Pseudogap Pairing in Ultracold Fermi Atoms

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The Bose-Einstein condensate to Bardeen-Cooper-Schrieffer crossover in ultracold Fermi gases creates an ideal environment to enrich our knowledge of many-body systems. It is relevant to a wide range of fields from condensed matter to astrophysics. The nature of pairing in strongly interacting Fermi gases can be readily studied. This aids our understanding of related problems in high-temperature superconductors, whose mechanism is still under debate due to the large interaction parameter. Here, we calculate the dynamical properties of a normal, trapped strongly correlated Fermi gas, by developing a quantum cluster expansion. Our calculations for the single-particle spectral function agree with recent rf spectroscopy measurements, and clearly demonstrate pseudogap pairing in the strongly interacting regime.

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Ultracold Fermi atom experiments allow interparticle interactions, geometries, and spin species of atomic gases to be precisely controlled and tuned at will, leading to an exactly known model Hamiltonian [1]. Since rapid experimental progress is able to provide accurate data on both static [2–4] and dynamic [5–8] properties, this type of quantum simulation can definitively settle fundamental issues. An interesting example is momentum-resolved rf quantum simulation can definitively settle fundamental issues. The calculation of the pseudogap—the precursor of fermionic superconductivity—is entirely determined by knowledge of a single-particle excitation gap or pseudogaps in the Cooper-Schrieffer (BEC-BCS) crossover [6,8], which can be readily studied. This aids our understanding of related problems in high-temperature superconductors, whose mechanism is still under debate due to the large interaction parameter. Here, we calculate the dynamical properties of a normal, trapped strongly correlated Fermi gas, by developing a quantum cluster expansion. Our calculations for the single-particle spectral function agree with recent rf spectroscopy measurements, and clearly demonstrate pseudogap pairing in the strongly interacting regime.

In this Letter, we develop a quantum virial or cluster expansion [14–18] in describing strong pairing fluctuations at the BEC-BCS crossover is notoriously difficult due to the lack of a small interaction parameter [19]. The situation is most severe for dynamical properties, where different crossover theories lead to qualitatively different predictions. For the single-particle spectral function in the strong-coupling regime, some crossover theories predict a pseudogap—the precursor of fermionic pairing in the normal state above $T_c$ [20–24]—while some others [25] claim no such effects. Quantum Monte Carlo simulations of the spectral function is not conclusive [26].

In this Letter, we develop a quantum virial or cluster expansion to solve this delicate problem of dynamic properties for a normal, trapped, and strongly interacting Fermi gas. The advantages of this method are clear. First, the expansion has a controllable parameter [27,28]: the fugacity $z = \exp(\mu/k_BT)$ is small at high temperatures $T$. Second, the expansion coefficient or function at the $n$th order $(n \geq 2)$ is entirely determined by knowledge of a $n$-particle cluster. Multiparticle correlations, which are missing in most current crossover theories, can be easily accounted for and improved. Finally, the method is easily capable of treating external potentials or traps. We have estimated the validity of the expansion by comparing its predictions with experimental data for thermodynamics [19]. At the cusp of the crossover, where the $s$-wave scattering length $a_s$ diverges (unitarity limit [29]), it is applicable down to $0.47T_F$ for a trapped Fermi gas [19].

To develop the cluster expansion for general dynamical properties, let us consider two arbitrary linear operators of physical interest, $\hat{R}$ and $\hat{S}$, and the related Green function or correlation function at different space-time points,

$$
G(\mathbf{r}, \mathbf{r'}; \tau) = \frac{\text{Tr}[e^{-\beta(\mathcal{H}-\mu N)}\hat{R}(\mathbf{r}, \tau)\hat{S}^+(\mathbf{r'})]}{\text{Tr}e^{-\beta(\mathcal{H}-\mu N)}},
$$

where at finite temperatures we are working with an imaginary time $\tau$ in the interval $0 < \tau \leq \beta = 1/k_BT$. At high temperatures, both numerator and denominator may be expanded into the powers of $\beta \ll 1$, leading to $G(\mathbf{r}, \mathbf{r'}; \tau) = (X_0+zX_1+\cdots)/(1+zQ_1+\cdots) = X_0+z(X_1-X_0Q_1)+\cdots$, where $X_n = -\text{Tr}[e^{-\beta H}\hat{R}(\mathbf{r}, \tau)\hat{S}^+(\mathbf{r'})]$ is the expansion function and $Q_n = \text{Tr}[e^{-\beta H}]$ is the cluster partition function. The above expansion is to be referred to as the cluster expansion of correlation function, $G(\mathbf{r}, \mathbf{r'}; \tau) = G^{(0)}(\mathbf{r}, \mathbf{r'}; \tau) + zG^{(1)}(\mathbf{r}, \mathbf{r'}; \tau) + \cdots$, where

$$
G^{(0)}(\mathbf{r}, \mathbf{r'}; \tau) = X_0, \quad G^{(1)}(\mathbf{r}, \mathbf{r'}; \tau) = X_1 - X_0Q_1, \quad \text{etc.}
$$

The experimentally measured spectral function $A(\mathbf{k}, \omega)$ can be calculated from the correlation function via analytic continuation, so that we may write accordingly, $A(\mathbf{k}, \omega) = A^{(0)}(\mathbf{k}, \omega) + zA^{(1)}(\mathbf{k}, \omega) + \cdots$. The calculation of the $n$th expansion coefficient $G^{(n)}(\mathbf{r}, \mathbf{r'}; \tau)$ or $A^{(n)}(\mathbf{k}, \omega)$ requires the knowledge of solutions up to the $n$-body problem, including both energy levels and wave functions (see Appendix). In this work we aim to calculate the leading effects, which give the second-order expansion function.
The next-order expansion function [28] is not treated here for simplicity.

To calculate the single-particle spectral function $A(k, \omega)$, we take the annihilation field operators $\hat{\Psi}_\sigma(r, \tau)$ ($\sigma = \uparrow, \downarrow$) for $\hat{R}$ or $\hat{S}$ (see Appendix). Figure 1 shows contour plots of the occupied spectral intensity of a trapped Fermi gas in the crossover at $T = 0.7T_F$. At this temperature, our results are quantitatively reliable [19]. We observe that, in addition to the response from coherent Landau quasiparticles (black lines), there is a broad incoherent spectral weight centered about $\omega + \mu = -\epsilon_k - \epsilon_F$ (white dashed lines), where $\epsilon_k = h^2k^2/(2m)$ and $\epsilon_F = h^2/(ma_F^2)$ is the binding energy. Thus, the spectra clearly exhibit a gaplike double peak structure in the normal state. This is a remarkable feature: the dispersion at negative energies seems to follow the BCS-like dispersion curve, $\omega = -\sqrt{(\epsilon_k - \mu)^2 + \Delta^2}$, and behaves as if the gas were superconducting, even though we are above the critical temperature $T_c$. Therefore, the incoherent spectral weight indicates the tendency of pseudogap: the precursor of fermionic pairing due to strong attractions, i.e., it arises from the atoms in the paired state or “molecules.” The pairing interaction necessarily implies a finite spectral weight at negative energies. At $k \approx k_F$, we anticipate that many-body correlations will become increasingly important.

For an absolute comparison with experiment [6], we perform calculations using realistic experimental parameters, including the measurement resolution. Figure 2 presents the results on the BEC side of crossover with $1/(k_Fa_F) = 1.1$. The temperature $T = 0.45T_F$ is estimated from an initial temperature $T_i = 0.17T_F$ obtained before the field sweep to the BEC side [6]. The experimentally observed upper and lower features, caused, respectively, by unpaired atoms and molecules, are faithfully reproduced. In particular, the experimental data for the quasiparticle dispersion of molecules, marked by white symbols, agrees with our theory (lower red dashed line). There is also a qualitative agreement for the energy distribution curves [Figs. 2(b) and 2(e)] and the occupied density of states [Figs. 2(c) and 2(f)]. A narrow peak due to free atoms and a broader feature due to molecules are reproduced theoretically with very similar width at nearly the same position. It is impressive that our simple quantum cluster expansion is able to capture the main feature of the experimental spectra. In contrast, a more complicated crossover theory with adjustable parameters fails to account for the free-atom contribution with similar parameters [24].

![Figure 1](https://example.com/fig1.png)

**FIG. 1 (color online).** Contour plots of the occupied spectral intensity at crossover. The intensity $I(\omega) = A(k, \omega)f(\omega)k^2/(2\pi^2)$ increases from blue ($10^{-3}I_{\text{max}}$) to red ($I_{\text{max}}$) in a logarithmic scale. The calculations were performed with harmonic traps at $T = 0.7T_F$ and $1/(k_Fa_F) = +1, 0, -1$, with a resulting fugacity at the trap center of $\zeta \approx 0.14, 0.42, \text{and } 0.48$, respectively.

![Figure 2](https://example.com/fig2.png)

**FIG. 2 (color online).** Single-particle excitation spectra on the BEC side of crossover. (a)–(c) Cluster expansion predictions ($\zeta = 0.1$ and $\mu \approx -1.08\epsilon_F$). (d),(e) Corresponding experimental data [6]. (a) The linear-scale intensity map. Our results were convoluted with a Gaussian broadening curve of width $\sigma = 0.22\epsilon_F$, to account for the measurement resolution [6]. The black line shows upper free-atom dispersion. The red dashed line is the lower dispersion curve of molecules, obtained via fitting each fixed-$k$ energy distribution curve [in (b)] with a two Gaussian distribution. It agrees fairly well with the experimental result (white symbols). (b) Energy distribution curves for selected values of $k$. (c) The occupied density of state (DOS). Blue dashed lines show the experimental peak positions.
Figure 3 reports the spectra in the unitarity limit at the critical temperature $T_c = 0.2T_F$. At such low temperatures, the use of a cluster expansion becomes highly questionable as the fugacity at the center $z = 6 \gg 1$. Nevertheless, we find that the dispersion curve is lowered by the attractions by an amount comparable to the Fermi energy $\epsilon_F$, as shown clearly by the red dashed line in Fig. 3(a). The calculated energy distribution curves bifurcate from a single peak with increasing $k$ and becomes dominated by the lower molecular branch [Fig. 3(b)], which eventually leads to the bending back of the dispersion curve to negative energy. This picture is suggestive of the existence of a pseudogap and is consistent with the experimental findings [Fig. 3(e)]. This surprisingly good agreement merits further investigation. We conjecture that even at these relatively low temperatures the virial expansion captures the dominant two-body correlations measured in these experiments, apart from a possible overall scaling factor due to the missing higher-order terms.

To study the temperature dependence of pseudogap pairing, we show in Fig. 4 the unitary spectral intensity at $T/T_c = 1.2$, $1.5$, and $2.0$, to be compared with the most recent measurement at JILA [8]. In this logarithmic scale, a pseudogap structure is clearly visible at about $k \sim 0.5k_F$ and $\omega + \mu \sim -0.5\epsilon_F$. The response is reduced with increasing temperature and becomes significantly weak once $T > 2T_c$. However, it seems difficult to accurately determine a characteristic temperature above which the pseudogap response disappears.

In conclusion, the results obtained here provide a good qualitative explanation for the recent single-particle spectral function measurement in trapped strongly interacting ultracold fermions. It demonstrates the precursor of fermionic pairing in the normal but strongly interacting regime. In the near future, tomographic rf spectroscopy may be used to reveal locally the homogeneous spectral function. Our calculation can be extended to a uniform gas, for which we expect a stronger pairing response and a wider temperature window for pseudogap. Our method is also applicable directly to multicomponent atomic Fermi gases and can be used to understand the intriguing triplet and quadruplet pairing in their dynamic responses.

Appendix: General rules of cluster expansion.—To calculate the Green function or correlation function, it is convenient to separate out the contribution arising from interactions. To this aim, for any physical quantity $Q$ we may write $Q = Q^{(0)} + Q^{(N)}$, where the superscript “$N$” in $Q^{(N)}$ denotes the part of a noninteracting system having the same fugacity. The operator $\{\}^{(0)}$ then picks up the residues due to interactions. We then may write

$$G(r, r'; \tau) = \{G(r, r'; \tau)\}^{(0)} + G^{(N)}(r, r'; \tau),$$

where $\{G\}^{(0)}$ can be expanded in terms of $\{X_{\alpha}\}^{(0)}$.

For the single-particle spectral function, we determine first the Green’s function $G_{\alpha\sigma}(r, r'; \tau)$ by taking $\hat{R} = \hat{\Psi}_\sigma$ and $\hat{S} = \hat{\Psi}_{\sigma'}$. Then, we take the Fourier transformation with respect to $\tau$, to obtain $G_{\alpha\sigma}(r, r'; i\omega_n)$. The spectral

FIG. 3 (color online). Single-particle excitation spectra of a strongly interacting Fermi gas. (a)–(c) Cluster expansion predictions ($z = 6$ and $\mu = 0.37\epsilon_F$). (d), (e) Corresponding experimental data [6]. In (e), for the experimental energy distribution curves, we use a larger value of $k$ (i.e., enlarged by a factor of $5/3$) to account for a scaling discrepancy due to many-body correlations.

FIG. 4 (color online). Temperature dependence of the spectral intensity at unitarity. (a)–(c) The intensity increases from blue ($10^{-3}\omega_{\text{max}}$) to red ($\omega_{\text{max}}$) in a logarithmic scale. (d), (e) Temperature dependence of the fugacity and chemical potential at unitarity. Our leading cluster expansion appears to be applicable at $T \geq 0.4T_F$, where $z \sim 1$ or $\mu \sim 0$ [19].
A final Fourier transform on $r - r'$ leads to $A_{\sigma\sigma'}(k, \omega)$, as measured experimentally. For a normal, balanced Fermi gas, $A_{\parallel} = A_{\parallel} = A(k, \omega)$ and $A_{\parallel} = 0$.

Leading expansion of spectral function.—The leading term of \{G(k, \omega', \tau)\} takes the form

$$- \frac{\alpha^2}{2} \exp[-\beta(\omega' - \omega - \mu) + i\omega' \tau] \delta(t - \tau) \delta(k - k'),$$

where $\alpha^2$ is the superfluid density, $\omega'$ is the frequency, $\tau$ is the time delay, and $k'$ is the momentum.

The leading term of $\{G_{\parallel}(r, r', \tau)\}$ takes the form

$$- \frac{\alpha^2}{2} \exp[-\beta(\omega' - \omega - \mu) + i\omega' \tau] \delta(t - \tau) \delta(k - k'),$$

where $\alpha^2$ is the superfluid density, $\omega'$ is the frequency, $\tau$ is the time delay, and $k'$ is the momentum.

The trace has to be taken over all the single-particle states (i.e., $\psi_p$, with energy $\epsilon_p$) for a spin-down fermion. We insert in the bracket an identity $\sum_Q \langle Q | \langle Q | \delta(1 + e^{-\beta(\omega' - \omega - \mu)})e^{-\beta(\omega' - \omega - \mu)}F_{\rho \varphi}(r, r') \rangle$.

Accordingly, the leading interaction correction to the spectral function $A(k, \omega)$ is given by

$$z(1 + e^{-\beta\omega}) \sum_p \langle \delta(1 + e^{-\beta(\omega' - \omega - \mu)})e^{-\beta(\omega' - \omega - \mu)}F_{\rho \varphi}(r, r') \rangle,$$

where $F_{\rho \varphi}(r) = f d\tau dr_{1} dr_{2} \psi_{p}^{*}(r_{1}) \Phi_{Q}(r, r_{1}) \Phi_{Q}^*(r_{2}, r_{2}) \psi_{p}(r_{2})$.

In an isotropic harmonic trap with frequency $\omega_0$, we solve exactly the two-fermion problem for relative wave functions [28] and obtain $\{A(k, \omega)\}$ using the above procedure. In the end, we calculate

$$I(k, \omega) = \frac{k^2}{2\pi^2} \{[A(k, \omega)] f(\omega) + A(\omega) f(\omega)\},$$

as measured experimentally [6,8]. Here, $f(\omega) = 1/(e^{\beta\omega} + 1)$ and the ideal spectral function $A(\omega) = 4\pi^2/\hbar^2(\omega + \mu + i\epsilon)^{1/2}$. To account for the experimental resolution, we further convolute $I(k, \omega)$ with a Gaussian broadening curve.

In the BEC limit, we may show analytically that

$$\{A(k, \omega)\} f \propto \exp[-\beta(\sqrt{\epsilon_0} - \omega - \mu - \epsilon_B - \sqrt{\epsilon_0}^{1/2})],$$

where $\epsilon_B = \hbar^2/(ma^2)$ is the binding energy. Thus, at large $k$ the intensity peaks at $\omega + \mu = -\epsilon_0 - \epsilon_B$, with a width $\sim\sqrt{\epsilon_0} T \epsilon_B$.

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