Rise and Fall of Pseudogaps Throughout the Two-Band BCS-BEC Crossover

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We demonstrate the rise-and-fall of multiple pseudogaps in the Bardeen-Cooper-Schrieffer-Bose-Einstein-condensation (BCS-BEC) crossover in two-band fermionic systems having different pairing strengths in the deep band and in the shallow band. The striking features of this phenomenon are an unusual many-body screening of pseudogap state and the importance of pair-exchange couplings, which induces multiple pseudogap formation in the two bands. The multi-band configuration suppresses pairing fluctuations and the pseudogap opening in the strongly-interacting shallow band at small pair-exchange couplings by screening effects, with possible connection to the pseudogap phenomenology in iron based superconductors. On the other hand, the multiple pseudogap mechanism accompanies with the emergence of binary preformed Cooper pairs originating from interplay between intra-band and pair-exchange couplings.

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The discovery of unconventional superconductors, which started with heavy fermions, followed by organic superconductors, and then by cuprate compounds, has prompted an era of tremendous growth of activities in various fields of condensed matter research [1, 2]. The complex structure of the order parameter in these systems brought a plethora of unique phenomena and effects, with no counterparts in conventional superconductors, such as a broken time-reversal symmetry, collective modes, and an unusual Josephson effect [3, 4]. The new degrees of freedom in multi-component and multi-band superconductors has been anticipated to be a promising root toward the realization of room-temperature superconductivity [5]. Such unconventional superconductors can exhibit also anomalous normal state characteristics above their critical temperature $T_c$, which are well-known now and interpreted as the pseudogap state [6, 7], corresponding to the presence of gap-like features above $T_c$ but with a finite spectral intensity at low frequencies [8]. The origin of the pseudogap is considered as a key ingredient for the understanding of the pairing glue in unconventional superconductors. Pseudogap effects have also been discussed in the context of the Bardeen-Cooper-Schrieffer (BCS) to Bose-Einstein condensation (BEC) crossover, where the BCS state of overlapping Cooper pairs changes continuously to the BEC of tightly bound molecules with increasing attractive interaction [9–22]. It is experimentally achieved in ultracold Fermi atomic gases exploiting Fano-Feshbach resonances [23, 24, 25, 26]. It should be noted that also ultracold Fermi gases in the BCS-BEC crossover regime exhibit strong pairing fluctuations and pseudogap effects [26, 27].

Among the variety of unconventional superconductors, the recently discovered iron-based superconducting compounds attract attention, since some of them are expected to place in the BCS-BEC crossover regime due to their large ratio between the superconducting gap and the Fermi energy $29, 32$. This new class of unconventional superconductors opens a new frontier for the study of the multi-band BCS-BEC crossover, where non-trivial features have been discussed [32–47]. Like for other unconventional superconductors, there is now expanding experimental evidence that the pseudogap is realized in iron-based compounds [46–48], despite some reports about the missing of strong pairing fluctuations and pseudogap effects [50–51]. In order to understand the controversial pseudogap physics in multiband and multicomponent systems like iron-based superconductors, a unified description of the multi-band BCS-BEC crossover is required. It is important to note that such a theory can be useful to describe also many-body physics in Yb Fermi gases near the orbital Feshbach resonance [52–54], thus bridging these atomic systems with multiband superconductors. The multi-channel many-body theory is also of importance to unveil pairing properties in nanostructured superconductors [33, 34, 61] and electron-hole systems [62–64].

In this letter, we develop a theory of the two-band BCS-BEC crossover in the normal state above $T_c$ based on the $T$-matrix approach [65], which has been successfully applied to strongly interacting attractive Fermi gases [50]. We address the single-particle density of states (DOS) and elucidate competing mechanisms of screening and enhancement of the pseudogap in two-band systems. The screening of pairing fluctuations and resulting reduction of the pseudogap regime are found in our re-
spin-singlet pair annihilation operators in the i
spectively. In this work, we use
the Kronecker delta. We use equal effective masses
the first deep band (ℓ ℓ = 1) \[72, 73\], as described by the
Hamiltonian \[74\]

\[
H = \sum_{k,\sigma,\ell} \xi_{k,\ell} c_{k,\sigma,\ell} c_{k,\sigma,\ell}^\dagger + \sum_{i,j} U_{ij} \sum_q B_{q,i} B_{q,j},
\]

where \( \xi_{k,\ell} = k^2/(2m_\ell) - \mu + E_0 \delta_{\ell,1} \) is the kinetic energy measured from the chemical potential \( \mu \) with the energy separation \( E_0 \) between two bands and \( \delta_{\ell,2} \) is the Kronecker delta. We use equal effective masses \( m = m_1 = m_2 \), for simplicity. \( c_{k,\sigma,\ell} \) and \( B_{q,i} = \sum_{k} c_{-k+q/2,\ell,\sigma} \) are spin-\( \uparrow, \downarrow \) fermion and spin-singlet pair annihilation operators in the i-band, respectively. In this work, we use \( E_0 = 0.6E_{F,1} \) where \( E_{F,i} = (3\pi^2 n_i)^{2/3}/(2m) \) is the non-interacting Fermi energy in the i-band, defined in terms of the number density \( n_i \). The intra-band couplings \( U_{\ell \ell} \) can be characterized in terms of the intra-band scattering lengths \( a_{\ell \ell} \) as

\[
\frac{m}{4\pi a_{\ell \ell}} = \frac{1}{U_{\ell \ell}} + \sum_k \frac{m}{k^2},
\]

where \( k_0 \) is the momentum cutoff taken to be 100\( k_{F,1} \).

Here, \( k_{F,1} \equiv \sqrt{2mE_{F,1}} \) is the Fermi wavevector associated with the total Fermi energy \( E_{F,1} = (3\pi^2 n_1)^{2/3}/(2m) \), defined in terms of the total number density \( n \). In a similar way, one defines the Fermi wavevectors \( k_{F,\ell} \) in each band, which are used to define the dimensionless intra-band coupling strengths \( (k_{F,1}a_{11})^{-1} \) and \( (k_{F,2}a_{22})^{-1} \). In this work, we use \( (k_{F,1}a_{11})^{-1} \leq -2 \) and \( -1 \leq (k_{F,2}a_{22})^{-1} \leq 1 \). With this choice of couplings, pairs forming in the deep band (\( \ell = 1 \)) have a BCS character, while the BCS-BEC crossover is tuned in the shallow band (\( \ell = 2 \)). For convenience, we also introduce a dimensionless pair-exchange coupling \( \lambda_{12} = U_{12}(k_0/k_{F,1})^2n/E_{F, \ell} \) where \( U_{21} = U_{12} \mathbb{1} \).

The i-band self-energy in the multi-band \( T \)-matrix approach reads

\[
\Sigma_i(k, \omega_s) = T \sum_{q, \nu} \Gamma_i(q, \nu \omega_s) G_0(q - k, \nu \omega_s - \omega_s),
\]

where \( \omega_s = (2s + 1)\pi T \) and \( \nu_l = 2l(\pi T) \) (s and l integer) are fermionic and bosonic Matsubara frequencies, respectively. \( G_0^0(q, \omega_s) = [\omega_s - \xi_{k,\ell}])^{-1} \) is the bare Green’s function. The many-body \( T \)-matrix \( \{\ell j\}^{2 \times 2} \), which sums up the ladder-type diagram shown in Fig. 1(d), is given by

\[
\Gamma_{ij}(q, \nu \omega_s) = U_{ij} + \sum_{\ell \ell'} U_{\ell \ell'} \Pi_{\ell \ell}(q, \nu \omega_s) \Gamma_{\ell j}(q, \nu \omega_s),
\]

where the pair propagator \( \Pi_{\ell \ell} \) is

\[
\Pi_{\ell \ell}(q, \nu \omega_s) = -T \sum_{p, \nu \omega_s} G_0^0(p + q, \nu \omega_s + \nu \omega_s) G_0^0(p, -\nu \omega_s).
\]

Fixing \( \mu \) by solving the number equation \( n = n_1 + n_2 \) with

\[
n_i = 2T \sum_{k, \nu \omega_s} G_i(k, \nu \omega_s),
\]

where \( G_i(k, \nu \omega_s) = [\nu \omega_s - \xi_{k,\ell} - \Sigma_i(k, \nu \omega_s)]^{-1} \) is the dressed Green’s function, we obtain the superfluid/superconducting critical temperature \( T_c \) from the Thouless criterion \( \quad \Omega_{22}(q = 0, \nu = 0) = 0 \). While, in the presence of \( U_{12} \), all the matrix elements \( \Gamma_{ij}(q = 0, \nu_l = 0) \) diverge simultaneously at \( T_c \), in the case of vanishing \( U_{12} \) only \( \Gamma_{22} \) diverges, due to our choice of the coupling strengths.]

The DOS is obtained from

\[
N_i(\omega) = -\frac{1}{\pi} \sum_{k, \nu \omega_s} \text{Im} G_i(k, \nu \omega_s \rightarrow \omega + i\delta),
\]
shows the obtained phase diagram at the low band (becomes larger when the intra-band coupling in the shallow band is increased). Interestingly, the pair-exchange-induced pseudogap in $N_1(\omega)$ is the non-interacting DOS associated with total number density $n$.

The dimensionless pair-exchange coupling is taken as $\lambda_{12} = 0$, 2, and 4. For reference, we present the spectral weight $A_2(k, \omega)E_{F,2} = -\text{Im}G_2(k, \omega + i\delta)E_{F,2}/\pi$ at $\lambda_{12} = 0.5$ in the inset of panel (b2). The inset of (c2) shows $N_2(\omega)$ at $\lambda_{12} = 4$ because of the large energy gap. $N_0 = mk_F^2/(2\pi^2)$ is the non-interacting DOS associated with total number density $n$.

\[ \lambda_{12} = 0, 2, 4. \]

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These features can be qualitatively understood as follows. Quite generally, the size of pseudogap effects in the band $i$ can be roughly estimated by the energy scale $\Delta_{\infty,i}^c = -T\sum_{i,\nu} \Gamma_{ii}(q, \nu) \int_{-\infty}^\infty \text{Im}G_{ii}(k, \omega + i\delta)E_{F,i}/\pi$ for a single band, and here generalized to the multiband case. Even though in general $\Delta_{\infty}$ is related to the so-called Tani’s contact $C_{\infty}$, it was shown in Ref. [78] that in the intermediate crossover regime and close to $T_c$, $\Delta_{\infty}$ is close to the pseudogap scale energy determined from $N(\omega)$. In the two-band case in the presence of a finite $\lambda_{12}$, $\Delta_{\infty} = -T\sum_{i,\nu} \Gamma_{ii}(q, \nu)$ diverge simultaneously at $T_c$, for $q = 0$ and $\nu = 0$. For this reason, the scales $\Delta_{\infty,1}$ and $\Delta_{\infty,2}$ become interconnected, explaining in this way the pair-exchange-induced pseudogap in the deep band.

To characterize the pseudogap state, we introduce the band-dependent pseudogap temperatures $T_{i=1,2}^*$ where the minimum of $N_i(\omega)$ around $\omega = 0$ disappears [26]. Figure 3 shows the obtained phase diagram at the unitarity limit (crossover regime) of the shallow band coupled with the weakly interacting deep band, where $(k_{F,2}a_{2g})^{-1} = 0$ and $(k_{F,1}a_{11})^{-1} = -2$. In this figure, we plot the critical temperature $T_c$ and pseudogap temperatures $T_i^*$ as functions of $\lambda_{12}$. While the single pseudogap (SPG) appears in the region $T_{i=1}^* < T < T_{i=2}^*$, the double pseudogaps (DPG) can be found below $T = T_{i=1}^*$. In the case of vanishing $\lambda_{12}$, since the deep band does not exhibit pseudogap behavior, we obtain $T_{i=1}^* = T_c$. However,
if $\lambda_{12}$ is shifted from zero to the strong coupling, $T_1^*$ deviates from $T_c$ due to the interband pairing fluctuations. Thus, one can conclude that the pseudogap regime in the deep band ($T_c < T < T_2^*$) originates purely from the pseudogap induced by the transfer of pair-fluctuations due to the pair-exchange coupling (rise of induced pseudogap).

The inset of Fig. 4 shows the ratio $(T_2^* - T_c)/T_c$ as a function of $\lambda_{12}$. For a reference, we plot in this figure the numerical value obtained in the single-band counterpart at the unitarity limit. The pseudogap regime ($T_c < T < T_2^*$) in the two-band case with small $\lambda_{12}$ is clearly reduced compared to the single-band counterpart (fall of pseudogap). This tendency is indeed consistent with the experiments for FeSe multi-band superconductors in the BCS-BEC crossover regime as well as with previous theoretical work. This screening effect is related to the Pauli-blocking produced by the large Fermi surface in the deep band for our two-band configuration. However, such a regime is destroyed if one shifts $\lambda_{12}$ to the strong-coupling regime ($\lambda_{12} \gtrsim 1$) due to strong interband pairing fluctuations.

Figure 4 shows a comparison between the pseudogap energy scales $E_{pg,i}$ obtained from our $T$-matrix approach at $T = T_c$ and the mean-field gaps $\Delta_{0,i}$ at $T = 0$. Here, $E_{pg,i}$ is the half width of the dip structure in $N_i(\omega)$ around $\omega = 0$. Specifically, we define $E_{pg,i} = (\omega_i' - \omega_{LM,i})/2$ where $\omega_{LM,i} < 0$ is the frequency where $N_i(\omega)$ has a local maximum due to the pseudogap and $\omega_i' > 0$ is determined such that $N_i(\omega_i') = N_i(\omega_{LM,i})$. One sees that the dependence of $E_{pg,i}$ and $\Delta_{0,i}$ on $\lambda_{12}$ are qualitatively similar. As for the single-band BCS-BEC crossover, the pseudogap can be regarded as half the energy needed to excite a single-particle by breaking a preformed Cooper pair. The coexistence and different magnitudes of the pseudogap energy scales $E_{pg,1}$ and $E_{pg,2}$ indicates the emergence of binary coreformed Cooper pairs. It is consistent with our prediction of binary molecular BEC with different pair sizes in the strong-coupling regime. Indeed, different intraband pair-correlation lengths, corresponding to different Cooper pair size in each band, are obtained also within the mean-field approach at $T = 0$. The finding that $E_{pg,i}$ is smaller compared to $\Delta_{0,i}$ is also consistent with the single-band result. We note that in the strong pair-exchange coupling regime $\lambda_{12} \gtrsim 1.5$, $\mu_2 = \mu - E_0$ changes its sign due to the large two-body binding energy associated with $U_{22}$ as well as with $\lambda_{12}$ (see the inset of Fig. 4). In such a regime, $N_i(\omega)$ exhibits a fully-gapped structure and $E_{pg,i}$ progressively approaches the two-body binding energy. Although not shown here, $\mu_1$ also changes sign in the stronger coupling regime.

Finally, we report the phase diagram of the two-band BCS-BEC crossover for strong pair-exchange coupling $\lambda_{12} = 2$, as shown in Fig. 5. At weak intra-band couplings, two pseudogaps simultaneously open in the two bands. This multiple pseudogap formation originates from the strong pair-exchange coupling. On the other hand, when the intraband coupling in the shallow band increases, the two pseudogap temperatures deviate from each other, indicating multiple energy scales of pseudogaps as shown in Fig. 4. This multiple pseudogap regime evolves eventually into a molecular binary Bose gas regime. Although the boundaries between these regimes are not sharp, the temperature $T_{\mu=0}$ at which the chemical potential $\mu$ goes below the bottom of the deep band could be used as a qualitative crossover line separating the two regimes at low temperature.
In conclusion, we have demonstrated how multiple pseudogaps appear and when pair fluctuations are screened in the two-band BCS-BEC crossover at arbitrary pair-exchange couplings. While the pair fluctuations inducing the pseudogap are screened by multi-band effects at weak pair-exchange couplings, this screening regime turns into the multiple pseudogap formation at strong pair-exchange couplings due to interband pair fluctuations. We have constructed the phase diagram of the two-pseudogap state in the temperature and pair-exchange coupling plane, and show the pseudogap temperatures where single and multiple pseudogaps appear in the single-particle density of states. Examining the pseudogap temperature in the shallow band, we have confirmed that the screening of pairing fluctuations due to the multi-band nature can be found in the BCS-BEC crossover regime. Furthermore, the different magnitudes of the pseudogaps indicates the presence of binary preformed Cooper pairs with different binding energies and sizes, as also confirmed from the comparison between the pseudogap size at the critical temperature and the mean-field energy gaps at $T = 0$.

We believe our results to be quite general: by relaxing, if required, some restrictions of the model specifically considered here, such as the fixed energy shift and the electron-like character of bands, the idea of multi-channel pairing fluctuations could be applied to a variety of strongly correlated multi-component systems such as cold atoms, electron-hole systems, nuclear matter, as well as nanostructured materials.

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