

## Zero-density-limit extrapolation of the superfluid transition temperature in a unitary atomic Fermi gas on a lattice

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The superfluid transition temperature  $T_c$  of a unitary Fermi gas on a three-dimensional isotropic lattice with an attractive on-site interaction is investigated as a function of density  $n$ , from half filling down to  $5 \times 10^{-7}$  per unit cell, using a pairing fluctuation theory. We show that except at very low densities ( $n^{1/3} < 0.2$ ), where  $T_c/E_F$  is linear in  $n^{1/3}$ ,  $T_c/E_F$  exhibits a significant higher-order nonlinear dependence on  $n^{1/3}$ . This calls for extra caution against possible significant error in the zero-density-limit value of  $T_c/E_F$  from typical quantum Monte Carlo (QMC) simulations, obtained by linearly extrapolating data points at intermediate and high densities. Our result,  $T_c/E_F = 0.256$ , at the  $n = 0$  limit, is close to, and should be compared with, the maximum  $T_c/E_F$  near the Bose-Einstein condensation regime obtained from QMC calculations.

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Experimental realization of superfluidity in cold atomic Fermi gases has given the study of the BCS–Bose-Einstein condensation (BEC) crossover a strong boost over the past decade. More importantly, the main attention has been paid to the strongly interacting regime, where the  $s$ -wave scattering length  $a$  is large. In particular, the unitary limit, where the scattering length diverges, has become a test point for theories. As a consequence, the superfluid transition temperature  $T_c$  in a unitary Fermi gas has been under intensive investigation in recent years.

Apart from calculating  $T_c$  directly in the three-dimensional (3D) continuum with various analytical approximations [1–16], one important method is to calculate  $T_c$  on a lattice and then extrapolate to zero density. It has been argued that the zero-density limit is identical to the continuum case. Indeed, this is the approach used by various quantum Monte Carlo (QMC) simulations. For this approach to work, two conditions have to be met. First, the result obtained from the simulation at a given density has to be accurate; this requires that both the lattice size and the particle number have to be large enough. Second, the densities  $n$  at which the simulations are performed have to be in the asymptotic linear regime of  $T_c$  as a function of  $n^{1/3}$ .

It is extremely important to investigate this issue, because the results of QMC calculations have often been taken as highly credible in the cold-atom community, despite the large discrepancies between the results from different groups (as well as within the same group sometimes), and the small total fermion number and lattice size used. For example, using QMC simulation, Troyer and co-workers [17,18] reported  $T_c/E_F = 0.152$ , whereas Bulgac and co-workers [19,20] reported  $T_c/E_F = 0.23$  and  $0.15$  in different papers. The simulations in Ref. [17] were done for lattice fermions at finite densities and then extrapolated to zero density. Using the method of Ref. [17], Goulko and Wingate [21] found  $T_c/E_F = 0.171$ . Another recent result [22] from QMC simulation gave  $T_c/E_F = 0.245$ . These different results do not seem to be converging.

Without reproducing these QMC results, it is hard to understand what causes these large discrepancies. However, we have noticed that the simulations mentioned above have

been done only in the high- and intermediate-density regimes. A natural question one may ask is whether these densities are low enough to ensure a good linear extrapolation to the zero-density limit.

To answer this question, ideally one would like to perform QMC simulations in the very-low-density regime. While such a low-density regime is practically unreachable in QMC simulation at present, one may start by studying how  $T_c/E_F$  extrapolates to the zero-density limit in other theories. It is the purpose of the present paper to investigate, using an alternative approach, how low in density one needs to go so that the simulations are in the asymptotic linear regime to ensure the accurateness of the zero-density-limit extrapolation. We argue that the presence of the lattice effect is sensitive predominantly to the finite fermion density and the type of the lattice (or the band dispersion) instead of different analytical approximations, provided that the approximations involved do not exhibit explicit dependencies on the fermion density and lattice periodicity. Therefore, it is hoped that our result may shed light on how the extrapolation should be properly done in various formulations of the QMC method. In what follows, we will mostly compare with the QMC result of Ref. [17] because it has been widely cited and compared with recently.

In this paper, we will study the finite-density effect on the zero-density-limit extrapolation by calculating  $T_c$  on a 3D isotropic lattice with an attractive on-site interaction  $U$ , using a pairing fluctuation theory. This theory has been able to generate theoretical results in good agreement with experiment [12,23]. To show how the lattice effect evolves with fermion density, we drop the complication of the particle-hole channel, which does not depend explicitly on the density or the lattice periodicity. Indeed, the particle-hole channel has been neglected in most theoretical calculations since the very first  $T_c$  calculation in the study of the BCS-BEC crossover by Nozières and Schmitt-Rink (NSR) [1]. Our result reveals that, as the density approaches zero,  $T_c/E_F$  does reach the 3D continuum value within the present theory. However, linear extrapolation using data points calculated at intermediate densities, such as those in Ref. [17], will lead to a significant underestimate of  $T_c$  for the continuum limit. When particle-hole channel contributions are properly included [24], we expect that the zero-density

limit will yield  $T_c/E_F = 0.217$ , as directly calculated in the continuum.

Details of the pairing fluctuation theory can be found in Ref. [10] both in the continuum and on a lattice (see Ref. [24] for the treatment of the particle-hole channel effect). On a lattice, the fermion dispersion is given by  $\xi_{\mathbf{k}} = 2t(3 - \cos k_x - \cos k_y - \cos k_z) - \mu \equiv \epsilon_{\mathbf{k}} - \mu$ , where  $t$  is the nearest-neighbor hopping integral,  $\epsilon_{\mathbf{k}}$  is the kinetic energy, and we have set the lattice constant  $a_0$  to unity. We define the Fermi energy  $E_F$  for a given density  $n$  as the chemical potential  $\mu$  for a noninteracting Fermi gas on the lattice at zero  $T$ . In addition, a contact potential in the continuum now becomes an on-site attractive interaction  $U$ . Namely, we are now solving a negative- $U$  Hubbard model. The Lippmann-Schwinger relation reads  $m/4\pi a\hbar^2 = 1/U + \sum_{\mathbf{k}}(1/\epsilon_{\mathbf{k}})$ . Therefore, the critical coupling strength is given by  $U_c = -1/\sum_{\mathbf{k}}(1/\epsilon_{\mathbf{k}}) = -7.91355t$ . Here  $m = t/2$  is the effective fermion mass in the dilute limit, where the Fermi surface becomes spherical so that one may define the Fermi wave vector  $k_F$  by  $E_F = \hbar^2 k_F^2/2m$ . In what follows, we shall set  $k_B = \hbar = 1$ .

To recapitulate our theory, the fermion self-energy comes from two contributions, associated with the superfluid condensate and finite-momentum pairs, respectively, given by  $\Sigma(K) = \Sigma_{sc}(K) + \Sigma_{pg}(K)$ , where  $\Sigma_{sc}(K) = -\Delta_{sc}^2 G_0(-K)$  and  $\Sigma_{pg}(K) = \sum_Q t_{pg}(Q)G_0(Q-K)$ , with  $\Delta_{sc}$  being the superfluid order parameter.  $\Sigma_{sc}(K)$  vanishes at and above  $T_c$ . The finite-momentum  $T$  matrix  $t_{pg}(Q) = U/[1 + U\chi(Q)]$  derives from summation of ladder diagrams in the particle-particle channel, with pair momentum  $Q$ , where the pair susceptibility  $\chi(Q) = \sum_K G(K)G_0(Q-K)$  involves the feedback of the self-energy via the full Green's function  $G(K)$ . As usual, we use a four-vector notation,  $K \equiv (i\omega_l, \mathbf{k})$ ,  $Q \equiv (i\Omega_n, \mathbf{q})$ ,  $\sum_K \equiv T \sum_l \sum_{\mathbf{k}}$ , and  $\sum_Q \equiv T \sum_n \sum_{\mathbf{q}}$ , where  $\omega_l$  ( $\Omega_n$ ) are the odd (even) Matsubara frequencies.

By the Thouless criterion, the  $T_c$  equation, given by  $1 + U\chi(0) = 0$ , now contains the self-energy feedback. This is a major difference between our pairing fluctuation theory and those based on NSR [1] or saddle-point approximations [2].

After analytical continuation  $i\Omega_n \rightarrow \Omega + i0^+$ , one can Taylor-expand the (inverse)  $T$  matrix as  $t_{pg}^{-1}(\Omega, \mathbf{q}) \approx Z(\Omega - \Omega_{\mathbf{q}} + \mu_{\text{pair}} + i\Gamma_{\mathbf{q}})$ , and thus extract the pair dispersion  $\Omega_{\mathbf{q}} = 2B(3 - \cos q_x - \cos q_y - \cos q_z)$ , where  $B$  is the effective pair hopping integral. Here the imaginary part  $\Gamma_{\mathbf{q}}$  can be neglected when pairs become (meta)stable [10].

At and below  $T_c$ ,  $\mu_{\text{pair}} = 0$  and  $\Sigma_{pg}(K)$  can be approximated as  $\Sigma_{pg}(K) = \Delta_{pg}^2/(i\omega_l + \xi_{\mathbf{k}}) + \delta\Sigma \approx -\Delta_{pg}^2 G_0(-K)$ , with the pseudogap parameter  $\Delta_{pg}$  defined as

$$\Delta_{pg}^2 \equiv - \sum_Q t_{pg}(Q) \approx Z^{-1} \sum_{\mathbf{q}} b(\Omega_{\mathbf{q}}), \quad (1)$$

where  $b(x)$  is the Bose distribution function. Neglecting the incoherent term  $\delta\Sigma$  in  $\Sigma_{pg}$ , we arrive at the total self-energy  $\Sigma(K)$  in the BCS form:

$$\Sigma(K) \approx -\Delta^2 G_0(-K), \quad (2)$$

where the total gap  $\Delta$  is determined via  $\Delta^2 = \Delta_{sc}^2 + \Delta_{pg}^2$ . Therefore, the Green's function  $G(K)$ , the quasiparticle dispersion  $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}$ , and the gap (or  $T_c$ ) equation all

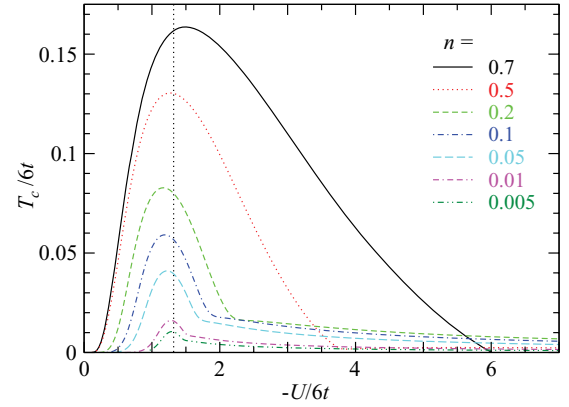


FIG. 1. (Color online) Behavior of  $T_c/6t$  as a function of the attractive on-site interaction  $-U/6t$  on a 3D isotropic lattice for various densities from high to low, as labeled. The unitary limit corresponds to  $-U/6t = 1.31893$ , as indicated by the vertical dotted line.

follow the BCS form, except that the total gap  $\Delta$  now contains contributions from both the order parameter  $\Delta_{sc}$  and the pseudogap  $\Delta_{pg}$ . Thus the gap equation is given by

$$1 + U \sum_{\mathbf{k}} \frac{1 - 2f(E_{\mathbf{k}})}{2E_{\mathbf{k}}} = 0, \quad (3)$$

where  $f(x)$  is the Fermi distribution function. In addition, the number equation  $n = 2 \sum_K G(K)$  is given by

$$n = \sum_{\mathbf{k}} \left[ 1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} [1 - 2f(E_{\mathbf{k}})] \right]. \quad (4)$$

Equations (3), (4), and (1) form a closed set. For given interaction  $U$ , they can be used to solve self-consistently for  $T_c$  as well as  $\Delta$  and  $\mu$  at  $T_c$ .

In Fig. 1 we plot  $T_c$  as a function of pairing strength  $-U/6t$  for various densities from high to low. Here  $6t$  is the half bandwidth. For  $n = 0.7$ , the maximum  $T_c$  occurs on the BEC side of unitarity. Then it moves to the BCS side as  $n$  decreases. As  $n$  further decreases, the maximum moves slowly back to the unitary point. This should be contrasted with the 3D continuum case, for which the maximum occurs slightly on the BEC side. The fact that the maximum occurs on the BCS side manifests a strong lattice effect at these intermediate densities; it is the lattice effect that causes difficulty for pair hopping and thus suppresses  $T_c$ . Even at density as low as  $n = 0.005$ , the maximum is still slightly on the BCS side.

In order to compare with the continuum  $T_c$  curves (see Fig. 10 in Ref. [12] for example) more easily, we normalize the  $T_c$  curves by the corresponding Fermi energy  $E_F$ , as shown in Fig. 2. For clarity, we have dropped the curves for the two high densities  $n = 0.7$  and  $0.5$ , for which  $T_c$  shuts off abruptly (for details, see Ref. [10]). The lattice effect has made the peak around unitarity much more pronounced and necessarily present in all different theoretical treatments of finite-temperature BCS-BEC crossover [25]. As  $n$  decreases, this peak becomes narrower and moves closer to unitarity. Beyond the unitary limit, the curve for  $n = 0.001$ , as a low-density example, exhibits a rapid falloff with pairing strength, and then decreases following the functional form  $T_c \propto -t^2/U$ .

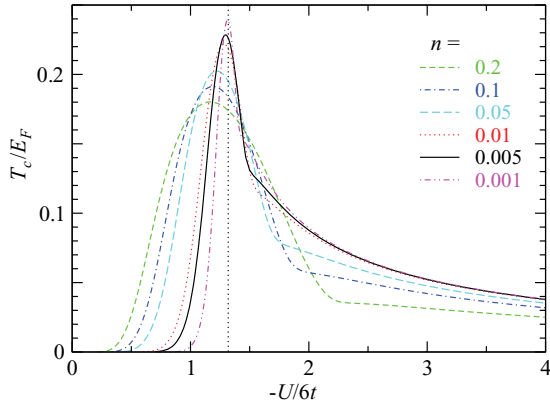


FIG. 2. (Color online)  $T_c/E_F$  as a function of  $-U/6t$  on a 3D isotropic lattice for various densities from  $n = 0.2$  to  $0.005$ . The unitary limit corresponds to  $-U/6t = 1.31893$ , as indicated by the vertical dotted line.

This is due to the virtual ionization during pair hopping in the BEC regime. At unitarity, a significant fraction of fermions form metastable pairs [10,11] already at  $T_c$ , and thus they also experience the lattice effect during pair hopping through virtual ionization. The tight-binding pair dispersion, restricted momentum space, and virtual ionization process suggest that the lattice effect does not readily go away completely as the  $n = 0$  limit is approached. Figure 2 also reveals that, as  $n$  approaches zero, the maximum  $T_c/E_F$  as well as  $T_c/E_F$  at unitarity gradually increase.

Finally, presented in the main figure of Fig. 3 is  $T_c/E_F$  as a function of (the cubic root of) the density  $n$  in the unitary limit, down to  $n = 5.0 \times 10^{-7}$ . For low  $n$ , the lattice effect is expected to vary as  $n^{1/3}$  to the leading order, namely,  $T_c(n)/E_F(n) = T_c(0)/E_F(0) - \alpha a_0 n^{1/3} + o(a_0^2/n^{2/3})$ , where  $\alpha$  is a proportionality coefficient. Note that  $a_0 n^{1/3}$  represents the ratio between the lattice period and the mean interparticle

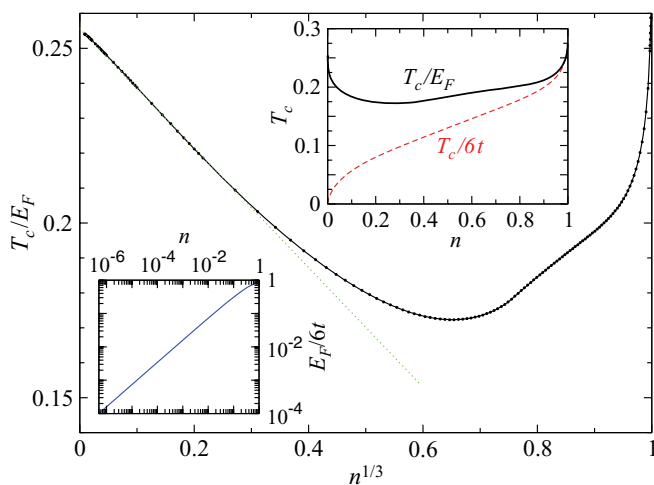


FIG. 3. (Color online)  $T_c/E_F$  as a function of  $n^{1/3}$  on a 3D isotropic lattice at unitarity. Shown in the lower left inset is  $E_F/6t$  as a function of  $n$ , and plotted in the upper inset are  $T_c/E_F$  (black solid curve) and  $T_c/6t$  (red dashed line) as functions of  $n$ . The (green dotted) linear extrapolation line obtained from fitting using data points below  $n^{1/3} = 0.2$  yields  $T_c/E_F = 0.2557$  at  $n = 0$ .

distance. At the same time,  $T_c/E_F$  and  $T_c/6t$  are plotted as functions of  $n$  in the upper inset. It shows that  $T_c/E_F$  increases rapidly near the very end of  $n = 0$ . The behavior of  $E_F/6t$  is shown in the lower inset, in a log-log plot. In units of  $6t$ , both  $E_F$  and  $T_c$  vanish at  $n = 0$  and reach a maximum at half filling [26]. In particular,  $E_F = 6t$  at half filling,  $n = 1$ , as expected.

It is evident that  $T_c/E_F$  is highly nonlinear as a function of  $n^{1/3}$ . Our result reveals that as  $n$  decreases from half filling,  $T_c/E_F$  decreases and reaches a minimum of  $0.172$  around  $n = 0.28$ , and then starts to recover slowly. It does not accelerate until the very end of  $n = 0$ . The main plot suggests that  $T_c/E_F$  eventually does recover its continuum counterpart value,  $0.256$ , but the curve exhibits a good linearity only for  $n^{1/3} < 0.2$ , i.e.,  $n < 0.008$ . At  $n = 5.0 \times 10^{-7}$ , we find  $T_c/E_F = 0.254$ , close to  $0.256$ . Using the data below  $n^{1/3} = 0.2$ , our extrapolation (the green dotted line) leads to  $T_c/E_F = 0.2557 \approx 0.256$  for the continuum limit. Note that the data points for  $n^{1/3} > 0.3$  show a rather obvious deviation from the lower- $n$  extrapolation line. It is possible that the  $T_c/E_F$  extrapolation in QMC simulations exhibits a similar behavior. Then this would suggest that the range of density for extrapolation used in Ref. [17] is still far from the asymptotic linear regime. In fact,  $n^{1/3} > 0.3$  (or equivalently,  $k_F a_0 > 0.9$ ) cannot be regarded as  $\ll 1$ . Indeed, the recent result of Gouliko and Wingate [21] seems to confirm this point. Being able to push their simulations down to  $n^{1/3} \approx 0.23$  (albeit with a big error bar for this lowest-density data point), they obtained  $T_c/E_F = 0.173$  for the zero-density limit using a linear extrapolation. One can also see from their Fig. 7 that, without this lowest-density data point, they would have obtained a lower value for  $T_c/E_F$ . In addition, their quadratic fit would yield  $T_c/E_F \approx 0.19$ . Finally, we note that a closer look at Fig. 3 of Ref. [17] suggests that the lowest-density point of those authors (also with a big error bar) actually already shows that their curve starts to bend upward, away from the straight extrapolation line. Although not conclusive, this observation does agree with the  $T_c/E_F$  curve in Fig. 3.

As argued above, despite the big difference between our theory and the QMC approach, it is not unreasonable to expect that the lattice effect has a rather similar impact (with possible minor quantitative differences) on  $T_c/E_F$ . Without a rigorous proof, the above examination of Refs. [21] and [17] does seem to support such an expectation. Even if the QMC approach may have a different scaling behavior of  $T_c/E_F$  versus  $n^{1/3}$ , it is highly unlikely that the linear regime extends up to  $n^{1/3} = 0.35$  (and all the way through  $n^{1/3} = 0.8$  as shown in Ref. [17]). Therefore, we propose that in order to obtain an accurate value of  $T_c/E_F$  in the zero-density limit using a linear extrapolation, one needs to perform QMC calculations down to  $n^{1/3} \sim 0.1$  (i.e.,  $n \sim 1.0 \times 10^{-3}$ ) or lower. A more careful study of the scaling behavior of  $T_c/E_F$  in various QMC formulations is required and extrapolation using a higher-order polynomial fit may be needed.

The authors of Ref. [18] reported that they confirmed their lattice fermion result of Ref. [17] by working in the continuum limit. However, here we argue that the lattice effect was actually introduced back through their Eqs. (3) and (4) and the periodic boundary condition, which is roughly equivalent to restricting consideration to the lowest energy band in the

zero-strength limit of the lattice potential [27]. Indeed, this has also been confirmed by Ref. [28]. In Ref. [18], simulations at unitarity were performed down to  $n \approx 0.05$  (with  $l_0 = 1$ ), or  $n^{1/3} \approx 0.37$  (or  $k_F l_0 \approx 1.1$ ). Above this density, the curve in the main figure of Fig. 3 shows significant deviation from linearity, caused by contributions of order  $n^{2/3}$  and higher. Our result suggests that the densities used for the QMC simulations in Ref. [17] were not low enough to ensure a good linear zero-density-limit extrapolation of  $T_c/E_F$  as a function of  $n^{1/3}$ .

The QMC simulations by Bulgac *et al.* were also done on a lattice, with a small atom number and a small lattice size (e.g., only 50–55 atoms on an  $8^3$  lattice in Refs. [19,20], equivalent to  $n = 0.1$ – $0.11$  or  $n^{1/3} = 0.46$ – $0.48$ ), rather far from the dilute limit. In the context of dynamical mean-field theory, Privitera *et al.* [29] studied the importance of nonuniversal finite-density corrections to the unitary limit and found that “densities around  $n \simeq 0.05$ – $0.01$  are not representative of the dilute regime”; a lower density is needed.

It should be noted that our  $E_F$  is the actual Fermi energy in the 3D lattice, whereas in Ref. [17] it is simply defined as  $E_F = tk_F^2 = t(3\pi^2 n)^{2/3}$ , which will become the true Fermi energy only in the dilute limit. This definition also introduced extra (unphysical) dependence of  $T_c/E_F$  on  $n^{1/3}$ , especially at high and intermediate densities (see the lower inset of Fig. 3). There is no reason to believe that this extra dependence will cancel out the intrinsic high-order dependence of  $T_c/E_F$  on  $n^{1/3}$ .

Finally, it is interesting to note that on the lattice, the interaction at unitarity,  $U_c$ , is density independent so that  $U_c/E_F$  will scale to infinity as  $n$  approaches 0; the lattice periodicity introduced a natural momentum cutoff  $k_0 = \pi/a_0$ . In contrast, in the continuum, a contact potential can be regarded as the cutoff momentum  $k_0 \rightarrow \infty$  limit of an  $s$ -wave interaction,  $U(k) = U\theta(k_0 - k)$ , which has  $U_c = -2\pi^2/mk_0$ . Apparently, this  $U_c$  is scaled down to 0 for a contact potential. This dramatic contrast for  $U_c$  between 3D lattice and 3D continuum seems to suggest that there exist some differences between the 3D continuum and the zero-density limit of a 3D lattice. Indeed, a single fermion has a tight-binding lattice dispersion defined in the first Brillouin zone due to the lattice periodicity. Only in the zero-strength limit of the lattice potential and with the summation of all the infinite number of energy bands can one recover the parabolic dispersion of the continuum model with an infinite momentum space. Therefore, the fermions are always subject to the lattice periodicity no matter how low the density is. This, however, may be regarded as a consequence of the single- (lowest-energy) band approximation of the lattice Hamiltonian.

Without including the particle-hole channel and the self-energy feedback in the  $T_c$  equation [11], the NSR theory [1,4,30] and the saddle-point approximation [2] predicted  $T_c/E_F = 0.22$ . Other approaches reported  $T_c/E_F \approx 0.26$  [3], 0.15 [5], and 0.16 [6], the last of which exhibits *unphysical* nonmonotonic first-order-like behavior in entropy  $S(T)$ .

Floerchinger *et al.* [7] found  $T_c/E_F = 0.264$  even after including particle-hole fluctuations. Within the present theory, Chen and co-workers reported  $T_c/E_F = 0.256$  [10–12].

Experimentally, the measurements of  $T_c/E_F$  have not reached a consensus yet. Kinast *et al.* [31], in collaboration with Chen *et al.*, found  $T_c/E_F = 0.27$  through a thermodynamic measurement in a unitary  ${}^6\text{Li}$  gas. Later, they [32,33] obtained 0.29 and 0.21 by fitting entropy and specific heat data with different formulas. The latter value was obtained assuming a specific heat jump at  $T_c$ , which may not be a good approximation in the presence of a strong pseudogap at  $T_c$  (see, e.g., Refs. [12,34,35]). According to our calculations,  $T_c$  at unitarity in the trap is only slightly higher than its homogeneous counterpart, 0.272 versus 0.256. A similar small difference in  $T_c$  between the trap and homogeneous cases is expected from other theories as well. Therefore, these measurements imply that the homogeneous  $T_c/E_F$  is about 0.25–0.19. Recently, Ku *et al.* [36] reported  $T_c/E_F \approx 0.167$  for a homogeneous Fermi gas by identifying the  $\lambda$ -like transition temperature.

Our result demonstrates that the  $n \rightarrow 0$  limit of the lattice  $T_c/E_F$  does approach that calculated directly in the continuum. We expect this to remain true when the particle-hole channel contributions are properly included. In that case, we obtain  $T_c/E_F = 0.217$  at unitarity [24], consistent with some of the above experimental measurements. In addition, the maximum  $T_c/E_F \approx 0.256$  is then shifted to  $1/k_{FA} \approx 0.35$ , leading to a positive slope of  $T_c/E_F$  vs  $1/k_{FA}$  at unitarity, in agreement with the QMC result [18]. In this way, our maximum  $T_c/E_F$  seems to be close to, and should be compared with, the maximum  $T_c/E_F$  around  $1/k_{FA} = 0.47$  in Ref. [18]. Finally, we note that inclusion of the incoherent self-energy  $\delta\Sigma$  in our calculations would further reduce the value of  $T_c/E_F$  at unitarity [24], bringing it closer to the result of Ku *et al.* [36].

In summary, we have investigated the lattice  $T_c/E_F$  as a function of  $n^{1/3}$  down to  $n = 5 \times 10^{-7}$ , using a pairing fluctuation theory. It turns out that only below  $n^{1/3} \approx 0.2$  does  $T_c/E_F$  exhibit a good linearity. Despite the difference between this approach and QMC simulations, which have difficulty reaching the low-density regime, this finding calls for extra caution when linearly extrapolating  $T_c/E_F$  to the zero-density limit using QMC simulation data points at intermediate and high densities. More careful studies of the scaling behavior of the lattice fermion  $T_c/E_F$  as a function of  $n^{1/3}$  in various QMC formulations are suggested.

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