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Collective excitations and the crossover from Cooper pairs to composite bosons in the attractive Hubbard model

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Motivated by the short coherence length of the high-temperature superconductors, we study in the negative-U Hubbard model the crossover from Cooper pairs for $U \ll t$ to composite bosons for $U \gg t$. We compute the collective-mode spectrum using a generalized random-phase-approximation analysis within the equations-of-motion formalism. We find a smooth evolution of the Anderson mode for weak coupling into the Bogoliubov sound mode for hard-core bosons.

One of the most striking characteristics of the superconducting cuprates,[1] in addition to their high transition temperatures, is their short coherence length. If one interprets the coherence length as a pair size one concludes that the number of fermions within a pair is rather small, in contrast to the standard BCS theory where the pairs are strongly overlapping. Following early work[2] on helium-3, and on excitonic condensates,[3] it is tempting to propose[4] that the high-T_c superconductors are in an interesting intermediate regime between the weak-coupling Cooper-pair limit, and the strong-coupling limit of tightly bound composite bosons. The normal-state experiments clearly show that the cuprates are, in fact, closer to the former limit than to the latter. However, the puzzling anomalies[5] of the normal state also suggest some deviation from the canonical Fermi-liquid state.

In this paper, we study the attractive (negative-U) Hubbard model. This is the simplest lattice model to display a crossover from BCS-like to Bose superconductivity as a function of the coupling U/t. In addition, it may also be relevant as a microscopic model for the bismuthates.[6] The analysis of the ground-state crossover in this,[3] and related[2,4,7] models has been done at the mean-field level (see below). While sufficient to establish the smooth evolution of the ground state and the single-particle excitations from weak to strong coupling, such an analysis cannot, for example, describe the important excitations in the $(U \gg t)$ composite-boson limit. The important excitations in weak coupling involve broken pairs; with increasing U/t these are pushed to very high energies. In the Bose limit the important excitations are the collective sound modes which, in terms of the constituent fermions, are bound pairs with a finite center-of-mass momentum. The collective modes in a Bose system depend in an essential way upon the interaction between the bosons, thus it is interesting to ask how they emerge from the analysis of the interacting Fermi system. Further, a satisfactory understanding of the intermediate regime at finite temperatures does not exist at the present time, and an analysis of the collective modes is a necessary first step in that direction.

Here we study the collective mode spectrum at $T=0$ using a generalized random-phase-approximation (RPA) formulation. We adapt the analysis of Anderson and others,[8] initially applied to weak-coupling superconductivity, and show that with some modifications it is capable of describing the evolution of the collective mode for *all* values of U/t. While one might not expect the RPA to be valid in the strong-coupling limit, we find that we recover the well-known Bogoliubov result[9] for the sound velocity of a repulsive Bose gas in the $U \gg t$ limit. We find a smooth evolution of the collective-mode spectrum in both two and three dimensions. We also generalize our results to the charged case. The details of the rather lengthy analysis will be presented elsewhere.[10]

While the RPA has been implemented in a variety of ways to study collective excitations above the superconducting ground state, we have used the linearized equations of motion method[8,11] since this has a certain intuitive appeal.

Our starting point is the attractive Hubbard Hamiltonian in d dimensions written in momentum space

$$H=\sum_{k,\sigma}(\varepsilon_k-\mu)c^\dagger_{k\sigma}c_{k\sigma}-\frac{U}{M}\sum_{kk'q}c^\dagger_{k+q\uparrow}c^\dagger_{k'-q\downarrow}c_{k'\downarrow}c_{k\uparrow}, \quad (1)$$

where $\varepsilon_k=-2t\sum_{i=1}^{d}\cos(k_i a)$. The chemical potential μ controls the band filling $f=N/2M$, where N is the average number of electrons and M the total number of sites. We will study the model at $T=0$ for arbitrary $U/t>0$ and $0\le f<\frac{1}{2}$; we stay away from half-filling where there is a competition between superconductivity and charge-density wave ordering.[12]

To establish notation, we quickly review the mean-field analysis. Recall that the BCS reduced Hamiltonian $H_{\rm BCS}$ is that part of (1) which describes the interaction between pairs with $k'=-k$. The BCS-Bogoliubov solution consists of determining the eigenoperators $\gamma^\dagger_{k\sigma}$ and $\gamma_{k\sigma}$ of $H_{\rm BCS}$. These operators define both the BCS ground state, via $\gamma_{k\sigma}|\Phi_0\rangle=0$, and the single-particle excitations $\gamma^\dagger_{k\sigma}|\Phi_0\rangle$ with energy E_k.

The first step is a linearization of the equations of motion for $c_{k\sigma}$ and $c^\dagger_{k\sigma}$ with respect to $|\Phi_0\rangle$ where $\langle c^\dagger_{k\sigma}c_{k\sigma}\rangle$ and $\langle c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}\rangle$ are nonvanishing. The Hartree shift in the chemical potential $\tilde{\mu}=\mu+fU$ is usually ignored; however, for large U it must be retained.

The second step is to diagonalize the linearized equations via the Bogoliubov transformation: $c_{k\uparrow}=u_k\gamma_{k0}+v_k\gamma^{\dagger}_{k1}$ and $c^{\dagger}_{-k\downarrow}=-v_k\gamma_{k0}+u_k\gamma^{\dagger}_{k1}$, with $u_k^2=1-v_k^2=\frac{1}{2}(1+\xi_k/E_k)$. Here $\xi_k=\varepsilon_k-\tilde{\mu}$, and the gap and the quasiparticle excitation energy are given by $\Delta=U\sum_k u_k v_k$, and $E_k=(\xi_k^2+\Delta^2)^{1/2}$, respectively.

Self-consistency is achieved by demanding that, for each value of the coupling U/t and filling f, Δ and the chemical potential $\tilde{\mu}$ satisfy the gap equation

$$1=\frac{U}{2M}\sum_k\frac{1}{(\xi_k^2+\Delta^2)^{1/2}} \tag{2}$$

and the number equation

$$f=\frac{1}{2M}\sum_k\left[1-\frac{\xi_k}{(\xi_k^2+\Delta^2)^{1/2}}\right]. \tag{3}$$

These equations may be analytically solved in the weak- and strong-coupling limits. [In the continuum limit in two dimensions an exact analytical solution is possible for all couplings.[4]] For $U/t\ll 1$ the chemical potential is at ε_F, the gap shows a characteristic essential singularity, and the pair size is much larger than the lattice spacing, as expected of a BCS ground state. In the opposite limit of $U/t\gg 1$, the pairs are on site, the chemical potential is one-half the pair binding energy, and the ground state is a condensate of composite bosons. There is a smooth crossover between these rather different limits, as can be seen by a numerical solution of (2) and (3). Figure 1(a) and 1(b) shows Δ and μ as a function of U for various fillings f in two dimensions; for the three-dimensional (3D) case, see Ref. 3. There is a gap to single-particle excitations $E_{\rm gap}=\Delta$ provided $\tilde{\mu}$ lies within the band. However, $E_{\rm gap}=(\tilde{\mu}^2+\Delta^2)^{1/2}$ once $\tilde{\mu}$ is below the bottom of the band.[2,4]

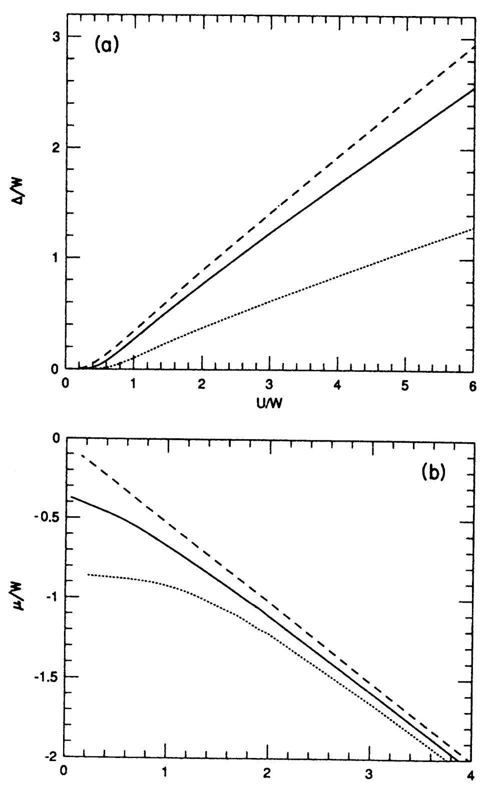

FIG. 1. (a) The order parameter Δ and (b) the chemical potential μ, as functions of the coupling U for two dimensions. All energies are plotted in units of the half-bandwidth $W=4t$. The dashed, solid, and dotted lines correspond to filling factors $f=0.45$, 0.25, and 0.05, respectively.

The (unnormalized) BCS ground state can be written as $|\Phi_0\rangle=(\sum_k\phi_k c^{\dagger}_{k\uparrow}c^{\dagger}_{-k\downarrow})^{N/2}|\text{vac}\rangle$, with $\phi_k=v_k/u_k$, which emphasizes the analogy with Bose condensation. Variationally, the mean-field solution corresponds to an optimal choice of the internal pair wave function ϕ. We thus see how, even in the strong-coupling limit where ϕ represents an on-site singlet, a BCS-like analysis is able to describe a condensate of composite bosons.

To determine the collective mode spectrum we study the time evolution of density fluctuations $c^{\dagger}_{k+q\sigma}c_{k\sigma}$. Its equation of motion is coupled to that of pairs with a finite center-of-mass momentum $c^{\dagger}_{k+q\uparrow}c^{\dagger}_{-k\downarrow}$ and $c_{-k-q\downarrow}c_{k\uparrow}$, resulting from the particle-hole mixing due to the condensate.

The overall strategy of the RPA is simple. As in the analysis sketched above, the first step is to linearize the equations of motion with respect to the mean-field ground state, and the second to diagonalize them by finding the appropriate eigenoperators for the collective coordinates. At the mean-field level one has diagonalized only the $H_{\rm BCS}$ part of the full Hamiltonian $H=H_{\rm BCS}+H_{\rm int}$. At the RPA level we treat the small fluctuations introduced by $H_{\rm int}$ which describes the interaction between the Bogoliubov quasiparticles.

The actual implementation of this idea is algebraically messy. We follow the very clear presentation of Bardasis and Schrieffer,[13] adapt it to the lattice model, and retain terms which allow us to work at arbitrary U; for details, see Ref. 10. Instead of working with bilinear products of c and $c^{\dagger}$, it is convenient to consider the time evolution of $\gamma^{\dagger}_{k+q,\sigma}\gamma_{k,\sigma}$, $\gamma^{\dagger}_{k+q,0}\gamma^{\dagger}_{k,1}$, and $\gamma_{k+q,1}\gamma_{k,0}$, leading to the Anderson-Rickayzen equations of motions. The eigenoperators are found as linear combinations of the above operators by diagonalizing the equations. These define as usual both the "renormalized" ground state (which differs from $|\Phi_0\rangle$ through the inclusion of the zero-point collective oscillations) and the excited states.

To determine the collective excitation spectrum $\omega(q)$ we take the matrix elements of the equations of motion between the ground state, and a state containing exactly one quantum of excitation. We thus obtain the secular equation

$$\begin{vmatrix} [1+UI_{E,n,n}(q)] & UI_{\omega,n,l}(q) & 2UI_{E,n,m}(q) \\ UI_{E,n,m}(q) & [1+UI_{E,l,l}(q)] & 2UI_{\omega,l,m}(q) \\ (U/2)I_{E,m,n}(q) & (U/2)I_{\omega,m,l}(q) & [1+UI_{E,m,m}(q)] \end{vmatrix}=0 \tag{4}$$

with

$$I_{a,b,c}(q)=\frac{1}{M}\sum_k\frac{a(k,q)b(k,q)c(k,q)}{\omega(q)^2-E_{k,q}^2}. \tag{5}$$

Here a, b, c denote any one of the following quantities: the excitation energy $\omega(q)$, or the quasiparticle energy $E_{k,q}=E_{k+q}+E_k$, or the coherence factors $l(k,q)=u_k u_{k+q}+v_k v_{k+q}$, $m(k,q)=u_k v_{k+q}+v_k u_{k+q}$, and $n(k,q)=u_k u_{k+q}-v_k v_{k+q}$.

We will first analytically solve the above equations in the weak- and strong-coupling limits, where we can compare our answers with known results, and then give a numerical solution which interpolates between the two limits. We restrict attention to the long-wavelength $q\rightarrow 0$ regime.

In weak coupling Δ is exponentially small and $\tilde{\mu}$ tends to the Fermi energy ε_F. The integrals (5) are then peaked at ε_F. For $q=0$, the products of coherence factors $n(k,q)l(k,q)$ and $n(k,q)m(k,q)$ are odd under change of sign of ξ_k, which leads to vanishing integrals for $I_{\omega,n,l}$ and $I_{E,n,m}$. As a result we are left with a 2×2 determinant to solve. The small q and ω expansion of the various terms in (4) is conveniently written in terms of four quantities: $x=\sum_k E_k^{-3}$, $y=\sum_k(\nabla_k\xi)^2/E_k^3$, $w=\sum_k \xi\nabla_k^2\xi/E_k^3$, and $z=\Delta^2\sum_k(\nabla_k\xi)^2/E_k^5$. The dispersion relation of the collective mode is then found to be

$$\omega(q)=[(1-U\Delta^2 x/2)(3z+w-y)/dx]^{1/2}q\,. \quad (6)$$

The sums over k are peaked about ε_F and may be estimated by integrals over a thin shell of thickness $2\omega_c$, such that $\Delta\ll\omega_c\ll W=2dt$, centered around ε_F. We then find $x=2N(0)/\Delta^2$, $y=2N_v(0)/\Delta^2$, $w=-2a^2N(0)\times\log(2\omega_c/\Delta)$, and $z=4N_v(0)/3\Delta^2$, where the density of states

$$N(\xi)=(2\pi)^{-d}\int d^dk\,\delta(\xi_k-\xi)$$

and

$$N_v(\xi)=(2\pi)^{-d}\int d^dk\,(\nabla_k\xi_k)^2\delta(\xi_k-\xi)\,.$$

The only dependence on the (arbitrary) cutoff ω_c is in w, which, however, is negligible compared to the other terms in (6) in the weak-coupling limit where Δ is small. Substituting these results in (6) we obtain

$$\omega(q)=[\langle v_F^2\rangle/d]^{1/2}[1-UN(0)]^{1/2}q\,, \quad (7)$$

where the mean-squared Fermi velocity is defined by $\langle v_F^2\rangle=N_v(0)/N(0)$.

The filling dependence of this result comes from the fact that $\langle v_F^2\rangle$ depends upon the band structure. In general the f dependence is smooth except for the following cases. In the 3D case there is a sharp dip in the collective mode speed of sound at $f=0.215$ due to a van Hove singularity. In the 2D case the speed of sound goes to zero as $f\rightarrow\frac{1}{2}$ due to the nesting at half-filling.

In the continuum limit, with a parabolic dispersion, $(\langle v_F^2\rangle)^{1/2}=p_F/m$ and (7) reduces to Anderson's weak-coupling result.[8] The collective mode in weak coupling is essentially the same for the lattice and continuum models, as one might expect since the size of the bound pairs ξ_0 is much larger than the lattice spacing a.

In the strong-coupling limit the fermions bind into on-site singlet pairs, and the attractive Hubbard model can be mapped onto a system of hard-core bosons described by

$$H_{\text{Bose}}=(2t^2/U)\sum_{i,j}(n_i n_j-b_i^\dagger b_j)\,.$$

The composite bosons move only via virtual ionization and their effective hopping amplitude is $t_b=2t^2/U$. The hard-core constraint is due to the Pauli principle for the constituent fermions, and in addition the bosons interact with a nearest-neighbor repulsion $V=2t^2/U$. In the long-wavelength limit, the collective excitation of a dilute $(n_b a_s^3\ll 1)$ 3D Bose gas is the Bogoliubov sound mode[9] with dispersion $\omega=(4\pi n a_s/m_b^2)^{1/2}q$. Here the density of bosons $n_b=f/a^3$, the scattering length a_s is of the order of the lattice spacing a, and the effective mass $m_b\simeq 1/t_b a^2=U/2t^2a^2$.

We now show that one obtains the same result from strong-coupling limit of our RPA result (4). Using the gap and the number equations, (2) and (3), we find $\Delta=U[f(1-f)]^{1/2}(1-da^2)$ and $\tilde{\mu}=U(2f-1)(1+2da^2)/2$, to leading order in $a=2t/U\ll 1$. A similar expansion of the various quantities in (4), with the further simplification of the dilute limit $f\ll 1$, yields: $1+UI_{E,n,n}=4f(1+4da^2)$, $1+UI_{E,m,m}=1-16fda^2$, $UI_{E,n,m}=-2f^{1/2}(1+da^2)$, $UI_{\omega,n,l}=-\omega(1+2da^2)/U$, and $UI_{\omega,m,l}=2\omega f^{1/2}$

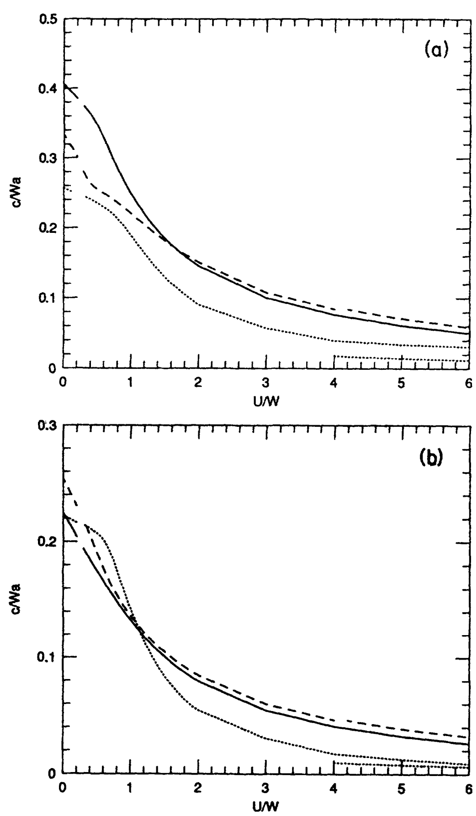

FIG. 2. Collective mode velocity as a function of coupling U for various fillings in (a) two and (b) three dimensions. $W=2dt$ is half the bandwidth, d the dimensionality, and a the lattice spacing. The dashed, solid, and dotted lines correspond to $f=0.45$, 0.25, and 0.05, respectively. The fourth curve in strong coupling is the analytical result for $f\ll 1$. See text for discussion of analytical results in the small and large U limits.

$\times(-1+7da^2)/U$. We also find, independent of the filling, $1+UI_{E,l,l}=a^2q^2a^2/2-\omega^2/U^2$. We thus obtain, for $f \ll 1$ and $U/t \gg 1$,

$$\omega(q)=\sqrt{4df}\,(4t^2a/U)q\,. \tag{8}$$

This result is clearly the same, up to an overall factor of order unity, as that expected for the dilute Bose gas. Quite remarkably, starting with interacting fermions and using RPA we were able to reach the regime of hard-core bosons in the strong-coupling limit. This suggests that RPA offers a reasonable interpolation scheme in the intermediate-coupling regime.

For intermediate couplings we have numerically solved the RPA equation (4) as a function of the coupling U/t, and for various fillings $f=0.05$, 0.25, and 0.45. As input to these equations we have used the numerical solutions for Δ and $\tilde{\mu}$ obtained from the mean-field gap and number equations, (2) and (3). To evaluate the k sums in (4) we numerically evaluated the density of states $N(\xi)$ and the function $N_v(\xi)$ in three dimensions; in two dimensions exact expressions for these in terms of complete elliptic integrals were used.

The collective mode velocity c is plotted in Fig. 2(a) (2D case) and Figs. 2(b) (3D case) as a function of the coupling. We see that the numerical results smoothly interpolate between the weak- and strong-coupling answers. The analytical results in the small U limit, obtained from (7), are separated for clarity from the numerical curves in Fig. 2(a) and 2(b). In strong coupling, the $f \ll 1$ result (8) is plotted as the fourth curve; clearly $f=0.05$ is not in the asymptotic low-filling limit in either the 2D or 3D case. The $f=0.45$ numerical result is compared in strong coupling with the analytical result for half-filling, which is much easier to obtain. However, at all fillings, the $1/U$ dependence of c is apparent in strong coupling. We see that c increases as a function of the filling in strong coupling, but, as discussed above, it has a nonmonotonic dependence on f in weak coupling.

We briefly summarize the results of an extension of the above analysis to charged systems, the details of which will be published elsewhere.[10] In weak coupling the sound mode is pushed up[8] to the plasma frequency in the 3D case; in the 2D case the plasmon has a $\sqrt{q}$ dispersion. We find[10] that the plasmon evolves smoothly as a function of the attraction, and in the strong-coupling, dense limit we recover the known plasma frequency for a dense charged Bose gas.[14] Using the methods of Ref. 15 we plan to generalize these results to layered superconductors.

Recently, the RPA has also been successfully applied to other crossover problems, for example, the evolution from itinerant to local moment antiferromagnetism,[16] and excitonic collective modes in a Bose condensed electron-hole gas.[17] The proven domain of validity[11] of the RPA is weak coupling. However, the results obtained in this paper, and the others cited above, clearly demonstrate that, at least in certain cases, it yields qualitatively reasonable results even for strong-coupling regimes and further provides a credible interpolating scheme in between. The reasons for this clearly need to be understood better.

The most important open question is a satisfactory treatment of finite temperatures,[18] and, in particular, of the normal state in the intermediate-coupling regime.

In conclusion, we have shown within the RPA that there is a smooth crossover in the collective excitation spectrum of the attractive Hubbard model. The collective mode evolves from an Anderson mode in the weak-coupling Cooper-pair limit to a Bogoliubov sound mode for a Bose gas in the strong-coupling composite boson limit. For the charged case we found a similar smooth evolution of the plasmon.

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