

## Temperature of a trapped unitary Fermi gas at finite entropy

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We present theoretical predictions for the equation of state of a harmonically trapped Fermi gas in the unitary limit. Our calculations compare Monte Carlo results with the equation of state of a uniform gas using three distinct perturbation schemes. We show that in experiments the temperature can be usefully calibrated by making use of the entropy, which is invariant during an adiabatic conversion into the weakly interacting limit of molecular BEC. We predict the entropy dependence of the equation of state.

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### I. INTRODUCTION

The past two years have witnessed many exciting developments in experiments on dilute Fermi gases of ultracold  ${}^6\text{Li}$  and  ${}^{40}\text{K}$  atoms [1–8]. In these systems the interaction strength between atoms, represented dimensionlessly as  $k_F a$ , where  $k_F$  is the Fermi wave vector and  $a$  is the  $s$ -wave scattering length, can be varied arbitrarily via a Feshbach resonance. One can therefore access the strongly interacting regime of  $-1 < 1/k_F a < 1$ , where a smooth crossover from a Bardeen-Cooper-Schrieffer (BCS) superfluidity to a Bose-Einstein condensate (BEC) occurs. Of particular interest is the unitary limit with negligible interaction range and divergent scattering length ( $k_F a \approx \infty$ ), in which a universal behavior is expected [9,10]. This remarkable feature renders the unitary Fermi gas an intriguing many-body system.

Evidence for the onset of fermionic superfluidity at the BCS-BEC crossover has been found in several ground-breaking experiments. These have measured condensate formation [1], density [2] and momentum distributions [4], collective excitations [5], rf spectroscopy [6], and vortices [7]. A thermodynamic measurement of the heat capacity of  ${}^6\text{Li}$  atoms has also been performed very close to the unitary limit [8], showing an abrupt jump at an estimated temperature of about  $0.27T_F$ , where  $T_F$  is the Fermi temperature. However, there is no model-independent method to measure the temperature of a strongly attractive, deeply degenerate Fermi gas. In experiments the gas is characterized indirectly by an empirical temperature (or thermometry) obtained by fitting integrated one-dimensional (1D) density profiles to an ideal Thomas-Fermi (TF) distribution [8]. For these isolated systems, the entropy is more readily measurable than the temperature. The goal of this work is to predict the equation of state in terms of measurable quantities such as the entropy.

In contrast to these rapid experimental advantages, theoretical progress on the crossover is quite limited [11–19]. In the strongly correlated unitary limit, it is extremely difficult to construct a quantitative theory in terms of a well-defined small parameter, especially at finite temperature. Therefore, current theoretical understanding of experimental data relies heavily on the simplest BCS mean field picture [8,20,21]. In particular, the heat capacity measurement has been explained by a crossover theory [8], where a BCS-like ground state is

generalized to accommodate thermal bosonic degrees of freedom in the long wavelength limit [22].

In the unitary limit of a Fermi gas there are strong pair fluctuations in the  $T$ -matrix approximation beyond the mean-field level. These must be included to predict the energy as a function of entropy in the unitary regime. The entropy in turn is a function of more readily measured temperatures in well-understood weakly interacting regimes, which are accessible via adiabatic changes in the coupling constant. The combination of measured temperatures of molecular BEC together with the state equation also allows one to estimate the corresponding strongly interacting temperatures. While entropy invariance under adiabatic passage is well understood, the crucial step here is to obtain a reliable state equation below threshold that covers the entire range from weak to strong interactions.

Without a controllable small parameter in the unitary regime, the determination of the equation of state is by no means a trivial task. In general, there are a number of alternative  $T$ -matrix schemes that can be implemented to tackle the crossover problem, and there is no *a priori* judgement of which one is the most accurate. In this regard, it is of particular relevance that Monte Carlo simulations have been performed in the unitary limit at finite temperature [23], which present useful benchmarks on the validity of different approximations. Here we present a comparative study of the equation of state of a *uniform* gas using three candidate  $T$ -matrix schemes, and show that, apart from a small region around the transition temperature, a below threshold version of the Nozières and Schmitt-Rink (NSR) scheme seems to be the optimal choice for the calculations [13] of the type required for thermometry. We then incorporate the effect of an harmonic trap using a local density approximation that holds for large particle number.

We characterize the entropy and temperature of the strongly interacting system by an isentropic sweep to the weakly interacting molecular BEC regime, and a consequent determination [2,6,24] of the entropy  $S$  from the final temperature  $T'$ . The  $T'$  dependence of the equation of state is predicted. Alternatively, we can view this as a predicted equation of state in terms of the entropy, which can be readily compared to completely model-independent experimental observations of quantities like the system energy as a function of entropy.

The manuscript is organized such that the equation of state of a uniform unitary Fermi gas is first determined by comparing three different perturbation schemes, and then used to calculate the equation of state of a trapped Fermi gas within local density approximation. In turn the resulting unitary entropy is used to match the entropy of a weakly interacting Bose gas to obtain the desired isentropic thermometry. Finally, a summary and conclusions are given.

## II. EQUATION OF STATE OF HOMOGENEOUS UNITARY GASES

To describe a gas of  ${}^6\text{Li}$  atoms at a broad Feshbach resonance  $B_0=834$  G, we adopt a single-channel model [25,26], in which the attractive interatomic interaction is characterized by a contact potential of strength  $U=4\pi\hbar^2 a/m$ . In the *normal* state above the superfluid transition temperature  $T_c$ , the model can be treated perturbatively with the inclusions of strong pair fluctuations in the many-body  $T$ -matrix approximation [22], which leads to a two-particle propagator  $\chi(\mathbf{q}, i\nu_n)$  given by

$$\chi(\mathbf{q}, i\nu_n) = \frac{1}{\beta} \sum_{\mathbf{k}, i\omega_m} G_a(\mathbf{k}, i\omega_m) G_b(\mathbf{q}-\mathbf{k}, i\nu_n - i\omega_m), \quad (1)$$

and a corresponding self-energy of the form

$$\Sigma(\mathbf{k}, i\omega_m) = \frac{1}{\beta} \sum_{\mathbf{q}, i\nu_n} \frac{U}{1 + U\chi(\mathbf{q}, i\nu_n)} G_c(\mathbf{q}-\mathbf{k}, i\nu_n - i\omega_m), \quad (2)$$

where  $\omega_m \equiv (2m+1)\pi/\beta$  and  $\nu_n \equiv 2n\pi/\beta$  are, as usual, the fermionic and bosonic Matsubara frequencies with inverse temperature  $\beta=1/k_B T$ . The superscript  $a$ ,  $b$ , and  $c$  in the above two equations can be set to “0,” indicating a noninteracting Green function  $G_0(\mathbf{k}, i\omega_m) = 1/[i\omega_m - \hbar^2 \mathbf{k}^2/2m + \mu]$ . If this superscript is absent, we refer to a fully dressed (interacting) Green function, and thereby a Dyson equation  $G(\mathbf{k}, i\omega_m) = G_0(\mathbf{k}, i\omega_m)/[1 - G_0(\mathbf{k}, i\omega_m)\Sigma(\mathbf{k}, i\omega_m)]$ , is required to self-consistently determine  $G$  and  $\Sigma$ . The only free parameter is the chemical potential  $\mu$ , which is fixed by using the number equation  $n=2/\beta \sum_{\mathbf{k}, i\omega_m} G(\mathbf{k}, i\omega_m)$ . According to the different combination of subscripts of  $a$ ,  $b$ , and  $c$ , on general grounds we may expect three obvious choices of the  $(G_a G_b)G_c$  will be used. These alternative choices distinguish themselves by the level of self-consistency contained in the Green function.

The simplest choice  $(G_0 G_0)G_0$  was proposed in a seminal paper [13] by NSR, although these authors approximated the Dyson equation using a leading order series, i.e.,  $G=G_0 + G_0 \Sigma G_0$ . This fully non-self-consistent scheme includes the least Feynman diagrams. In the other extreme limit, one can consider a fully self-consistent  $T$ -matrix approximation of  $(GG)G$ , which is a so-called conserving approximation [15]. An alternative intermediate scheme is to use an asymmetric form for the two-particle propagator, i.e.,  $(GG_0)G_0$  [22]. These candidate versions of  $T$ -matrix approximation have been extensively discussed for the attractive Hubbard model

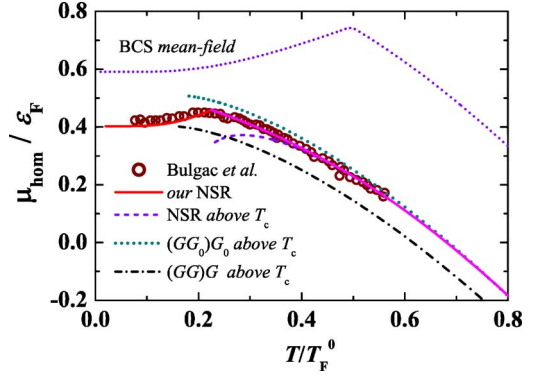


FIG. 1. (Color online) Chemical potential of a uniform Fermi gas in the unitary limit as a function of temperature, in units of Fermi energy  $\epsilon_F = \hbar^2 k_F^2/2m = k_B T_F^0$ . The lines plotted are our proposed results (solid lines), NSR  $(G_0 G_0)G_0$  predictions in Refs. [13,14] (dashed line), asymmetric  $(GG_0)G_0$  scheme (dotted line), and fully self-consistent  $(GG)G$  scheme (dot-dashed line). All these results are contrasted to the Monte Carlo data from Ref. [23] (open circles).

in the context of high- $T_c$  superconductors. The applicability of these theories to the single-channel model is under active debate, due to the complexity of numerical calculations. In this work, we have resolved the numerical difficulties by using a technique of adaptive step Fourier transformations [15,26], without additional approximation.

The situation in the broken-symmetry state is more subtle. Below  $T_c$ , the denominator in Eq. (2) develops a pole that signals the emergence of superfluid phases. To remove the instability, one may extend the different  $T$ -matrix approaches by using a BCS mean-field ground state as the starting point for a perturbation theory. For the  $(G_0 G_0)G_0$  scheme, this strategy has been recently adopted and investigated in depth by Strinati *et al.* [16] and by the present authors [17]. The advantage of the latter study is that a modified number equation was employed to obtain an (approximately) correct molecular scattering length, which therefore makes the theory quantitatively reliable over the entire crossover regime [17]. The other alternative versions of  $(GG_0)G_0$  and  $(GG)G$  along this line have not been explored yet. However, on physical grounds, below  $T_c$  one may expect only a slight difference among these schemes, as the ground state is well stabilized by the mean-field gap.

Figure 1 presents a comparative study of these candidate  $T$ -matrix approaches for a uniform unitary gas at finite temperature. In the superfluid state, we use the NSR-like formalism implemented in Ref. [17]. The calculated chemical potentials of the gas are compared with a recent Monte Carlo simulation from Ref. [23]. Just above the transition temperature  $T_c \sim 0.2T_F^0$ , all approximations appear poor, with errors of around  $\pm 10\%$ . In particular, the NSR approach suffers from an unphysical drop with decreasing temperature, which should be due to the lack of self-consistency in the two-particle propagator. At high temperatures above  $0.35T_F^0$ , the NSR result turns out to be very accurate. This observation, together with the excellent agreement between the NSR prediction and Monte Carlo data below  $T_c$ , suggest that the fully non-self-consistent NSR scheme is generally accurate, apart

TABLE I. The superfluid critical temperature for a homogeneous unitary Fermi gas obtained by various methods. The chemical potential, total energy, and entropy at the critical temperature are also listed. We note that all the methods, except the  $(GG_0)G_0$  scheme, satisfy an exact identity  $P=2/3E$  that holds in the unitary limit, where  $P=-\Omega=-(E-TS-\mu N)$  is the pressure of the gas. The energy and entropy for the  $(GG_0)G_0$  and  $(GG)G$  approximations are not available.

Methods	$T_c/T_F^0$	$\mu(T_c)/\epsilon_F$	$E(T_c)/(N\epsilon_F)$	$S(T_c)/(Nk_B)$
BCS-MF	0.50	0.743	1.022	1.92
$(G_0G_0)G_0$	0.225	0.340	0.290	0.64
$(GG_0)G_0$	0.178	0.508	N.A.	N.A.
$(GG)G$	0.150	0.404	N.A.	N.A.
our NSR	0.225	0.459	0.400	0.91
Monte Carlo	0.23(2)	0.45	0.41	0.99

from the regime just above  $T_c$ . The spurious structure about  $T_c$  in this scheme might be avoided by a phenomenological interpolation between the results at  $T_c$  and at a high temperature  $\sim 0.4T_F^0$ . The outcomes with this idea have been denoted in the figure by solid lines, and referred to later as “our NSR” results. From this, we are able to calculate the energy and entropy.

We emphasize that the equation of state obtained in this manner is certainly not *ab initio*, but it should be quantitatively valid, provided the Monte Carlo simulation data are accurate. More reliable Monte Carlo simulations with larger lattices may change these conclusions slightly in future, especially in the vicinity of  $T_c$ , where already there are reports of small discrepancies between the simulations carried out with different lattices and algorithms. The important issue here is that while there are discrepancies *above*  $T_c$  which make it difficult to decide which approximation is better, the below  $T_c$  region which is crucial for finite entropy thermometry methods shows excellent agreement between Monte Carlo data and our  $(G_0G_0)G_0$  scheme.

We close this section by listing in Table I the predictions for the superfluid transition temperature that were obtained by the various models we have discussed. The chemical potential, the total energy and the entropy at the transition temperature are also outlined.

### III. EQUATION OF STATE OF TRAPPED UNITARY GASES

With the knowledge of equation of state of a uniform gas, we incorporate the effects of harmonic traps by using the local density approximation, which amounts to determining the global chemical potential from the local equilibrium condition

$$\mu = \mu_{\text{hom}} \left[ n(\mathbf{r}), \frac{T}{T_F} \frac{T_F}{T_F^0(\mathbf{r})} \right] + \frac{m\omega_r^2}{2} (r^2 + \lambda^2 z^2), \quad (3)$$

with a density  $n(\mathbf{r})$  normalized to the total number of atoms,  $\int n(\mathbf{r}) d\mathbf{r} = N$ . Here  $\mu_{\text{hom}}$  is our proposed NSR chemical po-

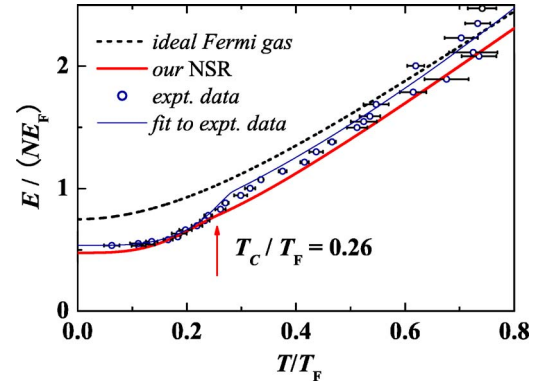


FIG. 2. (Color online) Energy of a trapped unitary gas is plotted as a function of temperature (thick solid line), and compared to experimental data (open circles with error bars). The comparison with respect to the prediction of an ideal Fermi gas (dashed line) is also shown. The thin solid line is an empirical power law fit to the measured energies [8], i.e.,  $E(T) = E_0[1 + 97.3(T/T_F)^{3.73}]$  for  $T < T_c \approx 0.27T_F$  and  $E(T) = E_0[1 + 4.98(T/T_F)^{1.43}]$  above  $T_c$ . Here  $E_0$  is the energy at zero temperature and  $T_c = 0.27T_F$  is the experimentally extracted superfluid transition temperature [8].

tential of a uniform gas in Fig. 1, and  $\omega_x = \omega_y = \omega_r$  and  $\omega_z = \lambda\omega_r$  are different frequencies for three axes. In this case, the energy and temperature can be taken in units of the (non-interacting) Fermi energy  $E_F = (3N\omega_x\omega_y\omega_z)^{1/3}$  and  $T_F = E_F/k_B$ , respectively. Once  $n(\mathbf{r})$  are obtained, the energy and the entropy of the gas can then be calculated straightforwardly, using  $E = \int n(\mathbf{r}) E_{\text{hom}} d\mathbf{r}$  and  $S = \int n(\mathbf{r}) S_{\text{hom}} d\mathbf{r}$ , with our proposed equation of state of a homogeneous gas  $E_{\text{hom}}[n(\mathbf{r}), T/T_F^0(\mathbf{r})]$  and  $S_{\text{hom}}[n(\mathbf{r}), T/T_F^0(\mathbf{r})]$ .

The temperature dependence of the energy and the specific heat of a trapped unitary gas are given in Figs. 2 and 3, and are compared to the experimental data obtained by Kinast *et al.* in the vicinity of unitary limit ( $1/k_F a \approx -0.03$ ) [8]. It is worth noting that these experimental data are not completely raw, since the measured empirical temperature requires a model-dependent theoretical recalibration [29].

Our results agree qualitatively with experimental data. In particular, our predictions for the specific heat show an apparent superfluid transition at about  $T_c \approx 0.26T_F$ , in excellent agreement with the experimental findings [30]. The peak structure resembles the  $\lambda$  transition for a BEC. The behavior of specific heat of a unitary Fermi gas thereby lies between that of ideal Fermi gases and that of BECs. The value of both theoretical and experimental  $T_c$  need further refinement, as the detailed equation of state of a uniform gas around the transition temperature is blurred by the semiempirical interpolation, and the experimental temperatures are not known accurately. Another noticeable feature of our result is that it deviates greatly from the noninteracting Fermi gas behavior for all the temperatures considered. This is suggestive of the strongly-correlated nature of unitary gases, and is in sharp contrast to the prediction of mean-field crossover theories by Chen *et al.* [8,22].

### IV. ISENTROPIC THERMOMETRY FOR TRAPPED UNITARY GAS

A quantitative comparison between our theoretical results and experimental findings is prohibited, as current esti-

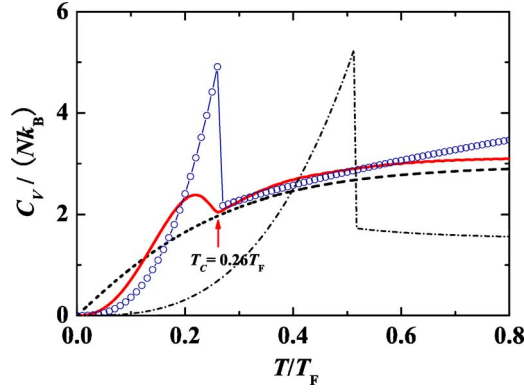


FIG. 3. (Color online) Specific heat  $C_V=dE/dT$  of a trapped unitary gas as a function of temperature. For comparison, the predictions of an ideal Fermi gas (dashed line) and of an ideal Bose gas with number of particles  $N_B=N/2$  (dot-dashed line) [27], together with the experimental extracted specific heat (line with open circles) are also presented. It should be noted that a precise determination of the specific heat from experimental data of energies is not permissible. The experimental specific heat shown here is calculated from the empirical power law fit to the measured energies, which is outlined in Fig. 2. The resulting sharp jump at  $T_c$  is thereby possibly an artifact of the fit. We note also that the abrupt discontinuity in the specific heat of an ideal trapped Bose gas at  $T_c$  will be rounded off quickly with inclusions of boson-boson interactions, see, for example, Fig. 3 in Ref. [28].

mates of strongly interacting Fermi gas temperatures are based on empirical thermometry through density profile measurements, which are strongly dependent on the model used, but relatively insensitive to the actual temperature [31]. A better thermometry would be obtained by an adiabatic conversion of the unitary gas to the deep BEC limit, and a consequent measurement of BEC temperature  $T'$  of a resulting Bose gas [24]. Such techniques have been used in recent experiments for temperature estimates [2,6], but the conversion between  $T'$  and the unitary temperature  $T$  remains unknown. Below we quantify this important relation using the isentropic condition  $S'(T')=S(T)$ .

To be concrete, we consider a gas of  $2 \times 10^5$   $^6\text{Li}$  atoms with a potential  $\omega_r=1555$  Hz and  $\omega_z=127$  Hz, according to the typical setup [2]. Assuming that the gas is swept to a field of  $B=676$  G [2], we find  $1/k_F a \approx 4.9$ . Thus, the system after sweep can be well described by a weakly interacting Bose gas with molecular scattering length  $a_m=0.6a$ . The entropy  $S'(T')$ , calculated within the Hartree-Fock-Bogoliubov-Popov theory [32], has been compared with the unitary entropy  $S(T)$  in Fig. 4(a). This calibrates the unitary temperature, given in Fig. 4(b). Accordingly, the equation of state can also be determined in terms of the BEC temperature  $T'$ , as shown in Fig. 4(c). It is worth noticing that this kind of thermometry should be very accurate, thanks to the demonstrated perfect adiabatic sweep of magnetic fields [2] and a precise determination of BEC temperature [33].

## V. SUMMARY

In the present paper we have studied the equation of state of a trapped unitary gas with a perturbation theory that in-

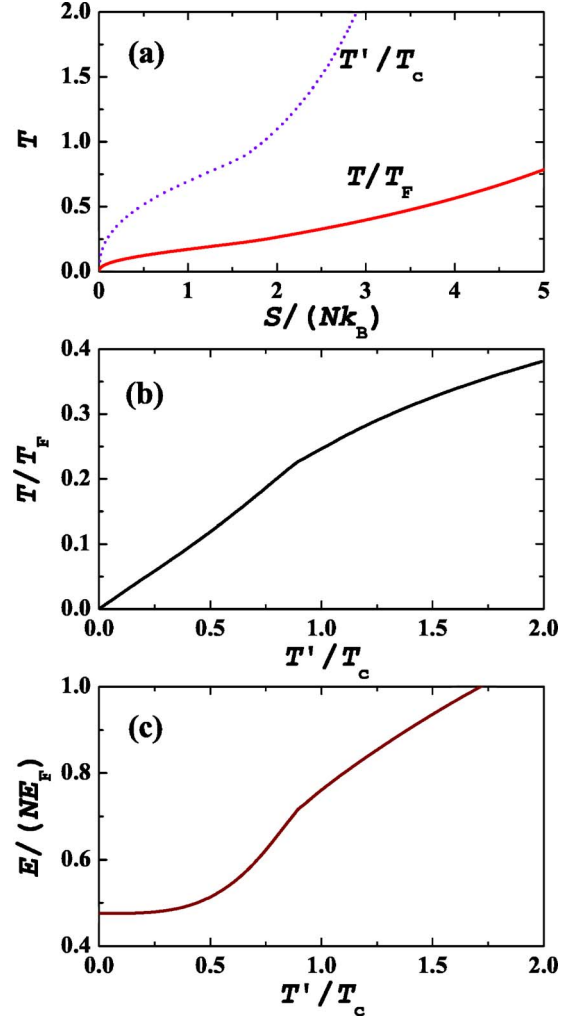


FIG. 4. (Color online) (a) The temperature as a function of entropy in the unitary limit (solid line) and in the deep BEC limit of  $1/k_F a \approx 4.9$  (dashed line), with  $T_c=0.518T_F$ . At low temperature, our calculated BEC entropy satisfies the scaling law for a weakly interacting Bose gas [32]:  $S'(T') \propto (T')^{5/2}$ . (b) Calibration curve of unitary temperature versus weakly interacting Bose gas temperature. (c) Unitary energy as a function of BEC temperature  $T'$ .

cludes fluctuations beyond the mean field. Our investigations, in contrast to mean-field theory [11,12,22], are in excellent agreement with Monte Carlo simulations below threshold, although there are still uncertainties of order 10% around threshold. We find a qualitative agreement between our theoretical predictions and the experimental findings. A fully quantitative comparison is not yet possible, as the experimental temperatures are not directly determined. We reach the conclusion that the empirical thermometry adopted in the experiment can be improved by using adiabatic sweeps at constant entropy to the weakly interacting molecular superfluid regime. The equation of state based on this type of thermometry has been predicted, allowing for experimental tests.

We emphasize that while our NSR result for the equation of state is very accurate at both low and high temperatures, its accuracy around the critical temperature  $T_c$  requires a further improvement beyond  $T$ -matrix approximation. In

terms of functional-integral methods [14], our NSR approach can be identified as a Gaussian expansion of the action of Cooper-pairs about the saddle point (mean-field solution). Therefore, a systematic refinement of equation of state around  $T_c$  might be achieved by expanding the action to fourth or higher order about the saddle point. We will address this issue in a later publication.

Our calculated equation of state can be used to predict other observables of experimental interest, such as the first sound and second sound velocities of trapped unitary Fermi gases at finite temperature [34,35], which soon may be mea-

sured. These sound modes, particularly the second sound, may provide us more accurate details about the equation of state in the unitary limit, and therefore discriminate various approximations that we have marked. This extension is under investigation and will be reported elsewhere.

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- [30] In contrast, the crossover theory of Chen *et al.* [22] fails to predict such apparent superfluid transition, although it has been used to recalibrate the measured empirical temperatures.
- [31] The resulting empirical temperature itself is model-independent. However, to recover the actual temperature, an assumption is used that the full three-dimensional density distribution in the unitary limit is close to an ideal TF functional form. We have checked this, and found that this essential assumption is not well-satisfied either in the mean-field or NSR theories. Hence, the mapping from empirical to actual temperatures can have large random and systematic errors.
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