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The Onset of the Pseudogap Regime in Ultracold Fermi Gases

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We show, using an *ab initio* approach based on Quantum Monte Carlo technique, that the pseudogap regime emerges in ultracold Fermi gases close to the unitary point. We locate the onset of this regime at a value of the interaction strength corresponding to $(k_F a)^{-1} \approx -0.05$ (a - scattering length). We determine the evolution of the gap as a function of temperature and interaction strength in the Fermi gas around the unitary limit and show that our results exhibit a remarkable agreement with the recent wave-vector resolved radio frequency spectroscopy data. Our results indicate that a finite temperature structure of the Fermi gas around unitarity is more complicated and involves the presence of the phase with preformed Cooper pairs, which however do not contribute to the long range order.

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The unitary Fermi gas is a dilute but an exceptionally strongly correlated ensemble of particles exhibiting universal properties and also a superfluid with a very large critical temperature, making it relevant to a wide range of systems including the quark-gluon plasma, neutron stars, nuclei [1], and to a certain extent to high T_c superconductors. A number of fundamental properties of the Fermi gas close to the unitary limit remain unknown and still pose an unprecedented challenge for the theory [2]. Although a convincing experimental proof of superfluidity was provided 6 years ago [3], the measurements of the pairing gap at finite temperatures are still in their infancy and only recently the technique of photoemission spectroscopy allowed to probe the low-energy excitations of the gas at finite temperatures [4]. The pairing gap measurements are believed to answer one of the most intriguing questions related to the strongly interacting Fermi gas: Does the simple picture of the phase transition from superfluid to normal state still holds around the unitary regime? Here we show, using an *ab initio* approach based on Quantum Monte Carlo (QMC) technique, that the pseudogap regime emerges in ultracold Fermi gases close to the unitary point. In the pseudogap regime fermions still have a strong tendency to be correlated with each other and behave to some extent as a system of bosons. Consequently above the critical temperature the system exists in an exotic state which is neither entirely normal nor superfluid and thus clearly eludes the understanding within the framework of classical BCS theory of superconductivity. This situation can be better understood from the viewpoint of the deep Bose-Einstein Condensation (BEC) limit, where the pairs of fermions form bound bosonic dimers. This implies the existence of two distinct temperature scales: the first one, T_c , related to the Bose-Einstein condensation of bosonic molecules and the second one, $T^* > T_c$, which is a temperature needed to break up a dimer into fermions. Somewhere around the unitary regime these two temperatures become practically

indistinguishable and eventually merge into the critical temperature for superfluid to normal phase transition [5]. The region between T_c and T^* is usually referred to as a pseudogap phase, where the system, although not being a superfluid, still exhibits the gap in the spectrum of quasiparticle excitations. Actually the term “pseudogap phase” may be somewhat misleading as, first, it is a strong depletion of the density of states in the spectrum and second, it is strictly speaking a particular regime, not a phase, as there is no phase transition between pseudogap regime and the normal Fermi gas.

The situation in the ultracold atomic gases at the unitary regime is somewhat similar to that encountered in high temperature superconductors (HTSC) [6], although the pseudogap regime in the cuprates is not exclusively related to Cooper-pair formation [7]. To appreciate these similarities one has to consider the ratio between the critical temperature and the pairing gap at zero temperature. According to the celebrated BCS theory this ratio is approximately equal to 1.76 (for the temperature expressed in energy units, $k_B = 1$). Any deviation from this value is an indication of the non-BCS superfluidity in the system. The origin of the deviation is usually related to the interaction strength and manifests itself in a rather large ratio of the pairing gap Δ to Fermi energy ε_F . It stands in contradiction to the implicit assumption of the BCS theory that the interaction is weak which imply $\Delta/\varepsilon_F \ll 1$. Clearly both ultracold gases and HTSC violate this assumption, see Fig. 1. Moreover the cold fermionic atoms constitute the system with the largest ratio Δ/ε_F and known HTSC only approach this limit [8].

Theoretically the single particle gap in the fermionic spectrum can be determined from the spectral weight function $A(\mathbf{p}, \omega)$, which carry information about the single particle excitation spectrum. In our approach we have used the Path Integral Monte Carlo (PIMC) technique on the lattice, which provides numerically essentially exact

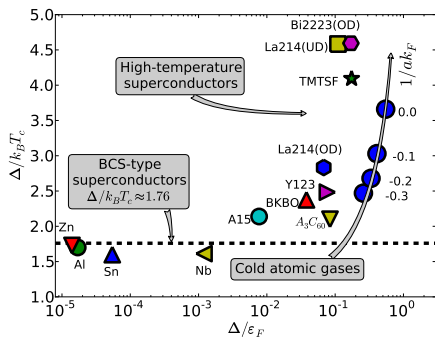


FIG. 1: (Color online) Ratio of the pairing gap and the critical temperature for various superconductors (data extracted from Ref. [10]). The clearly visible deviation from the typical ratio predicted by the BCS theory is a hallmark of HTSC. The same ratio for atomic Fermi gases close to the unitary limit are denoted by blue circles (data from Ref. [11]).

results with quantifiable uncertainties. The details of the approach have been described elsewhere [11–14]. Calculations presented here have been performed on a larger lattice than reported in Ref. [13], namely 10^3 , with particle number varying between 90 and 110. The number of Monte Carlo samples was chosen in such a way to decrease the statistical errors below 1%. The systematic errors, some due to finite lattice effects, others due to finite range effects, are estimated at no more than 10%, depending on physical quantity. In order to determine the size of the gap, we have used the one-particle temperature Green’s (Matsubara) function which can be easily calculated within the PIMC formalism and which is related to the spectral weight function [15]. The PIMC method provides us with a discrete set of values of the Green’s function. In the present calculations we have determined the Green’s function at 51 imaginary time points, equally spaced within the interval $[0, \beta = 1/T]$. We have found that due to the smooth behavior of the Green’s function the accuracy is not affected by increasing the number of points. We have used two methods to extract the spectral weight function from the Matsubara function: the maximum entropy method (MEM) and the Singular Value Decomposition method (SVD) [13, 16].

As an example in the Fig. 2 the spectral weight function is shown on the BEC side of the unitary regime for $(k_F a)^{-1} = 0.2$. The three temperature values correspond to three regimes realized in this system. At $T \approx 0.13\varepsilon_F < T_c = 0.19(1)\varepsilon_F$ the system is superfluid [11], at $T \approx 0.19\varepsilon_F$ the long range order is lost, but the gap in the single particle spectrum is still present. Finally, the lower panel shows the spectral weight function just above the crossover to the normal Fermi liquid. The negative energy branch is nonzero essentially up to $p \approx p_F$. For the momenta above the Fermi surface the negative energy branch has a tail which in the

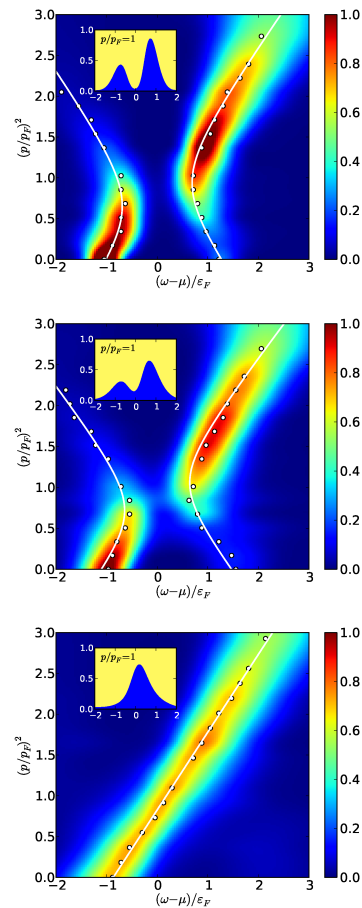


FIG. 2: (Color online) Spectral weight function $A(\mathbf{p}, \omega)$ at $1/k_F a = 0.2$ for three temperatures: $T = 0.13\varepsilon_F < T_c$ (middle panel), $T = 0.19\varepsilon_F \approx T_c$ (upper panel) and $T = 0.26\varepsilon_F > T^*$ (lower panel). White circles denote the position of the maxima of two branches of spectral weight function and the white line represents the quasiparticle energy $E(\mathbf{p})$ fit to the maxima of the spectral weight function. In the insets we show the section of the spectral weight function at the Fermi level.

case of the unitary Fermi gas is related to the behavior of the occupation probability $n(p)$ at large p which decay as $1/p^4$ [17]. The positive energy branch starts essentially around $p \approx p_F$ and the presence of the gap can be easily detected. The upper panel of Fig. 2 describes the superfluid system with no states at the Fermi surface (see inset). In the middle panel ($T \approx T_c$) the density of states at the Fermi level is significantly lowered. At large temperatures the two branches merge into a single branch extending from negative to positive values of $\omega - \mu$, characteristic for a normal state. Similarly like in [13, 18] we have fitted the formula for the quasiparticle energy $E(\mathbf{p}) = \sqrt{(p^2/2m^* + U - \mu)^2 + \Delta^2}$ to the maxima of the spectral weight function. The extracted values of gap Δ , self-energy U and effective mass m^* have been presented in the table I. One may notice

	T/ε_F	Δ/ε_F	U/ε_F	m^*/m
$(k_F a)^{-1} = -0.2$	0.122	0.21	-0.28	0.95
$T^*/\varepsilon_F = 0.14(2)$	0.146	0.06	-0.44	1.06
$T_c/\varepsilon_F = 0.125(10)$	0.17	0.0	-0.44	1.01
$(k_F a)^{-1} = -0.1$	0.12	0.42	-0.38	1.06
$T^*/\varepsilon_F = 0.14(1)$	0.144	0.02	-0.31	0.95
$T_c/\varepsilon_F = 0.135(10)$	0.17	0.0	-0.30	1.01
$(k_F a)^{-1} = -0.05$	0.144	0.25	-0.45	1.04
	0.18	0.04	-0.45	1.04
$(k_F a)^{-1} = 0.0$	0.12	0.47	-0.39	1.0
$T^*/\varepsilon_F = 0.19(2)$	0.15	0.42	-0.38	1.0
$T_c/\varepsilon_F = 0.15(1)$	0.165	0.19	-0.48	1.06
	0.184	0.05	-0.47	1.03
	0.21	0.05	-0.49	1.04
$(k_F a)^{-1} = 0.1$	0.14	0.57	-0.37	0.97
$T^*/\varepsilon_F = 0.24(2)$	0.17	0.31	-0.47	1.05
$T_c/\varepsilon_F = 0.17(1)$	0.22	0.15	-0.48	1.05
	0.24	0.0	-0.49	1.04
	0.28	0.0	-0.51	1.04
$(k_F a)^{-1} = 0.15$	0.18	0.46	-0.48	1.03
	0.21	0.22	-0.53	1.08
$(k_F a)^{-1} = 0.2$	0.13	0.66	-0.43	1.0
$T^*/\varepsilon_F = 0.26(2)$	0.17	0.62	-0.44	1.01
$T_c/\varepsilon_F = 0.19(1)$	0.22	0.46	-0.45	1.02
	0.26	0.03	-0.53	1.05
	0.30	0.0	-0.56	1.05

TABLE I: Pairing gaps Δ , self-energy U and effective masses m^* extracted from the spectral weight function for various temperatures T and scattering lengths (see left column). In the left column the extracted values of crossover temperature T^* have been shown together with the values of the critical temperatures (upper estimates) taken from Ref. [11]. All the results except of those for $(k_F a)^{-1} = -0.2$ have been obtained for the lattice 10^3 . The results on the BCS side at $(k_F a)^{-1} = -0.2$ have been obtained for the lattice 8^3 as described in [13]. The values of $\Delta/\varepsilon_F < 0.1$ should be treated as lying within the interval $[0, 0.1]$ due the finite resolution, see Ref. [16].

that the effective mass is practically constant and does not deviate from the bare mass by more than 10%. The self-energy U decreases with $(k_F a)^{-1}$. When compared to the experimentally extracted value at unitarity (see Ref. [19]) it agrees within a 10% accuracy. The values of T_c around unitarity have been determined elsewhere [11, 20]. The value of the gap at T_c is usually called the pseudogap, i.e. measure of the strength of the short range correlations at the critical temperature. These results can be subsequently used to estimate the value of T^* , where the gap tends to zero and also the value of

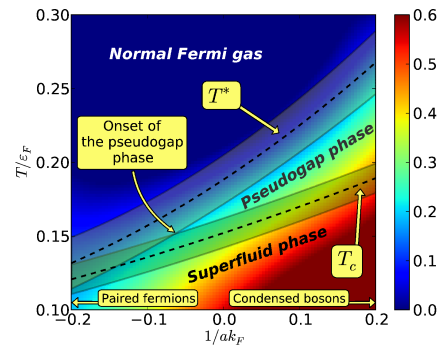


FIG. 3: (Color online) The gap Δ/ε_F extracted from the spectral weight function as a function of temperature and scattering length. The dashed lines denote two temperatures: critical temperature T_c and the crossover temperature T^* . Uncertainties (both systematic and statistic errors, estimated to be no more than 10%) of these temperatures, are denoted by shaded area.

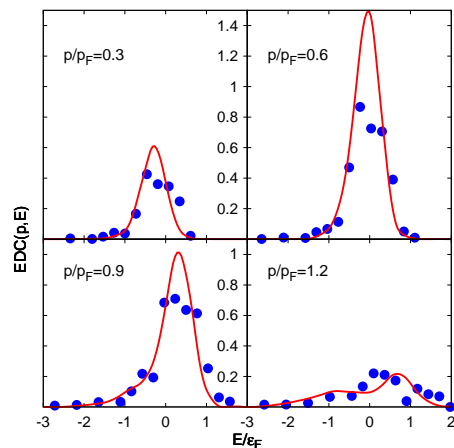


FIG. 4: (Color online) Experimental (dots) and theoretical (lines) energy distribution curves (EDC) for the trapped atomic gas in the unitary regime at the critical temperature (defined in the center of the trap) for various momenta p .

the gap at the critical temperature T_c for the superfluid to normal phase transition. We show the size of the gap Δ/ε_F plotted as a function both temperature and scattering length in Fig. 3. The two temperatures T^* and T_c become indistinguishable, due to uncertainties generated by Monte Carlo approach, between $-0.1 < (k_F a)^{-1} < 0$. Hence already at the unitary limit the system exhibits the pseudogap phase, albeit in a relatively small temperature interval. The temperature interval within which the pseudogap phase exists increases as one moves to the BEC side.

The present work is the first attempt to determine the evolution of the pseudogap as a function of temperature and interaction strength from fully *ab initio* calculations. Previous results obtained using this *ab initio*

method were used as a benchmark by other theoretical approaches and were as well validated by subsequent experimental results [21, 22]. On one hand, the most recent calculations of Ref. [23], based on the pairing-fluctuation theory, indicated the presence of the pseudogap without however specifying its size and evolution as a function of the scattering length. On the other hand the recent measurements of the magnetic susceptibility of the trapped atomic gases were explained within the Fermi liquid theory without invoking the pseudogap model [22, 24], a description challenged in Ref. [23]. The Fermi liquid parameters in Ref. [24] were extracted in a QMC calculation at zero temperature, in which the formation of pairs was artificially suppressed, and the spectral functions were approximated with δ -functions. Here we present the comparison of the experimental results based on the wave-vector resolved spectroscopy [23, 25]. Since the experimental data are for a trap which is inhomogeneous and likely composed of spatially separated and coexisting phases it is difficult to relate the particular behavior of the extracted energy distribution curves to the appearance of the pseudogap phase. However the agreement of the experimental and theoretical results supporting the existence of the pseudogap provides an implicit confirmation of the quality of the theoretical calculations. We use the Local Density Approximation [26] to relate the PIMC input to trap data, see Fig. 4 (without using any fitting parameters, see [16] for details). Over the years there was a significant body of work addressing the physics of preformed pairs, pseudogap and dissociation temperature T^* , see Refs. [5, 27–30] and earlier references, based on a variety of theoretical models and approximations. The theoretical predictions for some or all of these entities either varied widely or were at most of qualitative nature and the values obtained in these references for the pseudogap and T^* are significantly different from ours. The lack of quantifiable error bars makes essentially impossible to re-conciliate these earlier predictions and to judge their accuracy.

In summary we have determined in *ab initio* calculations the spectral weight function for various temperatures around the unitary regime. We have confirmed the existence of the pseudogap phase (we have reported the evidence of this phase at unitarity in Ref. [13]) and located the onset of this phase at a value of the interaction strength corresponding to $(k_F a)^{-1} \approx -0.05$. To date the present results are the first *ab initio* calculations which were able to determine the size of the pseudogap and its behavior as a function of interaction strength and temperature. Our results indicate that a finite temperature structure of the Fermi gas around unitarity is more complicated and involves the presence of the phase with preformed Cooper pairs, which however do not contribute to the long range order.

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