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Equation of state of a superfluid Fermi gas in the BCS-BEC crossover

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Abstract. – We present a theory for a superfluid Fermi gas near the BCS-BEC crossover, including pairing fluctuation contributions to the free energy similar to that considered by Nozières and Schmitt-Rink for the normal phase. In the strong coupling limit, our theory is able to recover the Bogoliubov theory of a weakly interacting Bose gas with a molecular scattering length very close to the known exact result. We compare our results with recent Quantum Monte Carlo simulations both for the ground state and at finite temperature. Excellent agreement is found for all interaction strengths where simulation results are available.

The recent experimental realization of strongly interacting Fermi gases of ^{6}Li and ^{40}K atoms near a Feshbach resonance has opened up the exciting possibility of investigating the crossover from a Bardeen-Cooper-Schrieffer (BCS) superfluid to a Bose-Einstein condensate (BEC) [1–5]. In these systems, the inter-atomic interaction strength can be varied by tuning the energy of a near-resonant molecular state with a magnetic field.

Below resonance where the s-wave scattering length a is positive, stable diatomic molecules are observed to form a BEC at low temperatures. Above resonance, with $a < 0$, the molecules dissociate and form a BCS superfluid of fermionic pairs. In the crossover region where the scattering length a is large one can access a new, strongly correlated regime known as the unitary limit [6]. Recent experiments in the crossover regime have found evidence for this transition by measuring low-lying collective modes [2, 7, 8] and heat capacity [4, 9].

These rapid experimental developments constitute an ideal testing ground for theoretical studies of the BCS-BEC crossover. However, theoretical results available in the literature are limited in the strongly correlated unitary regime. The first systematic study of the crossover at zero temperature was provided by Eagles and Leggett based on BCS mean-field equations [10, 11]. Later, the effects of pair fluctuations were considered by Nozières and Schmitt-Rink (NSR) at temperatures above the superfluid transition [12,13]. This was recently extended to the superfluid phase by Strinati *et al.* using finite-temperature Green functions [14,15].

Extensions of these approaches to take into account the bare Feshbach molecule have also been presented [16, 17], with the conclusion that additional two-channel effects can be

neglected for broad resonances and detunings near the crossover regime [18, 19]. All these studies give a qualitative description of the crossover: but none of them are quantitatively correct in the unitary limit, and in the BEC region. A major drawback of these theories is that the predicted value of the molecular scattering length in the deep BEC regime, $a_m = 2a$, does not agree with the exact result from the solution of the four-body problem [20–22], *i.e.*, $a_m \simeq 0.60a$. This much lower value is, however, consistent with Quantum Monte Carlo (QMC) simulations [23, 24].

The purpose of the present letter is to develop a *quantitatively* reliable theory for superfluid Fermi gases in the broad resonance or single-channel limit, at all interaction strengths and low enough temperatures. To this end, we extend the NSR analysis to the superfluid phase on top of the BCS mean-field approximation. An essential ingredient of our theory is that the number equation, *i.e.*, the relation $n = -\partial\Omega/\partial\mu$, is satisfied for the full thermodynamic potential Ω —not just for the mean-field contribution to Ω. In the deep BEC limit, where molecule-molecule correlations are important, this requirement renormalizes the mean-field molecular scattering length of $a_m = 2a$ to a value of $a_m \simeq 0.57a$ [25], which is very close to the exact four-body prediction [20]. As a consequence, our results for the equation of state at zero temperature along the full range of the BCS-BEC crossover are in excellent agreement with the QMC data [23]. The temperature-dependent results also agree with recent path integral Monte Carlo calculations [26].

The system we consider is a uniform gas of N Fermi atoms in two hyperfine states denoted as pseudo-spins $\sigma = \uparrow, \downarrow$, with $N_\uparrow = N_\downarrow = N/2$. To characterize the superfluid ground state, we introduce explicitly an order parameter Δ that will be determined at the mean-field level, and use the Nambu spinor representation, in which the system is described by the Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{V}_\Delta + \mathcal{V}_{int}$, with the terms

$$\mathcal{H}_0 = \sum_{\boldsymbol{k}} \psi^\dagger_{\boldsymbol{k}} \left[\xi_{\boldsymbol{k}}\sigma_z - \Delta\sigma_x\right] \psi_{\boldsymbol{k}} + \sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}}, \tag{1}$$

$$\mathcal{V}_\Delta = \sum_{\boldsymbol{k}} \psi^\dagger_{\boldsymbol{k}} \Delta\sigma_x \psi_{\boldsymbol{k}}, \tag{2}$$

$$\mathcal{V}_{int} = \frac{U_0}{2} \sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}} \left(\psi^\dagger_{\boldsymbol{k}+q}\sigma_z\psi_{\boldsymbol{k}}\right)\left(\psi^\dagger_{\boldsymbol{k}'-\boldsymbol{q}}\sigma_z\psi_{\boldsymbol{k}'}\right), \tag{3}$$

where $\psi^\dagger_{\boldsymbol{k}} = (c^\dagger_{\boldsymbol{k}\uparrow}, c_{-\boldsymbol{k}\downarrow})$ is the Nambu creation field operator for Fermi atoms with the kinetic energy $\xi_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}} - \mu = \hbar^2\boldsymbol{k}^2/2m - \mu$, μ is the chemical potential, and σ_x and σ_z are the 2×2 Pauli matrices. The contact interaction U_0 for atom-atom interactions is renormalized by introducing the s-wave scattering length a. This is defined by the low-energy limit of the two-body scattering problem via $(4\pi\hbar^2 a/m)^{-1} = U_0^{-1} + \sum_{\boldsymbol{k}}(2\epsilon_{\boldsymbol{k}})^{-1}$.

After taking into account anti-commutators, the "unperturbed" term $\mathcal{H}_0$ can be identified as the standard BCS mean-field Hamiltonian. In variational calculations, the approximate ground state would be an eigenstate of $\mathcal{H}_0$, with Δ varied to minimize the total energy [16]. However, this approach is inappropriate on the BEC side of the transition, where molecule-molecule scattering gives rise to strong density correlations involving four particles rather than just two. The purpose of the present letter is to describe an approximate perturbation expansion which takes this into account.

A diagrammatic expansion is performed in terms of the propagator of the "free" Hamiltonian $\mathcal{H}_0$, which is given by

$$\boldsymbol{G}_0(\boldsymbol{k}, i\omega_m) = \begin{bmatrix} \mathcal{G}(\boldsymbol{k}, i\omega_m) & \mathcal{F}(\boldsymbol{k}, i\omega_m) \\ \mathcal{F}(\boldsymbol{k}, i\omega_m) & -\mathcal{G}(\boldsymbol{k}, -i\omega_m) \end{bmatrix}. \tag{4}$$

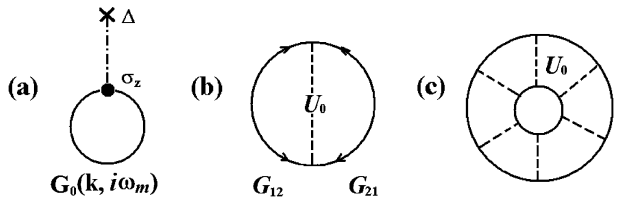

Fig. 1 – Diagrammatic representations of the mean-field contributions ((a) and (b)) and the pairing fluctuation contributions (c) to the thermodynamic potential. The full line represents $\boldsymbol{G}_0(\boldsymbol{k}, i\omega_m)$, the line with arrows describes the anomalous Green function $G_{12} = G_{21} = \mathcal{F}(\boldsymbol{k}, i\omega_m)$, and the dashed line is U_0.

Here $\mathcal{G}(\boldsymbol{k}, i\omega_m) = -[i\omega_m + \xi_{\boldsymbol{k}}]/[\omega_m^2 + E_{\boldsymbol{k}}^2]$ and $\mathcal{F}(\boldsymbol{k}, i\omega_m) = \Delta/[\omega_m^2 + E_{\boldsymbol{k}}^2]$ are, respectively, the BCS normal and anomalous Green functions, while $E_{\boldsymbol{k}} = [\xi_{\boldsymbol{k}}^2 + \Delta^2]^{1/2}$ denotes the single-particle excitation energy and $\omega_m = (2m+1)\pi/(\hbar\beta)$ is the fermionic Matsubara frequency with inverse temperature $\beta = 1/k_B T$. The associated "unperturbed" thermodynamic potential then takes the form, $\Omega_0 = 1/\beta \sum_{\boldsymbol{k},m} \mathrm{Trln}\, \boldsymbol{G}_0(\boldsymbol{k}, i\omega_m) + \sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} = \sum_{\boldsymbol{k}}[(\xi_{\boldsymbol{k}} - E_{\boldsymbol{k}}) + 2/\beta \ln f(-E_{\boldsymbol{k}})]$, where $f(x) = 1/(e^{\beta x}+1)$ is the Fermi function.

The contributions of interactions to the thermodynamic potential consist of a static mean-field part and a fluctuation part originating from the particle-particle Cooper channel. As shown diagrammatically in figs. 1a and b, the mean-field corrections from $\mathcal{V}_\Delta$ and $\mathcal{V}_{int}$ read, respectively, $\delta\Omega_\Delta = 1/\beta \sum_{\boldsymbol{k},m} \Delta \mathrm{Tr}[\sigma_x \boldsymbol{G}_0(\boldsymbol{k}, i\omega_m)] = -2\Delta^2/U_0$ and $\delta\Omega_{mf} = U_0 \times [1/\beta \sum_{\boldsymbol{k},m} \mathcal{F}(\boldsymbol{k}, i\omega_m)]^2 = \Delta^2/U_0$, where we have used the mean-field gap equation

$$-\frac{m}{4\pi\hbar^2 a} = \sum_{\boldsymbol{k}} \left[\frac{1 - 2f(E_{\boldsymbol{k}})}{2E_{\boldsymbol{k}}} - \frac{1}{2\epsilon_{\boldsymbol{k}}} \right] . \tag{5}$$

Here the coupling U_0 is eliminated in favor of the s-wave scattering length a. These corrections, together with Ω_0, give rise to an overall mean-field thermodynamic potential of $\Omega_{mf} = \Omega_0 + \delta\Omega_\Delta + \delta\Omega_{mf}$,

$$\Omega_{mf} = \sum_{\boldsymbol{k}} [\xi_{\boldsymbol{k}} - E_{\boldsymbol{k}} + \frac{\Delta^2}{2\epsilon_{\boldsymbol{k}}} + \frac{2}{\beta} \ln f(-E_{\boldsymbol{k}})] - \frac{m\Delta^2}{4\pi\hbar^2 a} . \tag{6}$$

Fluctuation corrections beyond mean field are illustrated in fig. 1c. A sum of the resulting geometrical series thus leads to [12, 13, 17]

$$\Omega_{pf} = -\frac{1}{\pi} \sum_{\boldsymbol{q}} \int_{-\infty}^{+\infty} \mathrm{d}\omega \frac{1}{e^{\beta\omega} - 1} \delta(\boldsymbol{q}, \omega) , \tag{7}$$

where, following NSR, we have written Ω_{pf} in terms of a phase shift defined by $\delta(\boldsymbol{q}, \omega) = -\,\mathrm{Im}\ln[-\chi_{11}(\boldsymbol{q}, \omega + i\eta)] - 1/2\,\mathrm{Im}\ln\{1 - \chi_{12}^2(\boldsymbol{q}, \omega + i\eta)/[\chi_{11}(\boldsymbol{q}, \omega + i\eta)\chi_{11}^*(\boldsymbol{q}, -\omega + i\eta)]\}$. Here the analytic continuation is performed and η is a positive infinitesimal, while $\chi_{11} = 1/U_0 + 1/\beta \sum_{\boldsymbol{k},m} \mathcal{G}(\boldsymbol{q} - k, i\nu_n - i\omega_m)\mathcal{G}(\boldsymbol{k}, i\omega_m)$ and $\chi_{12} = 1/\beta \sum_{\boldsymbol{k},m} \mathcal{F}(\boldsymbol{q} - k, i\nu_n - i\omega_m)\mathcal{F}(\boldsymbol{k}, i\omega_m)$ are the diagonal and off-diagonal parts of the Cooper-pair propagator, with $\nu_n = 2n\pi/\beta$ being the bosonic Matsubara frequency.

Putting together the mean field and the pairing fluctuation corrections to the thermodynamic potential, we obtain the total contributions, $\Omega = \Omega_{mf} + \Omega_{pf}$. We emphasize that the gap (5) is chosen at the mean-field level, *i.e.*, $\partial\Omega_{mf}/\partial\Delta = 0$. Non-trivial effects beyond the BCS mean-field approximation enter into the theory through the modified number equation $N = -(\partial\Omega/\partial\mu)_T$. Explicitly, we obtain $N = N_{mf} + N_{pf,\mu} + N_{pf,\Delta}$, where

$N_{mf} = -(\partial\Omega_{mf}/\partial\mu)_{T\Delta}$, $N_{pf,\mu} = -(\partial\Omega_{pf}/\partial\mu)_{T\Delta}$, and $N_{pf,\Delta} = -(\partial\Omega_{pf}/\partial\Delta)_{T\mu}(\partial\Delta/\partial\mu)$. The coupled gap and particle number equations, together with the thermodynamic potentials (6) and (7), form the basis of our NSR theory in the broken-symmetry state. Once μ and Δ are obtained as a function of the interaction strength and temperature, the entropy and the energy of the gas can then be calculated straightforwardly, using $S = -(\partial\Omega/\partial T)_{\mu}$ and $E = \Omega + TS + \mu N$.

There is a key difference between our method and the diagrammatic theory proposed by Strinati *et al.* [14,15]. The term $N_{pf,\Delta}$, which ensures number conservation, is not included in the diagrams considered by Strinati *et al.* This term becomes increasingly important in the BEC regime. Physically, it generates the dominant part of the four-fermion correlations, which are increasingly important for tightly bound Cooper pairs. This constitutes a major advantage of our NSR theory.

To give more insight, in the strong coupling limit we re-interpret our formalism in the framework of the functional integral method [13], in which a Cooper-pair Bose field $\Delta(x,\tau)$ is introduced through the Hubbard-Stratonovich transformation. Integrating out the fermionic degrees of freedom in the usual fashion and setting $\Delta(x,\tau) = \Delta + \delta\Delta(x,\tau)$, the resulting effective bosonic action is then expanded up to quadratic order in fluctuations $\delta\Delta(x,\tau)$: $S_{eff} \approx S^{(0)} + S^{(2)}$. After performing a Fourier transformation we find that $S^{(0)} = \beta\Delta^2/U_0 - \mathrm{Trln}[-\boldsymbol{G}_0^{-1}] + \beta\sum_{\boldsymbol{k}}\xi_{\boldsymbol{k}}$, and

$$S^{(2)} = \sum_{\boldsymbol{q},n}[-\delta\Delta_q^{\dagger}\chi_{11}(\boldsymbol{q},i\nu_n)\delta\Delta_q + \chi_{12}(\boldsymbol{q},i\nu_n)(\delta\Delta_q^{\dagger}\delta\Delta_{-q}^{\dagger} + \delta\Delta_{-q}\delta\Delta_q)/2]\,, \tag{8}$$

where $\delta\Delta_q = \delta\Delta(\boldsymbol{q},i\nu_n)$ is the Fourier transformation of $\delta\Delta(x,\tau)$. The saddle point solution of $S^{(0)}$gives the standard mean-field theory, while the next-order Gaussian expansion $S^{(2)}$ leads to exactly the same contribution as in eq. (7). It is easy to see that in the long-wavelength and low-frequency limits, $-\chi_{11}(\boldsymbol{q},i\nu_n) \sim -i\nu_n + \hbar^2\boldsymbol{q}^2/4m + \Delta^2/(-4\mu)$ and $\chi_{12}(\boldsymbol{q},i\nu_n) \sim \Delta^2/(-4\mu)$. Hence, $S^{(2)}$ acquires the familiar form of Bogoliubov excitations [27]. Our formalism therefore incorporates interactions between condensed and non-condensed Cooper pairs at the level of Bogoliubov theory, which *must* be the dominant part of four-fermion correlations at low temperature.

The crucial observation of the present letter is that in the deep BEC limit ($\Delta/(-\mu) \to 0$) $N_{pf,\Delta} \sim \Delta^2/(-\mu)^{1/2}$ is of the *same* order of N_{mf}, or more precisely, $N_{pf,\Delta} = CN_{mf}$ with $C \simeq 2.5$, as shown analytically in a forthcoming publication [28]. In contrast, $N_{pf,\mu} \sim \Delta^3/(-\mu)^{3/2} \sim \Delta/(-\mu)N_{mf}$ becomes negligible. We thereby find that the molecular condensate density $N_B^0 \simeq N/2 \simeq (1+C)N_{mf}/2$. Mean-field number and gap equations provide the expressions, $N_{mf} \simeq \Delta^2 m^2 a/(4\pi\hbar^2)$, and $\mu_B = 2\mu + \hbar^2/(ma^2) \simeq \Delta^2 ma^2/(2\hbar^2)$, where μ_B is the molecular chemical potential. Assembling together these three expressions and eliminating Δ, one finds that $\mu_B = 4\pi\hbar^2\left[2a/(1+C)\right]/(2m) \times N_B^0$, implying $a_m = 2a/(1+C) \simeq 0.57a$ —a value close to the exact result ($a_m \simeq 0.60a$). The residual 5% difference occurs because we exclude interactions between non-condensed Cooper pairs.

Our diagrammatic procedure is also different from the works in refs. [20,22], where molecule-molecule scattering processes are considered in isolation. These calculations perturb around the free-fermion state and therefore require additional terms beyond the ladder structures in fig. 1 to obtain correct results. By comparison, we perturb around a BCS state of *correlated* fermions *below* T_c. A dominant part of the molecule-molecule scattering is therefore already included in the ladder diagrams due to the inclusion of $N_{pf,\Delta}$, as we have shown using the functional integral method. To contain the full four-body correlations, a more complicated wave function has to be implemented [21]. Equivalently, within the functional integral

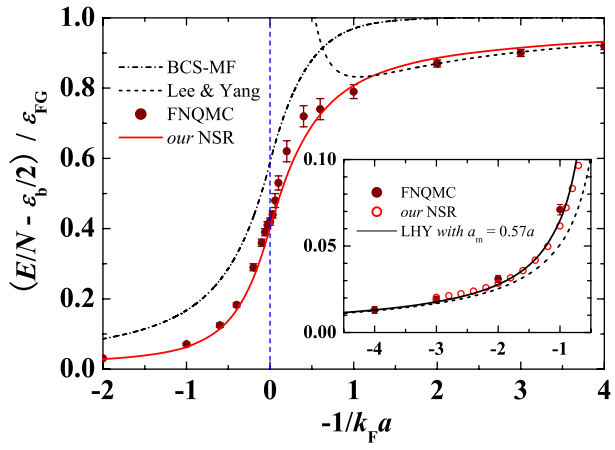

Fig. 2 – (Color online) Energy per particle E/N, in the BCS-BEC crossover (with the binding energy $\epsilon_b = -\hbar^2/ma^2$ subtracted). Lines plotted are: our result (solid line); fixed node QMC data from ref. [23] (circles with error bars), Lee and Yang perturbation theory (dashed line); BCS mean-field predictions (dot-dashed line). Inset: enlarged view of the BEC regime. The solid line corresponds to the equation of state of a repulsive gas of molecules given by LHY [29], $(E/N - \varepsilon_b/2)/\epsilon_{FG} = 5/(18\pi)k_F a_m[1 + 128/(15\sqrt{6\pi^3})(k_F a_m)^{3/2} + ...]$, with our analytic result of $a_m = 0.57a$.

method, we may include four-fermion correlations by expanding the action to fourth order of the gap [25]. However, this calculation is difficult to extend to the crossover regime.

Figure 2 presents our results for the energy per particle as a function of the interaction strength $1/k_F a$ at a low temperature $T = 0.02T_F$. The energy scale is given by the noninteracting energy, $\epsilon_{FG} = (3/5)\epsilon_F = (3/10)\hbar^2 k_F^2/m$, where $k_F = (3\pi^2 n)^{1/3}$ is the Fermi wave vector. As a benchmark, the approximate fixed node QMC data at zero temperature is shown [23], to-

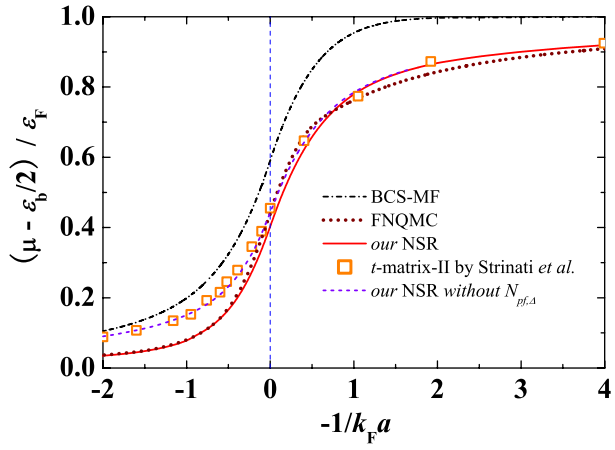

Fig. 3 – (Color online) Chemical potential in the BCS-BEC crossover, as predicted by various approaches. The QMC curve shown as a dotted line is calculated from a best fit to the QMC energies, as outlined in ref. [23]. The diagrammatic predictions (empty squares) by Strinati *et al.* are taken from ref. [15] without the inclusion of the self-energy shift.

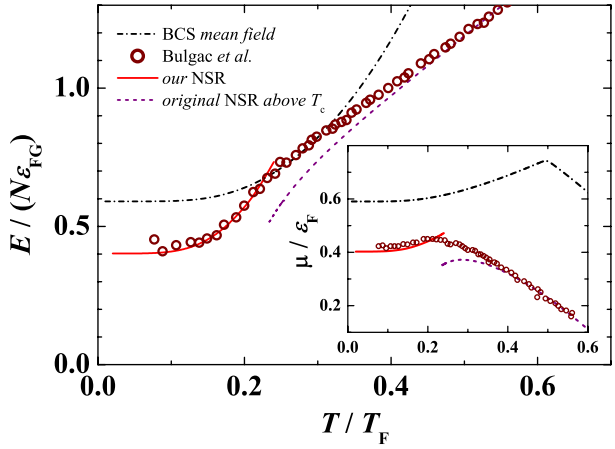

Fig. 4 – (Color online) Temperature dependence of the energy per particle (main plot) and the chemical potential (inset) in the unitary limit. Lines plotted are: our results (solid lines); path integral Monte Carlo data from ref. [26] (circles); BCS mean field (dot-dashed lines); the original NSR prediction in refs. [12, 13] (dashed lines).

gether with the perturbation results $E/(N\epsilon_{FG}) = 1+10/(9\pi)k_Fa+4/(21\pi^2)(11-2\ln 2)(k_Fa)^2$ obtained by Lee and Yang [30]. In the BCS region, $1/k_Fa < -0.5$, we find that our results agree with the QMC data, apart from residual differences due to the energy dependence of the scattering amplitude. In the BEC region, $1/k_Fa > 0.5$, our predictions coincide perfectly with QMC calculations, and thereby agree with the equation of state of a repulsive gas of molecules with $a_m \simeq 0.60a$, as shown in the inset. In the range $-0.5 \lesssim 1/(k_Fa) \lesssim 0.5$ spanning the most interesting crossover region, our results differ only slightly from that of QMC simulations. In particular, in the unitary limit we predict $E/N = \xi\epsilon_{FG}$ with $\xi = 0.401$, compatible with the QMC findings $\xi = 0.42(1)$ [23]. The overall agreement between the two alternative calculations is therefore excellent, especially in the challenging strong coupling regime.

We have also calculated the chemical potential at the BCS-BEC crossover, predicted by different theories (fig. 3). We find again an excellent quantitative agreement between our NSR results and QMC calculations. To emphasize the similarity between our formalism and the diagrammatic theory given by Strinati *et al.* [15], we compared the results obtained *without* the inclusion of the crucial term $N_{pf,\Delta}$ in the number equation, with Strinati's diagrammatic findings [15]. These asymptotically approach the mean-field predictions in the deep BEC limit, which would (incorrectly) imply that $a_m = 2a$. This observation thereby unambiguously verifies that $N_{pf,\Delta}$ is responsible for obtaining the correct molecular scattering length.

Finally, in fig. 4, we compare our predictions at finite temperature with recent path integral Monte Carlo calculations of spin-(1/2) fermions [26] in the strongly coupled unitary limit. At low temperature up to $T_c \approx 0.22T_F$, these results are in good qualitative agreement with each other. The residual discrepancy is possibly due to finite-size effects in the simulations.

To conclude, we have presented an NSR-type formalism for a Fermi gas at the BCS-BEC crossover, in the broken-symmetry phase. A notable achievement of our formalism is that a Bogoliubov theory of composite Cooper pairs is reproduced in the BEC limit, with a molecular scattering length very close to the exact value. We have compared our predictions of the equation of state of the gas with available Monte Carlo calculations, and find excellent agreement. Our results also make quantitative contact with a previous diagrammatic theory in

the weak and intermediate coupling regimes. We believe, therefore, that the present formalism provides a quantitatively reliable description of superfluid Fermi gases at low temperature over the entire range of the crossover.

* * *

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