Comment on "Is the π Particle Responsible for the 41 meV Peak in $YBa_2Cu_3O_7$?"

In a recent paper, Greiter [1] claimed erroneously that the π excitation [2] of the Hubbard model has an energy of the order of U. The source of this mistake can be traced both in the strong coupling and weak coupling limits.

The strong coupling limit.—If one inserts a single electron into the Hubbard model less than half filling, its energy can lie within the lower Hubbard band when the electron goes into an empty site. The coherent part of the quasiparticle bandwidth is of the order of J. However, its energy can also lie within the upper Hubbard band when it goes into a site already occupied by another electron. Very similar arguments go through for the π particle. It consists of a pair of electrons in a spin triplet state. Because of the spin triplet nature, the mutual interaction among the inserted pair of electrons can only be of the order of J. If both electrons go into empty sites, there is a finite spectral weight at low energy of the order of J. On the other hand, one or both of the inserted electrons can go into sites already occupied by other electrons. In this case, the energy of the π pair will be of the order of U and $2U$, respectively. Therefore, while the spectral function of a single electron Green's function decomposes into the lower quasi-particle-like band, the spectral function of the π pair should consist of three bands in the strong coupling limit, a low energy peak of the order J, and two higher energy peaks centered around U and $2U$. The spectral weight of the low energy peak is proportional to doping x, which is a rough estimate of the number of unoccupied sites. Exact diagonalization studies of the Hubbard clusters verify the above picture for all dopings away from half filling: The low energy π resonance peak scales *inversely* with U in the large U limit, and its spectral weight scale with x [3].

Greiter may have confused the *mean energy* of the π particle with the *spectral distribution* of the π peaks. In comparing with the resonant neutron scattering experiment in YBCO, one is only interested in the *low energy* portion of the π peaks. In computing the contribution of the π peak to the dynamic spin correlation function, one has to *divide* the normalization factor coming from the low energy portion of the π spectral weight [2]. This leads to the prediction that the resonant neutron scattering peak scales *inversely* with x. This prediction has been recently verified in underdoped YBCO [4].

The weak coupling limit.—Greiter used our calculation of the commutator between the Hamiltonian and the π operator in his equation (4). The leading U term in this commutator is a four electron operator, *only within the Hartree-Fock approximation this term reduces to a two electron operator expressed in (4).* It is imperative to point out that the bulk of Greiter's argument relies on this *approximate* equation, therefore, one is forced to discuss Hartree-Fock approximation consistently. Greiter seems to have overlooked the important fact that if one applied the same approximation to the one electron operator rather than the π operator, one finds a shift of the chemical potential due to the U interaction, $\delta\mu = Un_\downarrow$. This shift in chemical potential exactly cancels the leading order U term in Eq. (4).

The physical origin of this cancellation is obvious. In the resonant neutron scattering experiment, there is no net change in the total number of particles. Therefore, when one talks about a two particle intermediate state, one has to measure its energy with respect to the energy of inserting two separate electrons. Within the Hartree-Fock approximation, the interaction between an inserted electron and the background electrons is treated on average, leading to the term $\delta\mu = Un_\downarrow$. But it is clear that this argument applies to a single inserted electron as well as—within Hartree-Fock—to two inserted electrons, which is the physical origin of their cancellation when one measures the relative energies.

Greiter also commented on our interpretation of the numerical results. Close to half filling, where there is considerable pairing fluctuations on a finite sized system, there is indeed an ambiguity on whether the spin peak is due to π peak or the other way around. However, it is extremely important to point out that the π peak has been observed in our exact diagonalizations for *all densities* away from half filling where this ambiguity does not exist. Therefore, the π peak is a genuine collective mode. He also commented on the effect of the Gutzwiller projection on the approximate SO(5) symmetry [5]. We would like to point out that SO(5) multiplet patterns have recently been observed on 18 site t-J clusters [6] where the projection is incorporated *exactly.*

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