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Constraints on s-wave pairing in the Hubbard model

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We present an exact identity between the on-site and the extended s-wave pairing amplitudes in the Hubbard model. We prove that the extended s-wave pairing amplitude vanishes identically at half filling for both signs of U. Away from half filling, the existence of an on-site s-wave pairing is a necessary and sufficient condition for the existence of an extended s-wave pairing. This result gives rise to constraints on the possible symmetries of the superconducting gap in the Hubbard model.

Ever since the discovery of high-T_c superconductivity, most theoretical approaches have focused on the Hubbard model. Theorists are fascinated by the simplicity of the model and the complexity of the phases that emerge from it. However, understanding the physics of strongly correlated systems has always been a major theoretical challenge. Many approximation schemes have been developed to treat the Hubbard model, including weak-coupling random-phase approximations (RPA's), mean-field theories, variational approaches, and numerical simulations. However, because of the intrinsic complexity of the correlations, no universally accepted results have emerged, despite these intense efforts.

In view of this, it is desirable to develop some exact results which may yield powerful constraints on the different approximation schemes. While physically interesting correlation functions are generally difficult to calculate from first principle, exact identities between them can be derived without ever solving the model. The Ward identity is an excellent example of this approach. In the following, we shall present an exact identity between the on-site and the extended s-wave pairing amplitudes in the Hubbard model and discuss various implications that result from it.

Consider the Hubbard model given by the Hamiltonian

$$H=-t\sum_{\langle r,r'\rangle;\sigma}(c^\dagger_{r,\sigma}c_{r',\sigma}+\text{H.c.})+U\sum_r n_{r\uparrow}n_{r\downarrow}-\mu\sum_{r,\sigma}n_{r,\sigma}\,. \tag{1}$$

In the domain of strong couplings, Cooper pairs are expected to have sizes comparable to the lattice spacing. In the s-wave channel, one generally considers two possibilities, the on-site s-wave pairing, described by the operator

$$\Delta_r=c_{r\uparrow}c_{r\downarrow}\,, \tag{2}$$

and the extended s-wave pairing, described by the operator

$$\tilde{\Delta}_r=\sum_\delta(c_{r\uparrow}c_{r+\delta\downarrow}-c_{r\downarrow}c_{r+\delta\uparrow})\,, \tag{3}$$

where δ runs over nearest-neighbor bonds. The time evolution of the on-site pairing operator Δ_r is given by the Heisenberg equation of motion:

$$-i\frac{d\Delta_r}{dt}=[H,\Delta_r]=t\tilde{\Delta}_r-U\Delta_r+2\mu\Delta_r\,. \tag{4}$$

Equation (4) is a striking identity unique to the one-band Hubbard model. Generally, the commutator of a potential-energy term with a bilinear fermion operator gives a term quartic in fermion operators. In this case, however, since the Hubbard interaction acts only on site, the resulting quartic term actually reduces to a quadratic term since operators like $c^\dagger_{r\uparrow}c_{r\uparrow}c_{r\uparrow}c_{r\downarrow}$ have to vanish because of Fermi statistics. (This important observation was first made by Yang[1] in his construction of some exact eigenstates of the Hubbard model.) Therefore, *the equation of motion for the on-site pairing operator Δ_r closes at the two-particle level.* For any equilibrium state described by a time-independent density matrix ρ with $[\rho,H]=0$, one obtains from (4) that

$$\langle\tilde{\Delta}_r\rangle=f\langle\Delta_r\rangle,\ f=\frac{U-2\mu}{t}\,, \tag{5}$$

where $\langle A\rangle=\text{Tr}\rho A$ and $d\langle\Delta_r\rangle/dt=d[\text{Tr}\rho(t)\Delta_r]/dt=0$. For a state without spontaneous symmetry breaking, i.e. $[\rho,N_e]=0$, where N_e is the total number of the electrons, (5) is trivially satisfied since both sides vanish. In this case (5) should be replaced by a similar identity between the (off-diagonal long-range order) ODLRO correlation functions. We shall return to this case later. However, in the case where the symmetry is spontaneously broken, i.e. $[\rho,N_e]\neq0$, Eq. (5) states a nontrivial result relating the on-site and the extended s-wave pairing amplitudes. Note that (5) is an *exact* identity for the Hubbard model, valid for all dimensions, filling factors, and both signs of U.

Let us now consider some special cases of physical interest. Because of the particle-hole symmetry of the Hubbard model, the ground-state energy E_0 in the less than half-filled case is related to that in the more than half-filled case by the exact identity $E_0(N_e)=(N_e-N)U+E_0(2N-N_e)$, where N is the number of lattice sites. The chemical potentials in both cases are thus related by

$$\mu(N_e)=U-\mu(2N-N_e)\,. \tag{6}$$

Therefore, without loss of generality, we shall restrict ourselves to the cases of half and less than half filling in the following discussions, since $f(N_e)=-f(2N-N_e)$ from (6).

At half filling, $N_e=N$, thus $\mu=U/2$ from (6). We see that this is a special point at which $f=0$ or $\langle\tilde{\Delta}_r\rangle=0$. Therefore, *the extended s-wave pairing amplitude van-*

ishes identically at half filling both for the positive- and the negative-U Hubbard model. This is not a surprising result for the positive-U Hubbard model, since it is commonly believed that the ground state is Néel ordered. In fact, the absence of the ODLRO in the on-site s-wave pairing operators has been proven rigorously in the case,[2] i.e., $\langle\Delta_r\rangle=0$. Together with our result, the absence of both the on-site and the extended s-wave pairing in the half-filled positive-U Hubbard model is now established. For the negative-U Hubbard model, one generally expects pairing to be possible. However, (5) still implies that $\langle\tilde{\Delta}_r\rangle=0$ at half filling whereas $\langle\Delta_r\rangle\neq0$ is possible. While there are many ways to understand this less intuitive result, all based on the commensurability effect at half filling, a particularly instructive one is to consider the duality transformation[3] $c_{r\uparrow}\rightarrow(-1)^r d_{r\uparrow}^\dagger$ and $c_{r\downarrow}\rightarrow d_{r\downarrow}$ which at half filling exactly maps the negative-U Hubbard model to the positive-U Hubbard model. [$(-1)^r$ is 1 on the even sublattice and -1 on the odd sublattice.] Under this duality transformation, the on-site pairing operator Δ_r is mapped onto the spin-density wave (SDW) order parameter $S_r^\dagger=(-1)^r d_{r\uparrow}^\dagger d_{r\downarrow}$ which is nonvanishing in the Néel-like ground state, whereas the extended s-wave pairing order parameter $\langle\tilde{\Delta}_r\rangle$ is mapped onto

$$(-1)^r\sum_\delta\langle d_{r\uparrow}^\dagger d_{r+\delta\downarrow}+d_{r\downarrow}d_{r+\delta\uparrow}^\dagger\rangle\propto\frac{1}{N}\sum_{p,\delta}\cos(p\delta)\langle d_{p+Q\uparrow}^\dagger d_{p\downarrow}\rangle\,,$$

$$Q=(\pi,\pi,\dots)\,,$$

which vanishes due to the commensurability of the SDW with the underlying lattice, i.e., $S_p\equiv\langle d_{p+Q\uparrow}^\dagger d_{p\downarrow}\rangle=S_{p+Q}$. Physically, the Néel state in the positive-U Hubbard model corresponds to a pairing state in the negative-U Hubbard model in which all the even sublattice sites are doubly occupied and all the odd sublattice sites are empty. It is clear that $\langle\tilde{\Delta}_r\rangle$ vanishes in this situation.

Now let us proceed to the less than half-filled case. In this case, $f\neq0$ since $\mu\neq U/2$ and we conclude that *the extended s-wave pairing is possible if and only if the on-site s-wave pairing is possible.* To get some feeling about the order of magnitude of the ratio f, let us consider some special cases. For both signs of U, but with $|U|\ll t$, μ is of the order of t, therefore, $f\sim O(1)$ to the leading order. For large and positive U ($U\gg t$), μ is also of the order of t and $f\sim O(U/t)$ to the leading order. Finally, for large and negative U, the electrons are paired, μ is therefore given by $U/2$ to the leading order plus a correction of the order of $J\sim t^2/U$ due to the second-order hopping process of the paired electrons. Thus we have $f\sim O(t/U)$ in this case. Physically, the different leading behavior of f in the large-U limit is simple to understand. In the repulsive case, the wave function is pushed outwards whereas in the attractive case, it is pulled inwards.

Let us consider some theoretical implications of the above analysis. For the positive-U Hubbard model, it is generally believed that the on-site s-wave pairing is suppressed. This is strongly suggested by the numerical evidence based on Monte Carlo simulations[4] and variational studies.[5] This is to be expected since a state where electrons are paired on the same site would cost more potential energy than the free-fermion state due to the on-site Hubbard repulsion, and it certainly costs more kinetic energy since this is minimized by the free-fermion state. Therefore, many are led to consider extended s-wave[6] and d-wave pairing[7,8] or an appropriate mixture of the two.[9] In these cases, the pairing wave functions vanish when the electrons are on the same site, thus the on-site Hubbard repulsion is naturally avoided. However, our conclusion provides a strong constraint on these approaches since we proved that away from half filling, $f\neq0$, *the suppression of the on-site s-wave pairing therefore automatically enforces the suppression of the extended s-wave pairing.* This conclusion is consistent with the numerical results[4,5] in which one finds suppression of the extended s-wave pairing as well as the on-site s-wave pairing, whereas the d-wave pairing is slightly enhanced.

Finally, we consider the pairing identity for a finite system. In this case, spontaneous symmetry breaking is absent, and a nontrivial relation can be obtained if one studies the ODLRO correlation functions rather than the order parameters themselves. Let us define the general spectral functions associated with the dynamic Cooper susceptibilities

$$S(r,r';\omega)=\sum_n\langle0|\Delta_r|n\rangle\langle n|\Delta_{r'}^\dagger|0\rangle\delta(\omega-E_n+E_0) \tag{7}$$

and similarly

$$\tilde{S}(r,r';\omega)=\sum_n\langle0|\tilde{\Delta}_r|n\rangle\langle n|\tilde{\Delta}_{r'}^\dagger|0\rangle\delta(\omega-E_n+E_0)\,, \tag{8}$$

where $|0\rangle$ is the exact ground state with N_e electrons and $|n\rangle$ are the exact eigenstates with N_e+2 electrons. E_0 and E_n are respectively the energies of these eigenstates. The matrix elements of Δ_r and $\tilde{\Delta}_r$ are related through (4) by

$$\begin{aligned}(E_0-E_n)\langle0|\Delta_r|n\rangle=t\langle0|\tilde{\Delta}_r|n\rangle-U\langle0|\Delta_r|n\rangle\\+2\mu\langle0|\Delta_r|n\rangle\,.\end{aligned} \tag{9}$$

This relation implies that the various frequency moments of the spectral functions

$$\begin{aligned}S_n(r,r')&=\int d\omega\,\omega^n S(r,r';\omega)\,,\\ \tilde{S}_n(r,r')&=\int d\omega\,\omega^n\tilde{S}(r,r';\omega)\end{aligned} \tag{10}$$

are related by the following exact identity

$$\begin{aligned}\tilde{S}_0(r,r')=\frac{(U-2\mu)^2}{t^2}S_0(r,r')+\frac{2(U-2\mu)}{t^2}S_1(r,r')\\+\frac{1}{t^2}S_2(r,r')\,.\end{aligned} \tag{11}$$

Note that the zeroth-frequency moment is nothing but the static ODLRO correlation function, whose long-distance property characterizes the superconducting behavior.

In conclusion, we have found an exact identity between the on-site and the extended s-wave pairing amplitudes in the Hubbard model which is valid for all dimensions, filling factors, and both signs of U. At half filling, the extended s-wave pairing amplitudes vanish identically. Off of half filling, the on-site and the extended s-wave pairing amplitudes are proportionally related. While a rigorous proof is still lacking, the absence of the on-site s-wave pairing is plausible for the positive-U Hubbard model. Accepting this, one would conclude that the extended s-wave pairing is equally unlikely.

Experiments on the high-T_c superconductors strongly indicate that the Cooper pairs formed below the transition temperature are a spin singlet and there are no nodes of the superconducting gap over the Fermi surface. These facts are conventionally interpreted as the signature of the s-wave symmetry of the superconducting gap. Following our preceding analysis, this evidence seems to disfavor the positive-U Hubbard model as a model for the high-T_c superconductivity. However, other interpretations of the experiments are still possible. In a doped antiferromagnet, holes may form pockets in the magnetic zone boundary; in such a case, the superconducting gap can have a d-wave symmetry even though there are no nodes over the Fermi surface.[8] This case can only be distinguished from a conventional s-wave gap by experiments which not only measure the absolute value but also the phase of the superconducting gap.

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