Comment on "BCS to Bose-Einstein crossover phase diagram at zero temperature for a $d_{x^2-y^2}$ order parameter superconductor: Dependence on the tight-binding structure"

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The work by Soares *et al.* [Phys. Rev. B **65**, 174506 (2002)] investigates the BCS to Bose-Einstein crossover for *d*-wave pairing in the two-dimensional attractive Hubbard model. Contrary to their claims, we found that a nonpairing region does *not* exist in the density vs coupling phase diagram. The gap parameter at $T=0$, as obtained by solving analytically as well as numerically the BCS equations, is in fact finite for any nonzero density and coupling, even in the weak-coupling regime.

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In Ref. 1, Soares *et al.* analyzed the BCS to Bose-Einstein (BCS-BE) crossover at $T=0$ for *d*-wave pairing in the attractive Hubbard model, extending the work by den Hertog[2] by including the next-nearest-neighbor hopping t' in the tight-binding dispersion. As is evident from the insets of Figs. 1 and 3 as well as from the phase diagram of Figs. 2 and 4 of Ref. 1, in the weak-coupling regime and for any density, they obtained a non pairing metallic phase characterized by an exactly vanishing value of the BCS gap parameter at $T=0$ [$\Delta(T=0)=0$]. Similar results have been previously obtained by den Hertog in Ref. 2 for $t'=0$. In a related context, a metallic phase at $T=0$ in the weak-coupling regime could only result from the Capone *et al.* calculation in Ref. 3 (using a DMFT approach to the *s*-wave attractive Hubbard model at $T=0$) by suppressing superconducting pairing. On the other hand, results for the gap parameter obtained with Hubbard-like lattice models can be connected (in the weak-coupling and low-density limits) to the analytic results of the continuous models (see below) obtained in Refs. 4 and 5, where a *finite* value for the gap is found in the weak-coupling regime.

In this Comment, we show that the *d*-wave gap parameter at $T=0$ is *always finite* for any nonzero density and even in the weak-coupling regime, by performing both numerical and analytic calculations. This result was reported in Ref. 6 where it was explicitly contrasted with the results by den Hertog;[2] further comments on this point can be found in the review article by Loktev *et al.*[7] In particular, Soares *et al.* seem not to have been aware of the results of Ref. 6 concerning the weak-coupling regime. The difference in the results must be due to inaccuracy in the numerical calculations of Refs. 1 and 2.

To further support our previous finding about the existence of a *d*-wave BCS superconducting ground state [$\Delta(T=0)\neq 0$] in the weak-coupling regime, we solve the coupled self-consistent equations for the gap function and density at $T=0$, as given by BCS theory:

$$\Delta_{\mathbf{k}}=-\frac{1}{N}\sum_{\mathbf{k}'}\frac{V_{\mathbf{k},\mathbf{k}'}}{2\sqrt{\xi_{\mathbf{k}'}^2+\Delta_{\mathbf{k}'}^2}}\Delta_{\mathbf{k}'}, \quad (1)$$

$$n=\frac{1}{N}\sum_{\mathbf{k}}\left(1-\frac{\xi_{\mathbf{k}}}{\sqrt{\xi_{\mathbf{k}}^2+\Delta_{\mathbf{k}}^2}}\right). \quad (2)$$

Here, $\xi_{\mathbf{k}}=-2t(\cos k_x+\cos k_y)-4t'\cos k_x\cos k_y-\mu$ is the tight-binding dispersion with nearest- and next-nearest-neighbor hopping, μ the chemical potential, N the total number of sites, and $V_{\mathbf{k},\mathbf{k}'}=-V\gamma_{\mathbf{k}}\gamma_{\mathbf{k}'}$ (with $\gamma_{\mathbf{k}}=\cos k_x-\cos k_y$) the pairing interaction in the *d*-wave channel. (We set the lattice spacing to unity.) The wave-vector dependence of the gap parameter resulting from Eq. (1) is purely *d* wave, i.e., $\Delta_{\mathbf{k}}=\Delta\gamma_{\mathbf{k}}$, provided the interaction $V_{\mathbf{k},\mathbf{k}'}$ can be written in a separable form. This considerably simplifies the solution of the above equations.

We first solve the coupled Eqs. (1) and (2) by the standard Newton's method with high precision (using a *k*-space mesh up to 1024×1024 points), with the value $t'/t=-0.1$ to compare[8] with the inset of Fig. 3 of Soares *et al.* Our numerical results for the maximum value of the gap parameter $\Delta(T=0)$ are shown in Fig. 1 as a function of the interaction strength $V/4t$ and for different densities. In Fig. 1, the arrows locate the values of $V/4t$ below which the gap would vanish (for given density) according to the numerical results by Soares *et al.* We find instead *finite* values for the gap even well below the critical couplings identified by Soares *et al.* (and also by den Hertog[2] for the case $t'=0$). In the weak-

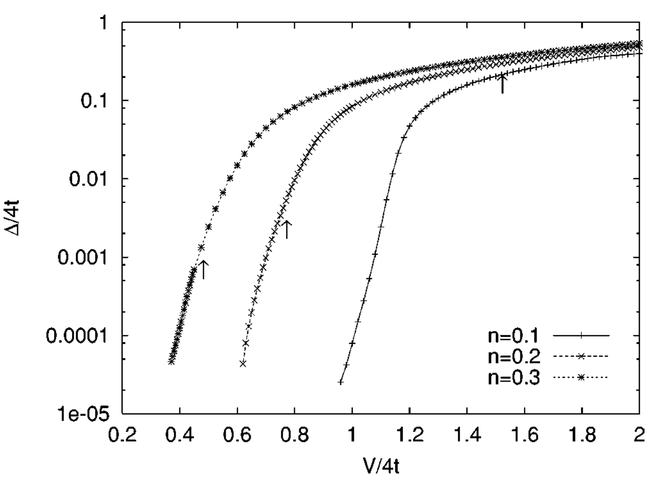

FIG. 1. Maximum value of the *d*-wave gap parameter Δ at $T=0$ as a function of the interaction strength V for different densities [$n=0.1$ (plus), $n=0.2$ (cross), $n=0.3$ (star)]. Energies are normalized with respect to the half bandwidth $4t$. The arrows locate the values of $V/4t$ below which Ref. 1 claims that $\Delta=0$.

coupling regime, our result is that the gap parameter decreases exponentially as the coupling is decreased, in agreement with the standard BCS result. We obtain the same result below by analytic calculations. Regarding instead the chemical potential, our results agree with those reported in Fig. 3 of Soares *et al.*, as expected by the smallness of the ratio Δ/μ in the weak-coupling region where our results for Δ disagree from those of Soares *et al.*

In the low-density regime, where the dispersion is parabolic, the d-wave BCS equations can be solved *analytically* in the weak-coupling limit. The expansion of the dispersion and of the d-wave factors for small wave vectors leads to $\xi_{\mathbf{k}} \simeq (t+2t')(k_x^2+k_y^2)-\mu-4t-4t' \equiv k^2/(2m^*)-\epsilon_F$ and $\gamma_{\mathbf{k}} \simeq (k_y^2-k_x^2)/2=(k^2/2)\cos 2\phi$, respectively, where the polar coordinates (k,ϕ) have been introduced together with effective mass $m^*=1/[(2(t+2t')]$ and Fermi level $\epsilon_F=\mu+4t+4t'$. In addition, in the weak-coupling regime it is convenient to limit the integral over the energy variable ϵ to a small window $|\epsilon-\epsilon_F|<\omega_0/2$ about the Fermi level, where ω_0 is a cutoff such that $\omega_0 \gg \Delta$. The integral outside this energy window gives subleading contributions that can only be evaluated numerically since the full wave-vector dependence of $\xi_{\mathbf{k}}$ and $\gamma_{\mathbf{k}}$ ought to be retained in this case. Note that, in the weak-coupling regime, the Fermi level coincides with the noninteracting value $\epsilon_F=k_F^2/(2m^*)=\pi n/m^*$ and Eqs. (1) and (2) can be decoupled. After these manipulations, we are led to the following expression for the d-wave gap equation at $T=0$:

$$1=\frac{2g_d}{\pi}\int_{-\omega_0/2}^{\omega_0/2} d\xi \int_0^{\pi/2} d\theta \frac{\cos^2\theta}{\sqrt{\xi^2+\Delta_d^2\cos^2\theta}}, \tag{3}$$

where $g_d=Vk_F^4 m^*/(16\pi)$, $\Delta_d=\Delta k_F^2/2$, $\theta=2\phi$, and $\xi=\epsilon-\epsilon_F$. Equation (3) has been written in a form which maps exactly into Eq. (A2) of Ref. 5. The analytic solution for the gap equation in the weak-coupling limit reported in Ref. 5 clearly shows that the gap is *always finite*, no matter how weak the effective attraction g_d. Since this point is crucial to the present discussion, we provide here some details of the derivation of the analytic result given by Eq. (A2) of Ref. 5. The integral over the angular variable in Eq. (3) can be performed exactly using known results for the elliptic integrals.[9] One obtains

$$\int_0^{\pi/2} d\theta \frac{\cos^2\theta}{\sqrt{\xi^2+\Delta_d^2\cos^2\theta}}=\frac{1}{\sqrt{\xi^2+\Delta_d^2}}\int_0^{\pi/2} d\theta \frac{\cos^2\theta}{\sqrt{1-\kappa^2\sin^2\theta}}$$
$$=\frac{1}{\sqrt{\xi^2+\Delta_d^2}}\left[\frac{1}{\kappa^2}E\left(\frac{\pi}{2},\kappa\right)-\frac{(1-\kappa^2)}{\kappa^2}F\left(\frac{\pi}{2},\kappa\right)\right], \tag{4}$$

where $\kappa^2=\Delta_d^2/(\xi^2+\Delta_d^2)$, and $F(\pi/2,\kappa)$ and $E(\pi/2,\kappa)$ are elliptic integrals of the first and second kind, respectively. Performing at this point the integral over the variable ξ, the expansion of the elliptic functions $E(\pi/2,\kappa)$ and $F(\pi/2,\kappa)$ up to second order in κ produces a log contribution in ω_0/Δ_d, leading to the usual BCS exponential dependence of the gap parameter on coupling. The prefactor of this exponential is obtained by considering the sum of the remaining terms of the above expansion, resulting in finite integrals over the variable ξ as $\omega_0/\Delta_d \to \infty$. These terms can be summed exactly by exploiting the analytic result

$$\int_0^1 d\kappa \frac{1}{\kappa\sqrt{1-\kappa^2}}\left[\frac{1}{\kappa^2}E\left(\frac{\pi}{2},\kappa\right)-\frac{(1-\kappa^2)}{\kappa^2}F\left(\frac{\pi}{2},\kappa\right)-\frac{\pi}{4}\right]$$
$$=\frac{\pi}{4}\ln\left(\frac{2}{\sqrt{e}}\right). \tag{5}$$

The final expression for the gap parameter Δ_d obtained in this way is

$$\Delta_d=\frac{2\omega_0}{\sqrt{e}}\ \exp(-1/g_d). \tag{6}$$

Note that the coupling constant $g_d=\pi n^2 V m^*/4$ entering the exponential in Eq. (6) depends on the squared density, leading to a marked exponential suppression of the gap parameter in the weak-coupling regime as the low-density limit $(n \to 0)$ is approached. We have verified that our numerical results for the gap parameter reproduce this dependence on coupling strength V and density n. We emphasize, however, that only the exponential dependence in Eq. (6) can be compared with the numerical results, since the subleading contributions to the energy integral in Eq. (3) outside the ω_0 window (which are not included in the present calculation) are expected to eventually modify the prefactor of Eq. (6) in such a way as to eliminate this cutoff completely (the energy scale ω_0 is absent in our starting model and has been introduced only for convenience in the analytic calculation).

Summarizing, we have found that a nonpairing region is completely absent in the phase diagram of the attractive Hubbard model for d-wave pairing describing the BCS-BE crossover. The gap parameter at $T=0$ is, in fact, finite for any nonzero density and coupling, even in the weak-coupling regime, contrary to the results of Soares *et al.*[1] and den Hertog.[2] In systems with dopant impurities,[10] on the other hand, a critical value of the fermion density at $T=0$ for the onset of d-wave superconductivity is instead possible.

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