Effects of intralayer correlations on electron-hole double-layer superfluidity

Filippo Pascucci,[1,2] Sara Conti,[3] Andrea Perali,[1] Jacques Tempere,[2] and David Neilson[3]

[1]*Supernano Laboratory, School of Pharmacy, University of Camerino, 62032 Camerino (MC), Italy*
[2]*TQC, University of Antwerp, Universiteitsplein 1, 2610 Antwerp, Belgium*
[3]*CMT, Department of Physics, University of Antwerp, Groenenborgerlaan 171, 2020 Antwerp, Belgium*

(Received 18 October 2023; revised 16 January 2024; accepted 26 February 2024; published 18 March 2024)

We investigate the intralayer correlations acting within the layers in a superfluid system of electron-hole spatially separated layers. In this system, superfluidity is predicted to be almost exclusively confined to the Bose-Einstein condensate (BEC) and crossover regimes where the electron-hole pairs are well localized. In this case, Hartree-Fock is an excellent approximation for the intralayer correlations. We find in the BEC regime that the effect of the intralayer correlations on superfluid properties is negligible but in the BCS-BEC crossover regime the superfluid gap is significantly weakened by the intralayer correlations. This is caused by the intralayer correlations boosting the number of low-energy particle-hole excitations that drive the screening. We further find that the intralayer correlations suppress the predicted phenomenon in which the average pair size passes through a minimum as the crossover regime is traversed.

DOI: 10.1103/PhysRevB.109.094512

I. INTRODUCTION

Recent reports of the likely observation of superfluidity with electron-hole pairs in spatially separated electron and hole conducting layers in zero magnetic fields [1–5] are currently attracting a lot of interest. The spatial separation opens a way to stable superfluids in equilibrium because it suppresses electron-hole recombination [6,7].

Theoretical investigations of these two-layer systems have mainly focused on the interlayer electron-hole correlations needed to generate the electron-hole pairs. Here we investigate the effect of the screened intralayer correlations acting within each layer on the superfluid properties. Reference [8] was the first attempt to include the effect of intralayer correlations on superfluidity in this system by including an unscreened repulsive intralayer interaction term in the Hamiltonian. However, there is no comparison of results with and without these correlations, and furthermore, Ref. [9] subsequently showed that screening plays a central role in exciton superfluidity. While quantum Monte Carlo simulations [10,11] include all correlations, and in fact all vertex corrections, they can yield no information at all about their separate contributions, nor where in the phase diagram the intralayer correlations become significant.

For superfluidity of spatially indirect excitons, the average separation between the excitons is generally much greater than the layer spacing separating the electrons and holes. The excitons are then well approximated by particles with dipole moments perpendicular to the layers and mutually interacting through repulsive dipole-dipole interactions acting parallel to the layers [12,13]. At the relatively low densities where superfluidity is found [2,11], kinetic energy effects tend to dominate over the intralayer correlations caused by the dipolar interactions. In this case, an expansion of the corrections due to the intralayer correlations will be dominated by the Hartree-Fock contribution. This is in striking contrast to Wigner crystallization in double-layer Coulombic systems, where at low densities the intralayer correlations from the Coulomb interactions are dominant over kinetic energy effects [14].

II. SCREENED HARTREE-FOCK APPROXIMATION

In this paper, we investigate the effect of intralayer correlations on superfluidity using the Hartree-Fock approximation. The coupled mean-field equations for the superfluid gap Δ_k and the layer density n at zero temperature are [9,15,16]

$$\Delta_k = -\frac{1}{S}\sum_{\mathbf{k}'} V^{sc}_{eh}(k-k')\frac{\Delta_{k'}}{2E_{k'}}, \tag{1}$$

$$n = \frac{g_s g_v}{S}\sum_{\mathbf{k}} \frac{1}{2}\left(1-\frac{\varepsilon_k-\mu_s}{E_k}\right). \tag{2}$$

$E_k = \sqrt{\xi_k^2+\Delta_k^2}$ is the excitation energy, $\xi_k = \varepsilon_k - \mu_s$, with ε_k being the single-particle energy band and μ_s being the single-particle chemical potential. g_s and g_v are the spin and valley degeneracies and S is the area of the system. $V^{sc}_{eh}(\mathbf{q})$ is the self-consistent electron-hole screened interaction, given by:

$$V^{sc}_{eh}(\mathbf{q}) = \frac{V_{eh}(\mathbf{q}) - \Pi_a(\mathbf{q})\left[V^2_{ee}(\mathbf{q}) - V^2_{eh}(\mathbf{q})\right]}{1-2[V_{ee}(\mathbf{q})\Pi_n(\mathbf{q}) - V_{eh}(\mathbf{q})\Pi_a(\mathbf{q})] + \mathcal{A}_{\mathbf{q}}\mathcal{B}_{\mathbf{q}}}, \tag{3}$$

where $V_{ee}(\mathbf{q}) = 1/q$ is the bare electron-electron (and hole-hole) interaction acting within each layer and $V_{eh}(\mathbf{q}) = -e^{-qd}/q$ is the bare electron-hole interaction between layers, where d is the interlayer distance. $\Pi_n(\mathbf{q})$ and $\Pi_a(\mathbf{q})$ are the normal and anomalous polarizabilities in the superfluid phase [9,17]. For brevity, we write $\mathcal{A}_{\mathbf{q}} = V^2_{ee}(\mathbf{q}) - V^2_{eh}(\mathbf{q})$ and $\mathcal{B}_{\mathbf{q}} = \Pi^2_n(\mathbf{q}) - \Pi^2_a(\mathbf{q})$.

In the Hartree-Fock approximation, the single-particle energy is given by [18,19]

$$\xi^{HF}_{\mathbf{k}} = \frac{\hbar^2\mathbf{k}^2}{2m} - \mu_s - \Sigma(\mathbf{k}), \tag{4}$$

where

$$\Sigma(\mathbf{k}) = \frac{1}{S}\sum_{\mathbf{p}} V_{ee}^{sc}(\mathbf{p}-\mathbf{k})v_{\mathbf{p}}^2, \tag{5}$$

with the Bogoliubov amplitude (density of states)

$$v_{\mathbf{k}}^2 = 1 - u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{\xi_{\mathbf{k}}^{HF}}{E_{\mathbf{k}}^{HF}}\right). \tag{6}$$

The self-consistent static screened electron-electron (hole-hole) interaction within each layer is [19,20]

$$V_{ee}^{sc}(\mathbf{q}) = \frac{V_{ee}(\mathbf{q}) - \Pi_n(\mathbf{q})\left[V_{ee}^2(\mathbf{q}) - V_{eh}^2(\mathbf{q})\right]}{1 - 2[V_{ee}(\mathbf{q})\Pi_n(\mathbf{q}) - V_{eh}(\mathbf{q})\Pi_a(\mathbf{q})] + \mathcal{A}_{\mathbf{q}}\mathcal{B}_{\mathbf{q}}}. \tag{7}$$

To determine the effect of the Hartree-Fock corrections within the layers, we solve the gap and number equations, Eqs. (1) and (2), using $\xi_{\mathbf{k}}^{HF}$ for the single-particle energy. The screened interactions, Eqs. (3) and (7), are modified similarly.

We take single-particle parabolic bands $\varepsilon_k = \hbar k^2/2m^*$, with equal effective masses $m^* = m_e^* = m_h^* = 0.04$. For the spin and valley degeneracy we consider $g_s g_v = 2$. We take hBN as the insulator between the layers with dielectric constant $\epsilon = 2$. We express lengths in units of the effective Bohr radius, $a_B^* = \epsilon a_0 m_e/m_r^* = 5.3$ nm, where $m_r^* = m^*/2$ is the reduced mass. Energies are in effective Rydberg, Ry$^* = 68$ meV. We consider equal electron and hole layer densities, $n = n_e = n_h$, corresponding to an average interparticle spacing in the layers of $r_0 = (\pi n)^{-1/2}$.

III. ACROSS BCS-BEC CROSSOVER

Figure 1(a) shows the resulting superfluid energy gap Δ_k for a layer separation $d = 0.2$. The intralayer distance r_0 shown spans the full range for superfluidity. Because of strong screening, there is a maximum threshold density for the superfluidity that corresponds to $r_0 \simeq 1$.

As the threshold density is approached, we see that the Hartree-Fock correlations have a strong effect on the superfluidity, reducing the gap Δ_k by as much as a factor of 2. Figure 1(b) demonstrates that this suppression of Δ_k comes from the effect of the Hartree-Fock correlations weakening the self-consistent electron-hole screened interaction, $V_{eh}^{sc}(\mathbf{q})$. The weakening is due to the Hartree-Fock corrections boosting the number of the low-energy particle-hole excitations that drive the screening [see Fig. 1(c)].

The effect of the intralayer correlations on the superfluidity weakens with decreasing density, and for $r_0 \gtrsim 3$ the correlations have negligible effect.

Figure 2 compares our results with diffusion quantum Monte Carlo (DQMC) numerical simulations [21] with the same physical parameters. We see in Fig. 2(a) that including the Hartree-Fock correlations significantly improves the agreement with DQMC for both the height and the position of the maximum of the superfluid peak $\Delta_{\max}$.

Figures 2(b) and 2(c) compare the condensate fraction (CF) and the single-particle chemical potential μ_s, respectively. We see that the Hartree-Fock corrections are significant and move these quantities closer to the benchmark DQMC results. DQMC shows a brief entrance into the BCS regime, specified by CF < 0.2, whereas our threshold density preempts entry

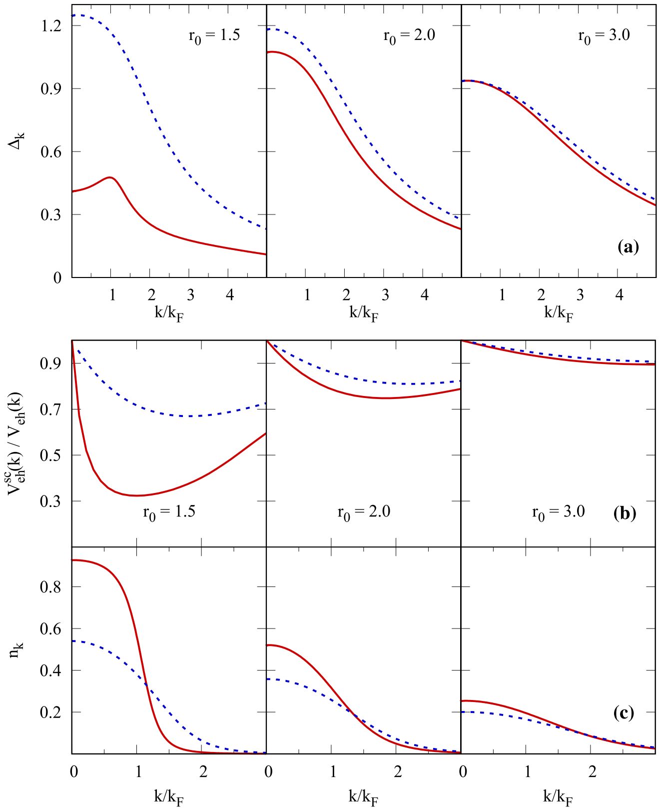

FIG. 1. (a) Superfluid gap Δ_k at densities characterized by r_0, the average interparticle spacing within each layer. Layer separation $d = 0.2$. Solid red line: Within the mean field including intralayer correlations. Dashed blue line: Within the mean field but neglecting intralayer correlations. (b) Ratio of self-consistent screened electron-hole attraction $V_{eh}^{sc}(k)$ to the bare attraction $V^{eh}(k)$ for the same densities. (c) Corresponding density of states $n_k = v_{\mathbf{k}}^2$. Lengths are in units of the effective Bohr radius and energies are in units of the effective Rydberg (see text).

into the BCS regime. This is associated with static screening underestimating the threshold density. Corrections from dynamical screening have been shown to increase this density [22].

An important feature of superfluidity in these electron-hole double-layer systems is that, by tuning the carrier density in the layers n using gate voltages, it is possible experimentally to sweep the superfluidity from a strong-coupled Bose-Einstein condensate (BEC) at the lowest densities to the intermediate-coupled BCS-BEC crossover regime, towards the weak-coupled BCS regime [9,23]. Figure 3 maps out the superfluidity and its regimes at very low temperatures in the r_0-d phase space. We set the boundary between the BEC and the BCS-BEC crossover regimes as the line at which the chemical potential μ_s changes sign from negative to positive [Fig. 2(b)] [24,25]. We can see from Fig. 3 that the inclusion of intralayer correlations strongly reduces the region of the r_0-d space in which superfluidity survives.

The smallest separation experimentally attained to date, in units of their effective Bohr radii, are in gallium arsenide double quantum wells $d \simeq 1.0$ (10 nm) [26–28], in double bilayer graphene $d \simeq 0.2$ (1 nm) [1], and in double-layer transition metal dichalcogenide $d \simeq 0.45$ (0.6 nm) [2,3].

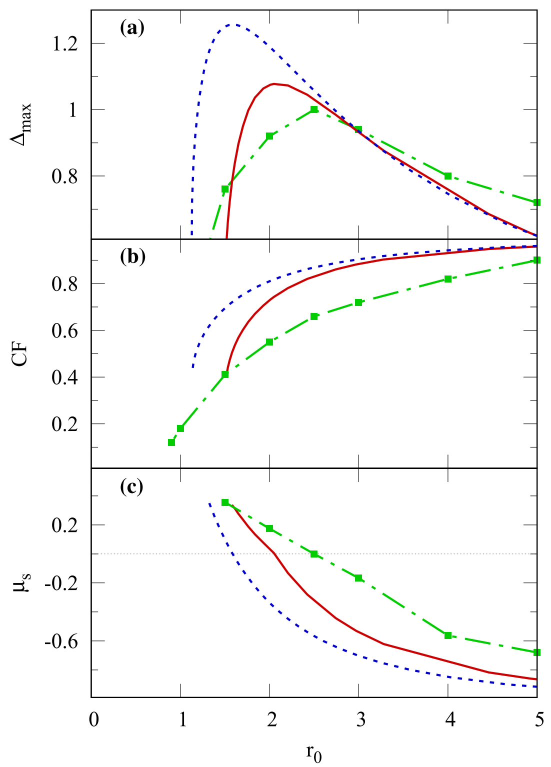

FIG. 2. (a) Maximum superfluid gap Δ_{max} as a function of r_0, the average interparticle intralayer distance within a layer. Solid red line: Within the mean field with intralayer correlations included. Dashed blue line: Within the mean field but neglecting intralayer correlations. We show for comparison (dash-dot green line) the Δ_{max} from diffusion Quantum Monte Carlo numerical simulations [21]. (b) The corresponding condensate fraction CF. (c) The corresponding single-particle chemical potential μ_s.

We compare in Fig. 4(a), for a fixed value of the layer interparticle spacing $r_0 = 3$, the evolution of the superfluid gap energy Δ_k when the Hartree-Fock correlations within

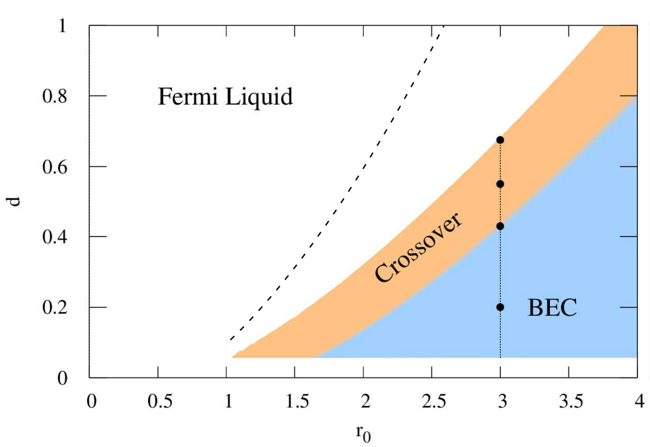

FIG. 3. Dependence of BEC and BCS-BEC crossover regimes on layer separation d and average interparticle spacing within each layer r_0. The BCS regime is preempted by strong screening that suppresses superfluidity at small r_0 and large d. The black dashed line is the boundary of the superfluid phase without the intralayer correlations. Marked are the points in the r_0-d phase space used in Fig. 4.

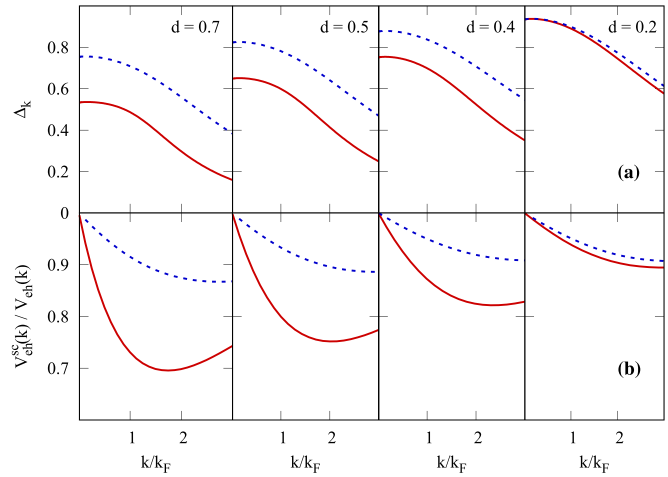

FIG. 4. (a) Superfluid gap $\Delta(k)$ for a fixed density corresponding to $r_0 = 3$, at different d points in the BEC and BCS-BEC crossover regimes (see Fig. 3). Solid red line: Within the mean field with intralayer correlations included. Dashed blue line: Within the mean field but neglecting intralayer correlations. (b) Ratio of the self-consistent screened electron-hole attraction $V^{sc}_{eh}(k)$ to the bare attraction $V_{eh}(k)$ for the same r_0-d points spanning the BEC and BCS-BEC crossover regimes.

the layers are either included or neglected, for different layer separations d. The corresponding (r_0-d) points are marked on the phase diagram (Fig. 3). Figure 4(b) compares the corresponding ratios of the screened electron-hole attraction $V^{sc}_{eh}(k)$ to the bare attraction $V_{eh}(k)$.

The layer spacing $d = 0.2$ lies deep in the BEC regime and Fig. 4(b) confirms that screening is indeed negligible there. Since the Hartree-Fock corrections primarily affect the screening, the correlations have almost no effect on Δ_k for $d = 0.2$. However, $d = 0.4$ lies on the BCS-BEC crossover boundary, and we see at that point that screening is no longer negligible, and as a consequence, Δ_k starts to develop a sensitivity to the Hartree-Fock corrections. As d is further increased and the crossover regime is traversed, both the screening and Δ_k become increasingly sensitive to the Hartree-Fock corrections. By $d = 0.7$, the correlations boost the low-lying density of states so much that the screening is strongly enhanced. This in turn strongly suppresses Δ_k, and $d = 0.7$ is close to the superfluid threshold where the screening kills the superfluidity.

IV. ELECTRON-HOLE PAIR SIZE

Figure 5 compares, with intralayer correlations included or neglected, the spatial size of the electron-hole pairs [25,29],

$$\xi_{pair} = \left[\frac{\sum_{\mathbf{k}} |\nabla_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}}|^2}{\sum_{\mathbf{k}} u_{\mathbf{k}}^2 v_{\mathbf{k}}^2} \right]^{1/2}, \tag{8}$$

as a function of r_0 for layer separation $d = 0.2$.

Without the intralayer correlations, starting from the low-density BEC regime, ξ_{pair} initially decreases as the density increases. In the BEC regime the pairs act as well-spaced composite bosons interacting primarily through exchange, and so, as the interparticle spacing decreases, exchange effects

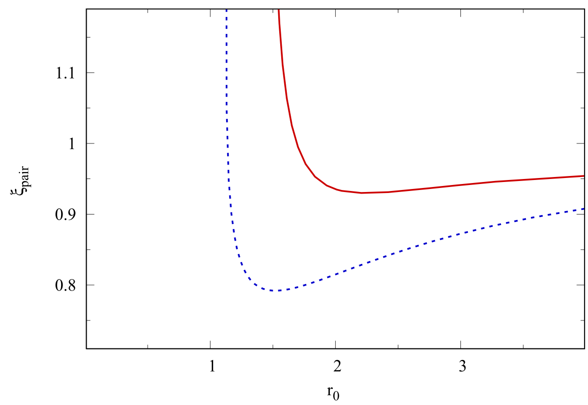

FIG. 5. The pair size of the exciton $\xi_{\rm pair}$ as a function of r_0, the average interparticle spacing in each layer. The layer separation is $d = 0.2$. Solid red line: Within the mean field with intralayer correlations included. Dashed blue line: Within the mean field but neglecting intralayer correlations.

strengthen causing the pairs to shrink [30]. In contrast, in the crossover regime the bosonic nature of the pairs is lost because there is significant overlap of the single-fermion wave functions. Thus $\xi_{\rm pair}$ will grow exponentially as the density is further increased. Reference [30] pointed out that this competing behavior leads to a minimum in $\xi_{\rm pair}$. In Fig. 5 this minimum is clearly visible when intralayer correlations are omitted.

However, we see that when intralayer correlations are included, the resulting buildup of screening strength with increasing density greatly weakens the shrinkage of $\xi_{\rm pair}$ and effectively eliminates the minimum. Then at higher densities, the very strong screening further weakens the superfluidity, causing the $\xi_{\rm pair}$ to grow exponentially. $\xi_{\rm pair}$ diverges at the threshold density for superfluidity. For $d > 0.2$ there is no minimum when intralayer correlations are included, and the minimum without correlations rapidly weakens. Our results can be compared with the Cooper pair radii from DQMC reported in Ref. [21]. We found that inclusion of intralayer correlations improves the agreement with the results for the Cooper pair radius from DQMC.

V. CONCLUSIONS

The primary effect of the Hartree-Fock correlations on superfluid properties in the present system is an increase in the strength of screening caused by a boost in the density of the low-lying states. Screening plays a crucial role in determining superfluid properties because the pairing interaction is long range [9,17], and we find that the strength of the screening can be as much as doubled by the Hartree-Fock corrections. The effects of screening on the superfluidity are negligible in the deep BEC regime [31] and therefore Hartree-Fock has minimal effect in that regime, but in the BCS-BEC crossover regime, where screening plays a crucial role in determining the superfluid properties, the increased screening strength results in (i) a diminution of the superfluid gap Δ by up to a factor of 2 within the BCS-BEC crossover regime, leading to a better agreement with the DQMC simulations, and (ii) a shift to lower densities of the boundary between the BEC and crossover regimes, which results in (iii) the disappearance of the minimum in the electron-hole pair-size as a function of density.

ACKNOWLEDGMENTS

We thank S. De Palo and G. Senatore for useful discussions. The work was partially supported by PNRR MUR Projects No. PE0000023-NQSTI, No. G061820N, No. G060820N, and No. G0H1122N and by the Flemish Science Foundation (FWO-Vl).

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