Pseudogap phenomena near the BKT transition of a two-dimensional ultracold Fermi gas in the crossover region

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Abstract We investigate strong-coupling properties of a two-dimensional ultracold Fermi gas in the normal phase. In the three-dimensional case, it has been shown that the so-called pseudogap phenomena can be well described by a (non-self-consistent) $T$-matrix approximation (TMA). In the two-dimensional case, while this strong coupling theory can explain the pseudogap phenomenon in the strong-coupling regime, it unphysically gives large pseudogap size in the crossover region, as well as in the weak-coupling regime. We show that this difficulty can be overcome when one improve TMA to include higher order pairing fluctuations within the framework of a self-consistent $T$-matrix approximation (SCTMA). The essence of this improvement is also explained. Since the observation of the BKT transition has recently been reported in a two-dimensional $^6$Li Fermi gas, our results would be useful for the study of strong-coupling physics associated with this quasi-long-range order.

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1 Introduction

An ultracold Fermi gas is well known as a system with high tunability of various physical parameters\cite{1,2}. For example, one can experimentally tune the strength of a pairing interaction associated with a Feshbach resonance. This has enabled us to systematically study how superfluid properties continuously change from the weak-coupling BCS (Bardeen-Cooper-Schrieffer) $\lambda$-type to the BEC (Bose-Einstein condensation) of tightly bound molecular boson with increasing the interaction strength, which is also referred to as the BCS-BEC crossover in the literature. In the crossover region, pairing fluctuations are expected to be strong near the superfluid phase transition temperature $T_c$, so that the so-called pseudogap phenomenon has been discussed there\cite{3,4}. Another example of the high tunability is the realization of a low dimensional Fermi gas by using an optical lattice technique. Since pairing fluctuations are enhanced by the

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low dimensionality of the system, together with the tunable pairing interaction, this is also use for the study of strong-coupling physics in a systematic manner. In particular, two-dimensional Fermi gases have recently attracted much attention in this field\cite{5, 6, 7, 8, 9, 10, 11, 12}, because the quasi-long-range superfluid order, called the Berezinskii-Kosterlitz-Thouless (BKT) phase is expected there\cite{13, 14}. Indeed, various physical quantities, such as photoemission spectra\cite{6}, as well as thermodynamic quantities\cite{9, 12}, have been measured in this system, and the observation of BKT transition has recently been reported in a two-dimensional $^6$Li Fermi gas\cite{10, 11}.

In the three-dimensional case, a (non-self-consistent) $T$-matrix approximation (the detail of which is explained in Sec. 2) has been extensively used to successfully explain various interesting phenomena observed in the BCS-BEC crossover region\cite{15, 16, 17}. In this regard, however, when TMA is applied to the two-dimensional case, while it is valid for the strong-coupling regime, it overestimates strong-coupling effects in the weak-coupling regime\cite{18, 19}. For example, TMA does not give free-particle density of states even in the weak-coupling regime, when the pairing interaction is very weak. Thus, in the current stage of research, it is a crucial theoretical issue to improve TMA so that one can correctly deal with the weak-coupling regime.

In this paper, we show that the self-consistent $T$-matrix approximation (SCTMA), which involves higher-order pairing fluctuations than TMA, meets our demand. Within this framework, we clarify how the so-called pseudogap phenomenon disappears in a two-dimensional Fermi gas as one approaches the weak-coupling regime from the strong-coupling side. Comparing SCTMA results with TMA ones, we also discuss the reason why the above mentioned problem in TMA can be eliminated in SCTMA.

Throughout this paper, we take $\hbar = k_B = 1$ and the two-dimensional system area is taken to be unity, for simplicity.

2 Formulation

We consider a two-dimensional uniform Fermi atomic gas consisting of two atomic hyperfine states, described by the BCS Hamiltonian,

$$H = \sum_{p, \sigma} \xi_p c_{p, \sigma}^\dagger c_{p, \sigma} - U \sum_{p, q} c_{p+q/2, \uparrow}^\dagger c_{p+q/2, \downarrow} c_{p, \uparrow} c_{p, \downarrow},$$

(1)

Here, $c_{p, \sigma}^\dagger$ is a creation operator of a Fermi atom with pseudospin $\sigma = \uparrow, \downarrow$ and the two-dimensional momentum $p = (p_x, p_y)$. $\xi_p = p^2/(2m) - \mu$ is the kinetic energy, measured from the Fermi chemical potential $\mu$, where $m$ is an atomic mass. The pairing interaction $-U (< 0)$ is assumed to be tunable by adjusting the threshold energy of a Feshbach resonance. As usual, we measure the interaction strength in terms of the two-dimensional $s$-wave scattering length $a_{2D}$, which is related to $U$ as\cite{20},

$$\frac{1}{U} = \frac{m}{2\pi} \ln(k_F a_{2D}) + \sum_{p \geq k_F} \frac{m}{p^2},$$

(2)

where $k_F = \sqrt{2\pi m N}$ is the Fermi momentum, with $N$ being the total number of Fermi atoms. Using this scale, $\ln(k_F a_{2D}) \ll -1$ ($\gg 1$) corresponds to the strong-coupling (weak-coupling) regime. $-1 \lesssim \ln(k_F a_{2D}) \lesssim 1$ is the crossover region.
Many-body corrections to Fermi single-particle excitations can be conveniently incorporated into the theory by considering the self-energy \( \Sigma(p, i\omega_n) \) in the single-particle thermal Green’s function,

\[
G(p, i\omega_n) = \frac{1}{i\omega_n - \xi_p - \Sigma(p, i\omega_n)}.
\]  

Here, \( \omega_n \) is the fermion Matsubara frequency. The self-energy \( \Sigma(p, i\omega_n) \) in the self-consistent \( T \)-matrix approximation (SCTMA) is diagrammatically described as Fig. 1(a), which gives

\[
\Sigma(p, i\omega_n) = T \sum_{q, iv_n} \Gamma(q, iv_n) G(q - p, iv_n - i\omega_n).
\]  

Here, \( \nu_n \) is the boson Matsubara frequency. The particle-particle scattering matrix \( \Gamma(q, iv_n) \) in SCTMA has the form (see the second line in Fig. 1(a))

\[
\Gamma(q, iv_n) = -\frac{U}{1 - U\Pi(q, iv_n)},
\]  

where

\[
\Pi(q, iv_n) = T \sum_{p, i\omega_n} G(p + \frac{q}{2}, iv_n + i\omega_n) G(-p + \frac{q}{2}, -i\omega_n).
\]

is a pair-correlation function, describing fluctuations in the Cooper channel.

The self-energy \( \Sigma^{TMA}(p, i\omega_n) \) in the non-self-consistent \( T \)-matrix approximation (TMA) is given by replacing all the dressed Green’s functions in the SCTMA \( \Sigma(p, i\omega_n) \) by the free Fermi Green’s functions \( G_0(p, i\omega_n) = (i\omega_n - \xi_p) \) as shown in Fig. 1(b). That is,

\[
\Sigma^{TMA}(p, i\omega_n) = T \sum_{q, iv_n} \Gamma^{TMA}(q, iv_n) G_0(q - p, iv_n - i\omega_n),
\]

where \( \Gamma^{TMA}(q, iv_n) = -U/(1 - U\Pi^{TMA}(q, iv_n)) \) and the TMA pair correlation function is given by

\[
\Pi^{TMA}(q, iv_n) = T \sum_{p, i\omega_n} G_0(p + \frac{q}{2}, iv_n + i\omega_n) G_0(-p + \frac{q}{2}, -i\omega_n).
\]

Because of this simplification, in contrast to SCTMA, strong coupling corrections to Fermi single-particle excitations, as well as the resulting pseudogap phenomenon, are completely ignored in evaluating the TMA particle-particle scattering matrix \( \Gamma^{TMA}(q, iv_n) \). We will show how this ignorance leads to the overestimation of the pseudogap phenomenon in the weak-coupling case when \( \ln(\xi_0 a_{2D}) \geq 0 \).

In both SCTMA and TMA, the Fermi chemical potential \( \mu \) is determined from the equation of the total number \( N \) of Fermi atoms,

\[
N = 2T \sum_{p, i\omega_n} G(p, i\omega_n).
\]
Calculated density of states $\rho(\omega)$ in a two-dimensional Fermi gas. The solid line and the dashed line show the results in SCTMA and TMA, respectively. $\rho_0 = m/2\pi$ is the density of state in a two-dimensional free Fermi gas. We set $\ln(k_F a_{2D}) = 0.57$, and $T = T_{BKT} = 0.146T_F$, where $T_{BKT}$ is the observed BKT phase transition temperature at this interaction strength in a $^6$Li Fermi gas[10,11]. (Color figure online.)

We then examine the pseudogap appearing in the single-particle density of states $\rho(\omega)$, given by

$$\rho(\omega) = -\frac{1}{\pi} \sum_p \text{Im} G(p, i\omega_n \to \omega + i\delta).$$  \hspace{1cm} (9)

We briefly note that neither SCTMA nor TMA can describe the BKT phase transition temperature $T_{BKT}$. Thus, this paper only deals with the normal phase above $T_{BKT}$.

### 3 Pseudogap Phenomena in the crossover regime

Figure 2 shows the density of states (DOS) $\rho(\omega)$ in a two-dimensional Fermi gas, when $\ln(k_F a_{2D}) = 0.57$ (in the crossover region) at the observed BKT phase transition temperature $T_{BKT} = 0.146T_F$ (where $T_F$ is the Fermi temperature) in a $^6$Li Fermi gas[10,11]. We see that SCTMA gives a pseudogap, that is, a dip structure around $\omega = 0$. As discussed in the three-dimensional case [15], this dip structure originates from pairing fluctuations around the Fermi surface, and the resulting formation of preformed Cooper pairs. Such an anomalous structure is also seen in the case of TMA, as shown in Fig.2. However, the pseudogap structure in this case is much more remarkable than that in the case of SCTMA, and the overall structure is rather close to the BCS-type superfluid density of states with the coherence peaks of the gaps edges (although the system in the present case is still in the normal state). At this interaction strength, the binding energy $E_b = 1/(ma_{2D}^2)$ of a two-body bound state equals $E_b = 0.64\epsilon_F$ (where $\epsilon_F$ is the Fermi energy). While this value is comparable to the pseudogap size seen in $\rho(\omega)$ in SCTMA in Fig. 2, the peak-to-peak energy in $\rho(\omega)$ in TMA ($\gg 4\epsilon_F$) is much larger than $E_b$. This implies that the pseudogap size in TMA does not reflect the binding energy of a preformed pair in this regime.

Figure 3 shows the interaction dependence of the density of states $\rho(\omega)$ when $T = 0.15T_F$. In the case of SCTMA shown in panel (a), the dip structure becomes less remarkable with decreasing the interaction strength, as expected. According to the preformed pair scenario for the pseudogap phenomenon [15], the pseudogap gradually disappears when $T \gtrsim E_b$. Noting that $E_b(\ln(k_F a_{2D}) = 1.23) = 0.17\epsilon_F$, and $E_b(\ln(k_F a_{2D}) = 1.72) = 0.064\epsilon_F$,}
one finds that the interaction dependence of the pseudogap structure seen in Fig. 3 (a) is consistent with this scenario.

However, a large gap still remains in the case of TMA even in the weak coupling case when \( \ln(k_Fa_{2D}) \approx 1.72 \), as shown in Fig. 3 (b). This is clearly contradict with the ordinary pseudogap case because \( T = 0.15T_F \) is much larger than the binding energy \( E_b = 0.064\epsilon_F \) at this interaction strength.

To explain the reason why TMA gives very different results form those in SCTMA in the weak-coupling regime (\( \ln(k_Fa_{2D}) \gg 0 \)), it is instructive to consider the weak-coupling limit \( \ln(k_Fa_{2D}) \rightarrow \infty \) at \( T = 0 \), where the system should become a free Fermi gas with no pseudogap. In a two-dimensional uniform system, although the Hohenberg-Mermin-Wagner theorem \([24, 25]\) prohibits the long-range superfluid order at \( T > 0 \), it may be realized at \( T = 0 \), when the Thouless criterion \([26]\),

\[
\Gamma^{-1}(q, iv_n) = 0, \tag{10}
\]

is satisfied. When one use \( \Gamma^{TMA}(q, iv_n) \) given below Eq. (7), the TMA Thouless criterion gives the chemical potential \( \mu_{TMA}(T = 0) = -E_b/2 \), indicating that all the Fermi atoms form two-body bound molecules with the binding energy \( E_b = 1/ma_{2D}^2 \). Even not in the weak-coupling limit but at \( \ln(k_Fa_{2D}) = 0.57 \), \( \mu_{TMA}(T) \) is found to approach \(-E_b/2 \approx -0.32\epsilon_F \) at low temperatures, as seen in Fig. 4. When the Thouless criterion in Eq. (10) is satisfied, one may approximate the self-energy in Eq. (7) to

\[
\Sigma^{TMA}(p, i\omega_n) \approx -\Delta_{PG}^2 G_0(-p, -i\omega_n),
\]

where \( \Delta_{PG} = \sqrt{-T \sum_{\mathbf{q}, iv_n} \Gamma^{TMA}(\mathbf{q}, iv_n)} \) is sometimes referred to as the pseudogap parameter in the literature \([15, 16, 19]\). In this so-called static approximation, the TMA Green’s function is approximated to

\[
G_{TMA}(p, i\omega_n) = -\frac{i\omega_n + \epsilon_p}{\omega_n^2 + \epsilon_p^2 + \Delta_{PG}^2}. \tag{11}
\]

Equation (11) just has the same form as the diagonal component of the mean-filed BCS Green’s function \([27]\), so that one has a clear energy gap with \( E_{PG} = 2\sqrt{|\mu_{TMA}|^2 + \Delta_{PG}^2} \). In addition, substituting Eq. (11) into the number equation (8) at \( T = 0 \), one obtains \( \Delta_{PG} = 2\sqrt{\epsilon_F(\epsilon_F - \mu_{TMA})} \), unphysically giving the large (pseudo) gap size as \( E_{PG} = 4\epsilon_F \gg 2E_b \), even in the weak-coupling limit.
In the case of SCTMA, the static approximation for the SCTMA Green’s function gives,

$$G_{\text{SCTMA}}(p, i\omega_n) = \frac{-i\omega_n + \xi_p}{\omega_p^2 + \xi_p^2 + 2\Delta_{\text{PG}}^2 \left[ 1 + \sqrt{1 + \frac{4\Delta_{\text{PG}}^2}{\omega_p^2 + \xi_p^2}} \right]^{-1}}.$$  

(12)

Apart from the factor $2 \left[ 1 + \sqrt{1 + \frac{4\Delta_{\text{PG}}^2}{\omega_p^2 + \xi_p^2}} \right]^{-1}$, Eq. (12) is still close to the diagonal component of the mean-filed BCS Green’s function. Indeed, when one uses Eq. (12) to evaluate the number equation (8), together with the Thouless criterion in Eq. (10), the resulting coupled equations are found to be formally close to the number equation at the gap equation in the mean-field BCS theory at $T = 0$, giving $\mu_{\text{SCTMA}} = \epsilon_F$, and $\Delta_{\text{PG}} = 0$, as expected.

The above discussions at $T = 0$ may be also applicable to the weak-coupling regime at the finite temperatures. In this case, although the Thouless criterion is, exactly speaking, not satisfied, the TMA chemical potential $\mu_{\text{TMA}}$ becomes very close to the value $\mu_{\text{TMA}}^\text{Th}$ (which satisfies Eq. (10) (where $\Gamma_{\text{TMA}}$ is used)) at low temperatures, as shown in Fig. 4. In the case of Fig. 4 the static approximation is considered to be valid for $T \lesssim 0.4T_F$, where an unphysically large pseudogap is expected in TMA density of states. In the case of SCTMA, $\mu_{\text{SCTMA}}$ becomes close to the value $\mu_{\text{SCTMA}}^\text{Th}$, which satisfies the Thouless criterion in Eq (10) (where $\Gamma$ in SCTMA is used), only when $T/T_F \lesssim 0.1$, so that the pseudogap structure in this case is not so remarkable as that in the TMA case.

Physically, when the Fermi chemical potential approximately satisfies the Thouless criterion ($\mu \approx \mu_{\text{Th}}$), strong pairing fluctuations cause a dip structure in the density of states $\rho(\omega)$ around $\omega = 0$. However, in the weak-coupling regime, since preformed pairs are dominantly formed around the Fermi surface, the appearance of the pseudogap would also suppress pairing fluctuations, as well as the pseudogap phenomenon. Such a feedback effect is, however, completely ignored in TMA, because the free propagator $G_0$ with no TMA self-energy is used in evaluating the particle-particle scattering matrix $\Gamma(q, i\nu_n)$. In this case, SCTMA treats pairing fluctuations in a consistent manner, so that the expected pseudogap behavior of the density of states is correctly obtained in the weak-coupling regime.
4 Summary

To summarize, we have discussed the pseudogap phenomenon in a two-dimensional ultra-cold Fermi gas in the crossover region, as well as in the weak-coupling regime. We showed that the pseudogap phenomenon associated with pairing fluctuations in this regime can correctly be treated by the self-consistent T-matrix approximation (SCTMA). In contrast to the ordinary (non-self-consistent) T-matrix approximation (TMA), which unphysically gives a large pseudogap in the density of states even in the weak-coupling regime, SCTMA gives a expected small pseudogap, which gradually disappears as one approaches the weak-coupling regime. We also pointed out the importance of a feedback effect in theoretically dealing with pairing fluctuations in this regime, which is completely ignored in TMA.

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References
1. V. Gurarie, and L. Radzihovsky, Ann. Phys. 332, 2 (2007).
2. I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008).
3. J.T. Stewart, J.P. Gaebler, D.S. Jin, Nature 454, 744 (2008)
4. J.P. Gaebler, et al., Nat. Phys. 6, 569 (2010).
5. K. Martiyanov, V. Makhalov, and A. Turlapov, Phys. Rev. Lett. 105, 030404 (2010).
6. M. Feld, et al., Nature 480, 75 (2011).
7. B. Fröhlich, et al., Phys. Rev. Lett. 106, 105301 (2011).
8. A. T. Sommer, et al., Phys. Rev. Lett. 108, 045302 (2012).
9. V. Makhalov, K. Martiyanov, and A. Turlapov, Phys. Rev. Lett. 112, 045301 (2014).
10. M. G. Ries, et al., Phys. Rev. Lett. 114, 230401 (2015).
11. P. A. Murthy, et al., Phys. Rev. Lett. 115, 010401 (2015).
12. K. Fenech, et al., Phys. Rev. Lett. 116, 045302 (2016).
13. V. L. Berezinskii, Sov. Phys. JETP 32, 493 (1971).
14. J. M. Kosterlitz, and D. J. Thouless, J. Phys. C 6, 1181 (1973).
15. S. Tsuchiya, R. Watanabe, and Y. Ohashi, Phys. Rev. A 80, 033613 (2009).
16. Q. J. Chen, and K. Levin, Phys. Rev. Lett. 102, 190402 (2009).
17. H. Hu, X.-J. Liu, P. D. Drummond, and H. Dong, Phys. Rev. Lett. 104, 240407 (2010).
18. F. Marsiglio, et al., Phys. Rev. B 91, 054509 (2015).
19. M. Matsumoto, D. Inotani, and Y. Ohashi, Phys. Rev. A 93, 013619 (2016).
20. S. A. Morgan, M. D. Lee, and K. Burnett, Phys. Rev. A 65, 022706 (2002).
21. R. Haussmann, Z. Phys. B: Condens. Matter 91, 291 (1993).
22. M. Bauer, M. M. Parish, T. Enss, Phys. Rev. Lett. 112, 135302 (2014).
23. B. C. Mulkerin, et al., Phys. Rev. A 92, 063636 (2015).
24. N. D. Mermin, and H. Wagner, Phys. Rev. Lett. 17, 1133 (1966).
25. P. C. Hohenberg, Phys. Rev. 158, 383 (1967).
26. D. J. Thouless, Ann. Phys. 10, 553 (1960).
27. J. R. Schrieffer, Theory of Superconductivity (Addison-Wesley, NY, 1964).
28. K. Miyake, Prog. Theor. Phys. 69, 6 (1983).