Ground State of the Attractive-U Hubbard Model

In a recent Letter [1] Singh and Scalettar showed that the η pairing proposed by Yang [2] for the attractive-U Hubbard model corresponds to the Nagaoka ferromagnetic phase [3] of the repulsive-U Hubbard Hamiltonian. Using the well-known mapping between the positive- and negative-U cases, they showed that the ground state of the attractive model with large U and $N_\uparrow - N_\downarrow > 0$, where $N_\uparrow$ and $N_\downarrow$ are the occupation numbers of the up and down spins, respectively, has off-diagonal long-range order (ODLRO). In contrast to the usual case the pair field order parameter is staggered corresponding to pairing with momentum $\mathbf{Q}=(\pi,\ldots)$. They also discussed the possibility of coexisting superconductivity and phase separation where the electron density becomes inhomogeneous.

In this Comment we wish to clarify some points which in fact highlight the richness of the problem.

First, we recall that in the case of the positive-U Hubbard Hamiltonian the Nagaoka theorem states that for strictly infinite U and one hole the ground state is ferromagnetic. If we make use of this theorem to learn about the properties of the negative-U case we conclude that the ground state of the attractive model in the *infinite-U* limit with an *odd* number of particles has ODLRO with a symmetry corresponding to $\mathbf{Q}=(\pi,\ldots)$. This statement was shown in Ref. [4]. To extrapolate this result to the case of finite U and states with $N_\uparrow - N_\downarrow > 1$ is quite dangerous. As we discussed in detail [4], the state of an odd number of particles $(2M+1)$ and large U corresponds to a state with an unpaired electron and M pairs which can be thought of as hard-core bosons. If U is noninfinite the unpaired electron will tend to produce in its neighborhood a domain with a local symmetry corresponding to $\mathbf{Q}=(\pi,\ldots)$ leaving unchanged the rest of the system with an order parameter corresponding to a symmetry $\mathbf{Q}=(0,\ldots)$. This produces an excitation which is the analog to the spin polaron. For a two-dimensional system the radius of the bag produced by the unpaired electron in a system with density n is $R=[U/4tn(2-n)]^{1/4}$. This type of excitation could be of relevance in the context of superconductivity in systems with very short coherence length.

As a second point, we want to refer to the possibility of phase separation. The mapping between the attractive- and repulsive-U models shows that the z component of the magnetization (M_z) in the repulsive case is related to the number of particles (N) in the attractive case. To study the attractive case with a given number of particles we could make use of the known solutions of the repulsive case with a given M_z. Although in the $U>0$ case the Nagaoka state has the full rotational symmetry, only one state with the proper M_z corresponds to the state with the desired particle density for the $U<0$ model. This state is homogeneous. This can be easily seen by generating it with successive application of the operator S^- to the state of maximum M_z.

The state with charge segregation in the attractive model corresponds to the ferromagnetic state in the positive-U representation with the magnetization along the z axis. In order to have the proper M_z one has to generate a Bloch wall, the region with $M_z>0$ $(M_z<0)$ corresponding to a high (low) electron density. This state, however, is not an eigenstate of the Hamiltonian even for infinite U if $N_\uparrow - N_\downarrow \neq 0$. If N is odd the composite bosons, corresponding to the strongly bound electron pairs, acquire a finite mass due to the presence of the unpaired electron and the ground state is homogeneous.

To conclude, although we find interesting the results which clearly indicate the existence of ODLRO in a nontrivial interacting electron model and its relation with the η pairing, we stress that (i) the analog of the Nagaoka ferromagnetic state is a state with a single unpaired electron. If U is finite the unpaired particle is dressed by superconducting fluctuations in analogy with the spin polaron of the positive-U model. Only if the radius R of the polaron is large compared with the characteristic dimensions of the sample, will the ground state of the system correspond to the Nagaoka state. (ii) The ground state for $N_\uparrow - N_\downarrow = 1$ is *homogeneous* and the segregated phase probably does not occur in this type of model.

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[1] R. R. P. Singh and R. T. Scalettar, Phys. Rev. Lett. **66**, 3203 (1991).
[2] C. N. Yang, Phys. Rev. Lett. **63**, 2144 (1989).
[3] Y. Nagaoka, Phys. Rev. **147**, 392 (1966).
[4] A. G. Rojo, J. O. Sofo, and C. A. Balseiro, Phys. Rev. B **42**, 10241 (1990); K. Hallberg, A. G. Rojo, and C. A. Balseiro, *ibid.* **43**, 8005 (1991).