Finite-Temperature Pairing Gap of a Unitary Fermi Gas by Quantum Monte Carlo Calculations

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We calculate the one-body temperature Green's (Matsubara) function of the unitary Fermi gas via quantum Monte Carlo, and extract the spectral weight function $A(p, \omega)$ using the methods of maximum entropy and singular value decomposition. From $A(p, \omega)$ we determine the quasiparticle spectrum, which can be accurately parametrized by three functions of temperature: an effective mass m^*, a mean-field potential U, and a gap Δ. Below the critical temperature $T_c = 0.15\varepsilon_F$ the results for m^*, U, and Δ can be accurately reproduced using an independent quasiparticle model. We find evidence of a pseudogap in the fermionic excitation spectrum for temperatures up to $T^* \approx 0.20\varepsilon_F > T_c$.

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Over the last few years, the field of cold atoms has drawn unprecedented attention, as documented in two recent review articles [1]. Within this field, the unitary Fermi gas, defined as the limit of vanishing interaction range and infinite scattering length, continues to be a fascinating area of research for a number of reasons. First, the properties of the unitary regime are universal, making this problem relevant to a wide range of fields including string theories, the quark-gluon plasma, neutron stars, nuclei, and to a certain extent to high T_c superconductors. Second, experimentalists can control the strength of the interaction by means of Feshbach resonances, which allows for the systematic exploration of weakly as well as strongly coupled regimes. Finally, these systems exhibit a rich variety of phenomena and properties (many of which await verification), creating an ideal playground for a large set of many-body techniques, possibly the largest ever applied to a single problem.

Properties established so far include energy as a function of temperature, entropy, frequencies of collective modes, speed of sound, critical temperature for the onset of superfluidity, and moment of inertia. In the case of polarized Fermi systems, the critical spin polarization at which superfluidity disappears has also been determined. All of these properties have been established quantitatively with a reasonable degree of certainty and accuracy, both experimentally and theoretically.

In spite of great efforts on the part of both theorists and experimentalists, some fundamental properties of these systems remain unknown. Among the most pressing questions is the magnitude of the pairing gap and its evolution with temperature. Theoretical progress in this direction has been nearly at a standstill, except for the theoretical determination of the pairing gap at $T = 0$ in Refs. [2–5], the recent analysis of experimental data of Ref. [6] and a recent experiment [7].

While theoretical models abound, predictions are mostly qualitative, and their validity and accuracy are difficult to assess due to the absence of a small parameter for a Fermi gas at unitarity. This work presents the first *ab initio* evaluation of the one-body temperature propagator of the unitary Fermi gas, free of uncontrolled approximations, which allows for the extraction of the temperature dependence of the pairing (pseudo)gap [8].

We begin by defining the one-body temperature Green's (Matsubara) function [9]:

$$\mathcal{G}(\boldsymbol{p}, \tau) = \frac{1}{Z}\,\mathrm{Tr}\{\exp[-(\beta - \tau)(H - \mu N)]\psi^\dagger(\boldsymbol{p}) \times \exp[-\tau(H - \mu N)\psi(\boldsymbol{p})]\}, \quad (1)$$

where $\beta = 1/T$ is the inverse temperature and $\tau > 0$. The trace Tr is performed over the Fock space, and $Z = \mathrm{Tr}\{\exp[-\beta(H - \mu N)]\}$. The spectral weight function $A(\boldsymbol{p}, \omega)$ can be extracted from the temperature Green's function using the relation

$$\mathcal{G}(\boldsymbol{p}, \tau) = -\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega A(\boldsymbol{p}, \omega)\frac{\exp(-\omega\tau)}{1 + \exp(-\omega\beta)}. \quad (2)$$

By definition, $A(\boldsymbol{p}, \omega)$ fulfills the following constraints:

$$A(\boldsymbol{p}, \omega) \geq 0, \qquad \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}A(\boldsymbol{p}, \omega) = 1. \quad (3)$$

Since our study focuses on the spin-symmetric system, and the Hamiltonian is spin symmetric as well, $\mathcal{G}(\boldsymbol{p}, \tau)$ is diagonal in the spin variables and these are suppressed in all formulas. The numerical evaluation of the one-body temperature propagator (1) is performed as described in Refs. [10,11], by using a Trotter expansion of $\exp[-\tau(H - \mu N)]$, followed by a Hubbard-Stratonovich transformation of the interaction and an evaluation of the emerging path-integral via Metropolis importance sampling. The number of imaginary time steps required to obtain an accuracy smaller than the statistical error varies with temperature. At low temperatures the number of time steps is $\mathcal{O}(10^3)$ [11]. All calculations presented here have been performed

with an average total particle number of 50–55 on an 8^3 lattice with periodic boundary conditions [10]. We have generated between 6000 and 10 000 uncorrelated samples at each temperature and the statistical errors are typically below 1%. The systematic errors, some due to finite lattice effects, others due to finite range effects, are estimated at about 10%–15%. Our $T = 0$ extrapolation results [11] for the energy per particle are systematically lower than previous fixed-node Monte Carlo results which are variational [2,3,12]. We have not used the fixed-node approximation and the value for $\xi = 5E/3N\varepsilon_F \approx 0.40$ that we extract at unitarity is in agreement with the auxiliary field Monte Carlo results of Ref. [13].

The numerical determination of $A(\boldsymbol{p}, \omega)$ via inversion of Eq. (2) is an ill-posed problem that requires special methods. We have used two, based on completely different approaches. The first approach is the maximum entropy method [14], which is based on Bayes' theorem. Quantum Monte Carlo (QMC) calculations provide us with a discrete set of values $\tilde{\mathcal{G}}(\boldsymbol{p}, \tau_i)$, where $i = 1, 2, \ldots, \mathcal{N}_\tau = 50$. We treat them as normally distributed random numbers around the true values $\mathcal{G}(\boldsymbol{p}, \tau_i)$. The Bayesian strategy consists in maximizing the posterior probability $P(A|\tilde{G}) \propto P(\tilde{G}|A)P(A)$ of finding the right $A(\boldsymbol{p}, \omega)$ under the condition that $\tilde{\mathcal{G}}(\boldsymbol{p}, \tau_i)$ are known. Here, $P(\tilde{G}|A) \propto \exp(-\frac{1}{2}\chi^2)$ is the likelihood function, where $\chi^2 = \sum_{i=1}^{\mathcal{N}_\tau}[\tilde{\mathcal{G}}(\boldsymbol{p}, \tau_i) - \mathcal{G}(\boldsymbol{p}, \tau_i)]^2/\sigma^2$. The quantity $\mathcal{G}(\boldsymbol{p}, \tau_i)$ is determined by the spectral weight function in the discretized form of Eq. (2) at frequencies ω_k. The prior probability $P(A)$, describing our ignorance about the spectral weight function, is defined as $P(A) \propto \exp[\alpha S(\mathcal{M})]$, where $\alpha > 0$ and $S(\mathcal{M})$ is the relative information entropy with respect to the assumed model $\mathcal{M}$:

$$S(\mathcal{M}) = \sum_k \Delta\omega \Big[A(\boldsymbol{p}, \omega_k) - \mathcal{M}(\omega_k) - A(\boldsymbol{p}, \omega_k) \ln\Big(\frac{A(\boldsymbol{p}, \omega_k)}{\mathcal{M}(\omega_k)}\Big)\Big]. \quad (4)$$

Hence the maximization of $P(A|\tilde{G})$ leads in practice to the minimization of the quantity $\frac{1}{2}\chi^2 - \alpha S(\mathcal{M})$ with respect to A. Note that the parameter α governs the relative importance of the two terms. The entropy term prevents excessive inclusion of unjustified structure into the shape of the spectral weight function. The constraints (3) are enforced by means of Lagrange multipliers.

The second approach is based on the singular value decomposition of integral kernel $\mathcal{K}$ of Eq. (2), which can be rewritten in operator form as

$$\mathcal{G}(\boldsymbol{p}, \tau_i) = (\mathcal{K}A)(\boldsymbol{p}, \tau_i). \quad (5)$$

The operator $\mathcal{K}$ possesses a singular system defined as

$$\mathcal{K}\, u_i = \lambda_i \vec{v}_i, \qquad \mathcal{K}^* \vec{v}_i = \lambda_i u_i, \quad (6)$$

where $\mathcal{K}^*$ denotes the adjoint of $\mathcal{K}$, the λ_i are the singular values, and the u_i, $\vec{v}_i$ are right-singular functions and left-singular vectors, respectively. The singular system forms a suitable basis for the expansion of the spectral weight

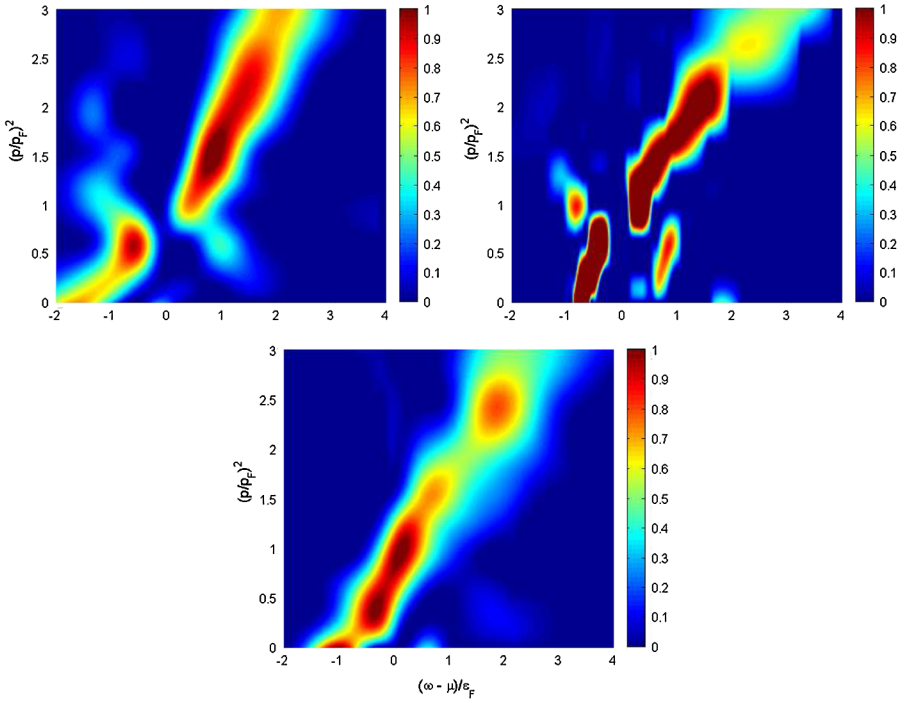

FIG. 1 (color online). Spectral weight function $A(\boldsymbol{p}, \omega)$ for three temperatures: $T = 0.15\varepsilon_F \approx T_c$ (left upper panel), $T = 0.18\varepsilon_F$ (right upper panel), and $T = 0.20\varepsilon_F$ (lower panel). The presence of a gap in clearly seen in the upper two panels.

function [15], which we can then write as

$$A(\boldsymbol{p},\omega)=\sum_{i=1}^{r} b_i(\boldsymbol{p})u_i(\omega), \qquad b_i(\boldsymbol{p})=\frac{1}{\lambda_i}[\vec{\mathcal{G}}(\boldsymbol{p})\cdot\vec{v}_i], \tag{7}$$

where $[\cdot]$ is a scalar product and r is the rank of the operator $\mathcal{K}\mathcal{K}^*$. Since $\mathcal{G}(\boldsymbol{p},\tau_i)$ is affected by the QMC errors σ_i, the coefficients b_i carry some uncertainty Δb_i. Each set of expansion coefficients $\tilde{b}_i \in (b_i-\Delta b_i, b_i+\Delta b_i)$ reproduces $\mathcal{G}(\boldsymbol{p},\tau_i)$ within its error bars. We use this flexibility of choosing the expansion coefficients to produce a solution satisfying constraints (3) [16].

The advantages and disadvantages of both methods will be discussed elsewhere [17]. Here we note only that since they are based on completely different approaches their agreement serves as a robust test for the determination of the spectral weight function. A sample of calculated spectral weight functions at unitarity are shown in Fig. 1. In order to characterize the quasiparticle excitation spectrum we have associated with the maximum of $A(\boldsymbol{p},\omega)$ the quasiparticle energy $E(\boldsymbol{p})$:

$$E(\boldsymbol{p})=\pm\sqrt{\left(\frac{p^2}{2m^*}+U-\mu\right)^2+\Delta^2}, \tag{8}$$

where m^* is an effective mass, the potential U and the "pairing" gap Δ depend on temperature, and μ is an input parameter. In Fig. 2 we compare the spectrum of elementary fermionic excitations evaluated in Ref. [4], with the one extracted by us from our lowest temperature spectral weight function. Such comparisons are legitimate because the temperature dependence of various quantities at $T\leq T_c$ is relatively weak, see Ref. [10] and the results below. The agreement between the $T=0$ Monte Carlo results and the low T limit of our finite-T unrestricted QMC data validates those results. One should keep in mind that the effective range corrections are noticeable, since $r_0=4/\pi\Lambda\approx 0.4$ (in lattice units), where Λ is the cutoff in momentum [10].

The extracted value of the single-particle potential U (see Fig. 3) shows essentially no temperature dependence in the range investigated by us. (Simulations at higher temperatures are not reliable with lattice sizes we considered here, see also Ref. [10].) The values of U and α are very close to the values determined in Ref. [18] at $T=0$ and show almost no temperature dependence.

A surprising feature of our results can be seen if we assume that the system is composed of independent quasiparticles with BCS-like dispersion relation, in which case the susceptibility can be easily evaluated:

$$\chi(\boldsymbol{p})=-\int_0^\beta d\tau\mathcal{G}(\boldsymbol{p},\tau)=\frac{1}{E(\boldsymbol{p})}\frac{e^{\beta E(\boldsymbol{p})}-1}{e^{\beta E(\boldsymbol{p})}+1}. \tag{9}$$

From the calculated one-body propagator, using Eqs. (1) and (9), one can extract the spectrum of the elementary fermionic excitations at finite temperature, which turns out somewhat unexpectedly to be accurately parametrized by Eq. (8). Extracted parameters are plotted in Fig. 3 with lines. While the agreement between the mean-field potential U and effective mass m^* obtained using the two procedures is almost perfect at all temperatures, the pairing gap is reproduced satisfactorily only up to $T\leq T_c$.

Another notable feature of our results is that both methods admit the "gapped" spectral function above the critical temperature, routinely referred to as the pseudogap [8]. Various aspects and the physics of a pseudogap in a Fermi gas in the unitary regime have been advocated and discussed for a number of years by several groups [19]. It is, however, notable that the pseudogap has not entered the mainstream of research in this field and the physics of the pseudogap is barely covered in the recent reviews [1], which reflects a rather widespread opinion in the cold

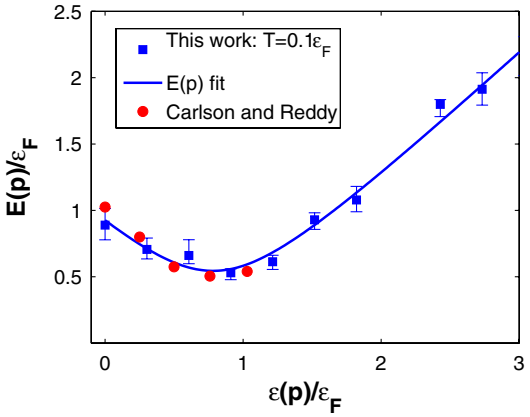

FIG. 2 (color online). Quasiparticle energies $E(\boldsymbol{p})$ (squares) extracted from the spectral weight function $A(\boldsymbol{p},\omega)$ at $T=0.1\varepsilon_F$. The line corresponds to the fit to Eq. (8). The circles are the results of Carlson and Reddy [4].

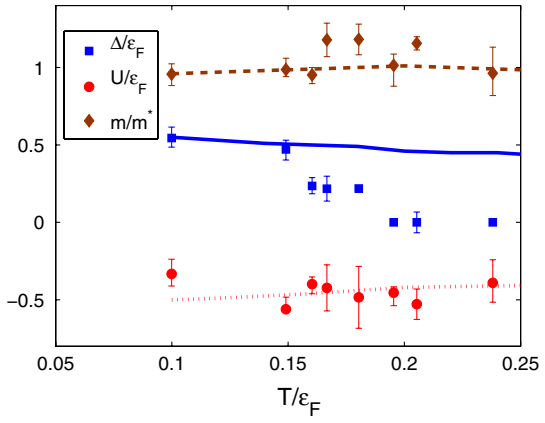

FIG. 3 (color online). The single-particle parameters extracted from the spectral weight function at unitarity. The dashed, solid, and dotted lines represent the quantities: m/m^*, Δ/ε_F, U/ε_F, respectively, extracted using the assumption of independent quasiparticle model.

atom community that the gap should vanish at T_c. There have been several experimental attempts to extract the pairing gap in ultracold dilute Fermi gases [20] and a theoretical explanation of these spectra was given in Refs. [21]. However, it was later shown in Refs. [22] that these initial interpretations of the rf spectra as revealing the pairing gap were in error, as strong final state interaction effects had been neglected. In particular the difficulties of determining the pairing gap using rf spectroscopy were discussed in Ref. [23]. In Ref. [24] the use of Bragg spectroscopy is advocated instead, in order to measure the onset of superfluidity as well as the appearance of a pseudogap. A recent theoretical calculation of the spectral function, based on summing all the particle-particle ring diagrams [25], does not reveal signs of a pseudogap. On the other hand, in Refs. [26,27] there are experimental indications that a pseudogap exists in a unitary gas.

Our calculations show that the spectral function reveals the presence of a gap in the spectrum up to about $T^* \approx 0.20\varepsilon_F$. This result is reproduced by both the maximum entropy and singular value decomposition methods, which indicate that the spectral function possesses a two peak structure around the Fermi level at temperatures above T_c. In the maximum entropy method this result is stable with respect to variation of the assumed model $\mathcal{M}$ and for $\sigma^2\alpha \leq 0.3$, see Eq. (4). In the range of temperatures $0.18 \ldots 0.25\varepsilon_F$ the singular value decomposition method can reproduce both two- and one-peak structures depending on the details of the method, due to finite size of the statistical errors in the imaginary time Green's function. In our case this resolution is at the level of $\Delta \approx 0.2 \ldots 0.3\varepsilon_F$, which means that the gap above T_c is barely visible by the singular value decomposition method. We note that T^* is the temperature at which, not surprisingly in hindsight, the caloric curve $E(T)$ has a shoulder [10], which in Ref. [11] we called T_0.

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