for the one-dimensional problem. It is not difficult to show that these terms are irrelevant and can be made to cancel by a suitable, but involved, redefinition of the Green's function. It follows that the energies determined by the poles of the single-particle Green's function are *exact* in one dimension and correct up to $O(t^6)$ and $(n_0)^2$ for a Bethe lattice.

The single-particle result, Eq. (4), is identical, for a Bethe lattice, to that for the uncorrelated problem, i.e., for $U=0$, when written in terms of the *regular* time-ordered Green's function, for a given spin direction. In the thermodynamic limit

$$g_{nm}(\epsilon)=\frac{1}{\epsilon-[z/(z-1)]\Sigma(\epsilon)}\,,$$

where

$$\Sigma(\epsilon)=\frac{(z-1)t^2}{\epsilon-\Sigma(\epsilon)}\,.$$

The solution, valid for a Bethe lattice for small n_0, is[4]

$$g_{nm\sigma}(\epsilon)=2(z-1)\frac{1}{iz[4(z-1)t^2-\epsilon^2]^{1/2}+(z-2)\epsilon}\,,$$

and corresponds to having band edges at $\pm D$, where $D=2t\sqrt{z-1}$. Near the band edges the density of states $\sim\sqrt{D\pm\epsilon}$.

The regular temperature-ordered Green's function G can be calculated, from the new time-ordered g, using the well-known analytic properties of such Green's functions,

$$G_{nm\sigma}(i\omega_n)=\int_{-\infty}^{\infty}d\omega'[n_0(\omega')+n_{\sigma}(\omega')]\times\frac{1}{i\omega_n-\omega'}\frac{1}{\pi}\,\mathrm{Im}[g_{nm}(\omega'+is)]\,, \quad (5)$$

where the probability that a state of energy ω will be filled by a hole is $n_0(\omega)=[1/(1+2e^{-\beta\omega})]$ and with an electron of spin σ is $n_{\sigma}(\omega)=[e^{-\beta\omega}/(1+2e^{-\beta\omega})]$. Notice the spin degeneracy factor of 2 in the denominators; these are the same statistics as encountered for the chain[5] and follow because the current approximation deliberately fails to couple the kinetic and spin degrees of freedom.

Finally, for the square lattice, the four-step loop term corresponds to

$$t\left(\frac{t}{\epsilon+\mu}\right)^{3}(A^{nm}A^{st}A^{uv}A^{st'})_{\sigma\sigma'}f^{\dagger}_{nm\sigma'}b_{nm0}\,,$$

which cannot be simplified to $f^{\dagger}_{nm\sigma}b_{nm0}$. As with the earlier $O(t^6)$ Bethe term, this implies a spin ground-state dependence to $g_{nm\sigma}(\epsilon)$ which is associated with the, sought for, coupling of the kinetic and spin degrees of freedom. It is found, *for a square lattice*, that the addition of the loop contributions leads to a ferromagnetic coupling between the kinetic energy and the spin degrees of freedom and are favorable to the Nagaoga ground state. On the other hand, the $O(t^6)$ interaction which comes from shunting particles at a node is antiferromagnetic. It follows that for a small enough concentration of holes, the former process dominates and the ground state is ferromagnetic while, for higher concentrations, the latter process takes over and the tendency is towards antiferromagnetic correlations. Trivially, the role of a finite J is also to favor the antiferromagnetic tendency, however there is not a *single* J_c associated with the instability of the Nagaoga state, as often assumed in the analysis of small systems, but rather J_c depends on the concentration of holes.

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