Interplay of the pseudogap and the BCS gap for heteropairs in $^{40}$K-$^{6}$Li mixture

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Abstract – The description of heteropairs like $^{40}$K-$^{6}$Li near and in the superconducting state requires a fully self-consistent theory (see Hanai R. and Ohashi Y., Phys. Rev. A, 90 (2014) 043622). We derive analytic pseudogap Green’s functions for the “normal” and superconducting states from the Luttinger-Ward theory with the $T$-matrix in the static separable approximation. The self-consistency in the closing loop of self-energy has two pronounced effects on the single-particle spectrum. First, the single-particle excitations decay before the asymptotic quasiparticle propagation is established, therefore the normal state is not a Fermi liquid. Second, the pseudogap has a V shape even for $s$-wave pairing. The V-shaped pseudogap and the U-shaped BCS gap interfere resulting in slope breaks of the gap walls and the in-gap states in the density of states. Various consequences of an incomplete self-consistency are demonstrated.

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The cold Fermi gas of 1:1 mixture of $^{40}$K and $^{6}$Li is expected to develop an unconventional superfluidity with Cooper pairs composed of different species [1]. If achieved, this phase transition offers experimental verification of theories of heteropairs condensation important also in other fields of physics, e.g., the color superconductivity [2]. Recently Hanai and Ohashi [3] have discussed the critical temperature using the Thouless criterion based on the instability of the normal state. They found that the two-particle $T$-matrix theory has to be fully self-consistent to describe the superconducting phase transition. Failure of partly or fully non-self-consistent approaches can be traced down to their ill-behaved density equation of state [4].

The fully self-consistent $T$-matrix approximation known as the Luttinger-Ward (LW) theory [5] results in a qualitatively correct density equation of state [6], but it suffers from two setbacks when applied to the pseudogap and superconducting states. First, there is no analytic formula for the pseudogap density of states (DOS) so that each observed signature requires independent numerical study. Second, although the $T$-matrix includes the pairing channel, the LW theory fails to describe the Bardeen, Cooper and Schrieffer (BCS) gap and it has to be modified to cover the superconducting state. This extension is not unique because several modifications are possible, which lead to distinguishable predictions for the DOS.

In this paper we derive an approximation convenient for eventual fits to experimental data on the BCS side of the BCS-BEC crossover. We start from analyses of single-particle excitations in the LW theory of the pseudogap state. Assuming the dominant role of low-lying preformed pairs, we adopt the static and separable approximation of the $T$-matrix. In this approximation we obtain an analytic Green’s function from which it is shown that the lifetime of excitations is the same as the time scale of binary correlations, therefore the quasiparticle concept is not applicable and the system is not a Fermi liquid. The corresponding DOS has the pseudogap. In spite of the $s$-wave pairing, the pseudogap has a V shape which compares well with numerical results of Hanai and Ohashi [3]. Then we modify the theory for the superconducting state and derive an analytic Green’s function which covers the combined effect of the V-shaped pseudogap and the U-shaped BCS gap on the single-particle excitation spectrum. We discuss approximations with and without feedback effect of the BCS gap on the pseudogap, which lead to substantially different resulting DOS.
Although we discuss a rather general effect of the self-consistent Green’s function in the closing loop on the single-particle energy spectrum, we prefer to relate all formulas to the specific example of $^{40}$K-$^6$Li gas and use the $^{40}$K and $^6$Li atomic masses in plots of the spectral functions.

The bare Green’s function for lithium atoms $G_{\text{FK}}^R(k) = 1/(\omega + i0 - \epsilon_{\text{Li}})$ depends on the kinetic energy $\epsilon_{\text{Li}} = |k|^2/(2m_{\text{Li}}) - \mu_{\text{Li}}$ counted from the chemical potential.

The only important interaction is between lithium and potassium atoms. It is tuned by the magnetic field with the Feshbach resonance enhancement in the scattering $s$-channel [1]. The self-consistent pseudogap-state Green’s function $G_{\text{FK}}^R(k) = G_{\text{FK}}^R(k) + G_{\text{FK}}^R(k)\Sigma_{\text{FK}}^R(k)G_{\text{FK}}^R(k)$ depends on the Li-K interaction via the self-energy

$$
\Sigma_{\text{FK}}^R(k) = \int \frac{d\Omega}{2\pi} \frac{dQ}{(2\pi)^3} T^R(Q)G_{\text{FK}}^A(Q - k) - \int \frac{d\Omega}{2\pi} \frac{dQ}{(2\pi)^3} T^< (Q) G_{\text{FK}}^A(Q - k),
$$

(1)

where $k \equiv (\omega, k)$ and $Q \equiv (\Omega, Q)$. We assume non-retarded contact interaction so that the $T$-matrix depends only on the four-momentum of the interacting pair. In the Fourier picture the contact interaction is independent of momentum, therefore, the wave function of pairs is isotropic having the $s$-wave symmetry.

The functions $G_{\text{FK}}^A(Q - k) = 2\text{Im}G_{\text{FK}}^A(Q - k)f_{\text{FD}}(\Omega - \omega)$ and $T^<(Q) = -2\text{Im}T^R(Q)f_{\text{BE}}(\Omega)$ include statistics. The potassium function remains small as $f_{\text{FD}} < 1$, while the two-particle function is large at very small frequencies $\Omega$ that appear only for very small pair momenta $Q$. Based on the dominant role of pairs with small four-momentum we adopt the approximation

$$
\Sigma_{\text{FK}}^R(k) \approx - D^2 G_{\text{FK}}^A (-k),
$$

(2)

with $D^2 = (2\pi)^{-4} \int d\Omega dQ T^<(Q)$. In the following we take the value of $D$ as a parameter and focus on properties of the single-particle spectral function and the density of states.

Equation (2) recalls the approximation of the pseudogap introduced by Maly et al. [7] who have numerically verified the dominant role of the low energy and momentum part of the $T$-matrix. In spite of this common point, our results sharply differ from [7], because we start from the LW theory so that the fully self-consistent Green’s function closes the loop of the self-energy (2), while studies of the pseudogap by Kathy Levin’s group [7,8] are based on the partly self-consistent and partly non–self-consistent theory of Kadanoff and Martin (KM) [9] with the bare Green’s function in the closing loop.

The advanced Green’s function of potassium satisfies an analogous equation with $\Sigma_{\text{FK}}^R(-k) \approx - D^2 G_{\text{FK}}^A(k)$. The set of these two equations has solution

$$
G_{\text{FK}}^R(k) = \frac{\omega + \epsilon_{\text{K}}}{2D^2} \left(1 - \eta \sqrt{1 - \frac{4D^2}{(\omega + \epsilon_{\text{K}})(\omega - \epsilon_{\text{Li}})}}\right),
$$

(3)

with $\eta = i \text{sign}(2\omega + \epsilon_{\text{K}} - \epsilon_{\text{Li}})$ if $0 < (\omega + \epsilon_{\text{K}})(\omega - \epsilon_{\text{Li}}) < 4D^2$ and $\eta = 1$ otherwise. The spectral function $A_{\text{FK}}(k) = (-1/\pi)\text{Im}G_{\text{FK}}^A(k)$ is shown in fig. 1(a). It is non-zero in two energy intervals $\frac{1}{2}(\epsilon_{\text{Li}} - \epsilon_{\text{K}}) - \frac{1}{\sqrt{2}}(\epsilon_{\text{Li}} + \epsilon_{\text{K}})^2 + 4D^2 < \omega < \min(-\epsilon_{\text{K}}, \epsilon_{\text{Li}})$, $\max(-\epsilon_{\text{K}}, \epsilon_{\text{Li}}) < \omega < \frac{1}{\sqrt{2}}(\epsilon_{\text{Li}} - \epsilon_{\text{K}}) + \sqrt{\frac{1}{4}(\epsilon_{\text{Li}} + \epsilon_{\text{K}})^2 + 4D^2}$.

For comparison we show in fig. 1(b) the spectral function of the KM theory which obtains using $\Sigma_{\text{FK}}^R(k) = - D^2 G_{\text{FK}}^A(-k)$ instead of the self-energy (2). The KM spectral function is of the BCS type having two $\delta$-functions at energies $\omega = \frac{1}{2}(\epsilon_{\text{Li}} - \epsilon_{\text{K}}) \pm \sqrt{\frac{1}{4}(\epsilon_{\text{Li}} + \epsilon_{\text{K}})^2 + 4D^2}$. Apparently, with the same approximation of the $T$-matrix, the KM and LW theories predict very different single-particle excitations. The KM theory results in quasiparticles of infinite lifetime, while the LW theory leads to excitations with non-exponential decay, see fig. 2. Both spectra show back-folding near the Fermi level which is experimentally confirmed for balanced gases [10–12]. The spectra differ, however, in the line shape. The $\delta$-peak of the KM theory broadened by the lifetime is symmetric while the LW “line” has higher weight on the side of the Fermi level in agreement with the momentum-dependent
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is shown for $\epsilon$ values of $\alpha$ the quasi-particle energy from 1 particle picture is not applicable. An attempt to define propagators and self-energies are comparable, the quasi-

The walls of the pseudogap (5) are convex functions, in contrast to the smeared BCS gap in which the concave region extends over more than a half of the gap bottom. The pseudogap found numerically by Hanai and Ohashi [3], see the lithium DOS in their fig. 5, has such convex walls. A wider but still narrow convex region resulted from the numerical study of the pure two-dimensional Li gas, see the low-temperature DOS in fig. 1 of [5].

The perturbation of the real part of the local Green’s function $g_{Li}(\omega) = N_{Li} \int_{-\infty}^{\infty} d\epsilon_{Li} \text{Re} \left[ G_{Li}^{R}(k) - G_{Li}^{0}(k) \right]$ is also analytic:

$$g_{Li}(\omega) = \frac{N_{Li}}{\pi} \text{Im} \left( \frac{1}{\omega - \epsilon_{Li}} \right).$$

Since the perturbation of the local Green’s function $g_{Li}(\omega) = i/\pi \int |h_{Li}(\omega)|^{2} d\epsilon_{Li} \text{Im} \left[ G_{Li}^{R}(k) - G_{Li}^{0}(k) \right]$ is large only in a very narrow region $|\omega| \sim 4D/(\alpha + 1/\alpha)$, the Kramers-Kronig relation $g_{Li}(\omega) = i/\pi \int d\omega' g_{Li}(\omega')/(\omega - \omega')$ provides an effective way to include the above neglected finite lifetime due to binary collisions of atoms, by shifting energies into the complex plane $\omega \rightarrow \omega + i/\tau$. We do not discuss this effect keeping $1/\tau \rightarrow 0$.

The T-matrix approach can be modified to cover the superconducting state in three ways, which we list in order of increasing level of self-consistency. First, building the loop in the self-energy from bare Green’s functions one obtains the KM theory in the version of Patton [13]. As shown by Hanai and Ohashi [3], partly self-consistent theories fail because the bare Green’s function depends on the self-consistent chemical potential and an effective Fermi surface of bare potassium atoms is strongly reduced. We remove this problem enforcing fixed Fermi momentum and show the KM theory for comparison. The second possibility is to postulate the pseudogap state as the normal state and add the BCS gap as $G_{Li}^{R}(k) = G_{Li}^{R}(k) - G_{Li}^{R}(k)\Delta^{2}/K_{Li}^{2}(k)$, which de-
of Cooper pairs, enabling formation of the BCS gap \([15]\) which enters the Green’s function as

\[
\hat{G}^R_{\text{Li}}(k) = G^R_{\text{Li}(k)}(k)
- G^R_{\text{Li}(k)}(k) \left[ D^2 G^A_{\text{K}}(-k) + \Delta^2 G^A_{\text{K}}(-k) \right] G^R_{\text{Li}(k)}. \tag{7}
\]

Here hats denote functions with the BCS gap included. Note that the gap does not enter the potassium propagator in the BCS self-energy \(-\Delta^2 G^A_{\text{K}}(-k)\) while the full self-consistency appears in the pseudogap self-energy \(-D^2 G^A_{\text{K}}(-k)\).

The three above theories can be classified as approximations of the \(T\)-matrix theory in terms of the Nambu-Gor’kov matrices \([16,17]\). Let us list them from the best to the crudest. In the Nambu-Gor’kov approach the gap function depends on energy and momentum due to the non-BCS off-diagonal self-energy emerging from relation \((1)\) with the anomalous function closing the loop. The multiple scattering theory \((7)\) obtains by neglecting this non-BCS off-diagonal term. The Gor’kov and KM theories obtain by approximating both potassium functions in eq. \((7)\) by \(G^A_{\text{K}}\) and \(G^A_{\text{0K}}\), respectively.

Equation \((7)\) together with the conjugated equation for \(\hat{G}^R_{\text{K}}(-k)\) are solved by

\[
\hat{G}^R_{\text{Li}}(k) = \frac{\omega + \epsilon_K}{2D^2/\Lambda} \left( 1 - \hat{\eta} \sqrt{1 - \frac{4D^2/\Lambda^2}{(\omega + \epsilon_K)(\omega - \epsilon_{\text{Li}})}} \right),
\tag{8}
\]

\[
\Lambda = 1 - \frac{\Delta^2}{2D^2} + \frac{\Delta^2}{2D^2\eta} \sqrt{1 - \frac{4D^2}{(\omega + \epsilon_K)(\omega - \epsilon_{\text{Li}})}} \]

\[
\hat{\eta} = \left\{ \begin{array}{ll}
\frac{\pi}{2} \arg \left( \frac{1 - 4D^2/\Lambda^2}{w^2 - \epsilon^2} \right), & 0 < w^2 - \epsilon^2 < 4D^2, \\
\i \text{ sign}(w\Lambda), & 4D^2 < w^2 - \epsilon^2 < 4D^2/\Lambda^2, \\
1, & \text{otherwise},
\end{array} \right.
\]

with \(\arg(\cdots) \in [-\pi, \pi]\) and \(w, \epsilon\) defined before \((4)\). The spectral function \(\hat{A}_{\text{Li}}(k) = (-1/\pi) \text{Im} \hat{G}^R_{\text{Li}}(k)\) is shown in Fig. 3: (Color online) Spectral function \(\hat{A}_{\text{Li}}(k)\) in the superconducting state for \((a)\) \(\Delta = 1.5D\) and \((b)\) \(\Delta = 3D\), with \(\epsilon_{\text{Li}} = \epsilon_0\), \(\epsilon_K = \epsilon/\alpha\), and different values of \(\epsilon\). The curves are shifted vertically for clarity. The sharp edges of the pseudogap spectrum persist in the superconducting state being more suppressed for the larger BCS gap \(\Delta\). For \(\Delta > 2D\) the spectrum is non-zero in four energy intervals, for \(\Delta < 2D\) these intervals merge in two intervals.

Fig. 4: (Color online) (a) Density of states for various BCS gaps \(\Delta\) in units of the pseudogap parameter \(D\). The “normal”-state pseudogap (thick line) has a \(V\) shape. As the density of the BCS condensate increases, it transforms into the \(U\) shape. Residual states in gap have non-analytic features like slope breaks and shoulders of in-gap states. (b) \(T\)-matrix with multi-ple scattering corrections (MSC) compared with the Kadanoff-Martin (KM) and Gor’kov theories. In all three theories the “normal”-state \(T\)-matrix is in the static approximation with the same value of the parameter \(D\).
The singular edges of the background pseudogap spectrum are maintained although their amplitude decreases with increasing BCS gap. These pseudogap edges result in the slope breaks and in-gap states seen in the DOS in fig. 4. When compared with single-particle spectroscopies [18], the sharp edges have to be smeared by the finite lifetime due to dissipative binary collisions omitted in the present approximation, and by thermal as well as other extrinsic effects affecting the energy resolution.

The DOS in the superconducting state displayed in fig. 4(a) for fixed pseudogap $D$ and a set of values of the BCS gap $\Delta$ shows that the gap maintains its V shape for small $\Delta < 2D$, develops into the U-shape gap with V-shape in-gap states for $\Delta > 2D$ which slowly vanish for $\Delta \gg 2D$. For $\Delta > 2D$ our model recalls the DOS of the 2D Hubbard model obtained by a Monte Carlo calculation restricted to static ($\Omega = 0$) correlations, see fig. 2(a) in [19]. In fig. 4(b) one can see that the gap region is very sensitive to self-consistency. The DOS resulting from KM theory have the fixed U shape with effective gap magnitude $\sqrt{\Delta^2 + D^2}$. The renormalized Gor’kov theory shows that the in-gap states are only slightly modified by the BCS gap effect on the non-condensed pairs, while the gap edges sharply differ.

In summary, we have derived analytic pseudogap Green’s functions for the “normal” and superconducting states. We have shown that the full self-consistency in the closing loop of the self-energy has pronounced effects on the single-particle spectrum. The “normal” state is not a Fermi liquid, because the quasiparticle formation time is the same as the quasiparticle lifetime. The pseudogap has a V shape in spite of the s-wave pairing. These features contrast with the partly self-consistent and partly non-self-consistent KM theory which predicts infinitely long-living quasiparticles and the U-shaped pseudogap. We have found that the V-shaped pseudogap has non-trivial interplay with the U-shaped BCS gap. In particular, the pseudogap features persist in the BCS gap causing slope breaks of the gap walls and in-gap states. The single-particle excitations in the superconducting state have non-exponential decay in time so that they escape a simple approximation by Bogliubov-Valatin quasiparticles.

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