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Finite-temperature behavior of an interspecies fermionic superfluid with population imbalance

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We determine the superfluid transition temperature T_c and related finite temperature phase diagrams for the entire BCS–Bose-Einstein-condensation crossover in a three-dimensional homogeneous mixture of ^{6}Li and ^{40}K atoms with population imbalance. Our work is motivated by the recent observation of an interspecies Feshbach resonance. Pairing fluctuation effects, which significantly reduce T_c from the onset temperature for pairing (T^*), provide reasonable estimates of T_c and indicate that the interspecies superfluid phase should be accessible in future experiments. Although a homogeneous polarized superfluid is not stable in the ground state near unitarity, our phase diagrams show that it stabilizes at finite temperature.

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Ultracold Fermi gases with tunable attractive interactions provide an exciting opportunity to study superfluidity in the crossover from BCS theory to Bose-Einstein condensation (BEC). Recently, there has been an emphasis on population imbalanced gases [1–5]. There is evidence for a number of exotic states including both homogeneously polarized (widely called [21] the "Sarma" phase) as well as inhomogeneously polarized (or phase separated [6]) states [2,4]. Adding to the excitement is the possibility of discovering a new form of superfluid involving interspecies pairing. A first step en route to the discovery is the recent observation of Feshbach resonances between ^{6}Li and ^{40}K atoms [7]. If the transition temperatures are accessible, this tunable attractive interaction should enable BCS-BEC crossover in superfluid phases associated with unequal mass pairing.

In this Rapid Communication we determine the transition temperatures for the entire BCS-BEC crossover in a three-dimensional homogeneous mixture of ^{6}Li and ^{40}K atoms with population imbalance. We present the temperature-polarization phase diagrams associated with interspecies superfluid phases at and around unitarity. Our calculations show the importance of including pairing fluctuations which greatly suppress the transition temperature T_c relative to the pair formation temperature T^*. Our finite T theory is chosen to be compatible with a generalized BCS-Leggett ground state which has been studied previously [8,9] in the strict $T=0$ limit. An understanding of finite temperature effects positions us to address actual experiments (which are never in the ground state).

Our theoretical findings have features in common with previous equal-mass polarized gas experiments [10] where superfluid phases appear which are constrained to an intermediate regime of nonzero temperatures and restricted to very low polarizations. That is, they are associated with a lower as well as upper critical temperature although the polarized superfluid (when stable) is not otherwise atypical. We show that, in the absence of a trap, this intermediate temperature superfluid will be extremely difficult to observe when the heavy species is the majority, but it should be more accessible for the case where the heavy species is the minority. Finally, we study how the phase diagram evolves as one crosses from BCS to BEC. In contrast to polarized Fermi gases with equal mass, close to, but on the BEC side of resonance, the intermediate temperature superfluid disappears when the lighter species is the majority, giving way to a superfluid with only one transition temperature.

Here we consider only a homogeneously polarized superfluid or "Sarma state," noting that while it is unstable in the deep BCS regime [11], it is stabilized toward and beyond unitarity. We exclude from consideration the phase separated state [6]. This is principally because it is now clear [5] that the normal regions in this heterogeneous phase correspond to a complicated correlated normal state, which is currently best addressed nonanalytically using quantum Monte Carlo (QMC) simulations [12]. We also omit from consideration Larkin-Ovchinnikov-Fulde-Ferrell (LOFF) phases which are of interest in optical lattices [13] and one-dimensional gases [14] since earlier work by our group [15] has indicated that the LOFF state is generally very fragile with respect to raising temperature. There have been extensive studies on zero temperature properties of homogeneous [8] as well as trapped interspecies Fermi gases [8,16,17]. This body of work (like that in the present Rapid Communication) is based on a natural generalization of the BCS-Leggett ground state to accommodate unequal populations. There are, similarly, QMC simulations at $T=0$ [18]. While a two channel model formalism may be more relevant to the narrow resonances seen in Ref. [7], all work to date (including our own) deals with the simpler one channel model. Theoretical studies at finite temperatures that are consistent with these $T=0$ calculations have been limited to a strict mean-field approach [9] which ignores the important effects of pair fluctuations or noncondensed pairs.

In our discussion of the generalized Sarma state, we choose the convention $m_\downarrow > m_\uparrow$. The mass ratio is $m_\downarrow/m_\uparrow=6.7$. We define $E_{k\uparrow,\downarrow}=E_k \pm \xi_k^-$ and $E_k=\sqrt{\xi_k^{+2}+\Delta^2}$, where $\xi_k^\pm=(\xi_{k\uparrow}\pm\xi_{k\downarrow})/2$. Here $\xi_{k\sigma}=(k^2/2m_\sigma)-\mu_\sigma$ and $\sigma=\uparrow,\downarrow$. The four unknowns that must be determined at general temperature T involve the two fermionic chemical potentials $\mu_\uparrow$ and $\mu_\downarrow$, the excitation gap Δ and the order parameter Δ_{sc}. The central physical idea is that in our treatment [19] of BCS-BEC crossover, the quantity Δ^2 contains a contribution from condensed (denoted as sc) as well as noncondensed [pseudogap (pg)] pairs:

$$\Delta^2 = \Delta_{sc}^2 + \Delta_{pg}^2. \tag{1}$$

Thus the gap component Δ_{pg} must be separately determined in order to establish the transition temperature T_c, above which Δ_{sc} vanishes. This pg contribution to Δ^2 results from the fact that the attractive interaction is stronger than in the BCS limit so that an extra energy must be input (beyond Δ_{sc}^2) to break pairs. The distinction between Δ (associated with an onset temperature T^*) and the order parameter Δ_{sc} (associated with T_c) is an important component of the present theory. Moreover, at unitarity, μ is positive and nevertheless $\Delta_{pg} \neq 0$ so that we do not require a molecular binding energy to obtain a pseudogap. Experimentally Δ_{pg} can be measured using radio-frequency spectroscopy above T_c [20].

There are then four equations which will be derived microscopically below. The equations for the total number $n=n_\uparrow+n_\downarrow$ and number difference $\delta n=n_\downarrow-n_\uparrow$ of fermions are

$$n = \sum_{\mathbf{k}} \left\{ \left(1 - \frac{\xi_k^+}{E_k}\right) + [f(E_{k\uparrow}) + f(E_{k\downarrow})]\frac{\xi_k^+}{E_k} \right\}, \tag{2}$$

$$\delta n = \sum_{\mathbf{k}} [f(E_{k\downarrow}) - f(E_{k\uparrow})]. \tag{3}$$

Here $f(x)=(e^{x/T}+1)^{-1}$ is the Fermi distribution function. The polarization is defined as $p=\delta n/n$. The gap parameter Δ is obtained from

$$-\frac{M}{2\pi a} = \sum_{\mathbf{k}} \left[\frac{1 - f(E_{k\uparrow}) - f(E_{k\downarrow})}{2E_k} - \frac{1}{\epsilon_k} \right]. \tag{4}$$

Here the coupling constant is regularized by $g^{-1}=M/(2\pi a)-\Sigma_{\mathbf{k}}(2\epsilon_k)^{-1}$, where a is the s-wave scattering length, $M=m_\uparrow m_\downarrow/(m_\uparrow+m_\downarrow)$ is the reduced mass, and $\epsilon_k=k^2/2M$.

Finally, an equation for Δ_{pg}^2 requires that we establish the dispersion of the noncondensed pairs. These noncondensed pairs or pseudogap effects appear at $T\neq 0$ and are included via a T-matrix contribution to the fermion self-energy. Following Refs. [19,21], the fermionic self-energy $\Sigma_\sigma(K)=\Sigma_Q t(Q)G_{\bar\sigma}(Q-K)$, where the four-momentum $Q=(i\Omega_l,\mathbf{q})$, $K=(i\omega_n,\mathbf{k})$, and $\Omega_l(\omega_n)$ is the bosonic (fermionic) Matsubara frequency, with $\Sigma_Q=T\Sigma_l\Sigma_{\mathbf{q}}$, $\Sigma_K=T\Sigma_n\Sigma_{\mathbf{k}}$, and $\bar\sigma=-\sigma$. The T matrix is presumed to have the structure $t(Q)=t_{sc}(Q)+t_{pg}(Q)$. The condensate contribution satisfies $t_{sc}(Q)=-(\Delta_{sc}^2/T)\delta(Q)$. Here the fermionic Green's function is $G_\sigma(K)=[G_{0\sigma}^{-1}(K)-\Sigma_\sigma(K)]^{-1}$, with $G_{0\sigma}^{-1}(K)=(i\omega_n-\xi_{k\sigma})$. We set $\hbar\equiv 1$ and $k_B\equiv 1$.

The excited pair propagator is given by $t_{pg}(Q)=[g^{-1}+\chi(Q)]^{-1}$, where the symmetrized pair susceptibility, $\chi(Q)=\Sigma_{K,\sigma}G_{0\sigma}(Q-K)G_{\bar\sigma}(K)/2$, is used. A natural assumption is the usual BEC condition that the pair chemical potential vanishes below T_c, which, in turn, allows us to derive Eq. (4). This BEC condition $[t_{pg}^{-1}(0)=0]$ implies that t_{pg} is dominated by terms with $Q\approx 0$. In this way the pseudogap is well approximated by $\Delta_{pg}^2\equiv-\Sigma_Q t_{pg}(Q)$. It follows that $\Sigma_\sigma(K)=-\Delta^2 G_{0\bar\sigma}(-K)$, and in that way we have derived Eq. (1). One arrives at the two equations for the number densities via $n_\sigma=\Sigma_K G_\sigma(K)$, and in this way one derives Eqs. (2) and (3).

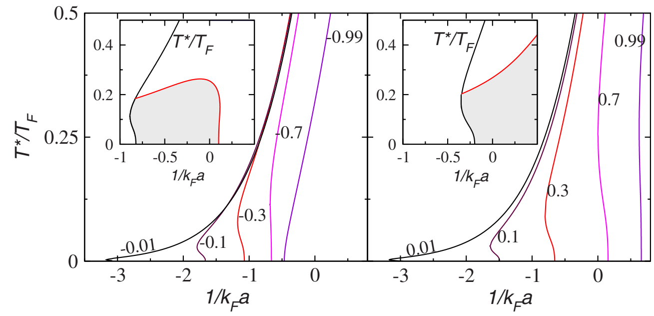

FIG. 1. (Color online) T^* as a function of $1/(k_Fa)$ for several values of $p=\delta n/n$ (as labeled). Here $p<0$ when the lighter (spin-up) species is the majority (left panel) and $p>0$ otherwise. Insets: The black solid, light (red) solid, and light (green) dashed lines are T^*, T_c, and the boundary of stable phases, respectively. Here k_F and T_F are the Fermi momentum and Fermi temperature of an unpolarized noninteracting Fermi gas with the same total particle density presuming a mass equal to the average mass of ^{6}Li and ^{40}K. The colored curves are to improve visibility but have otherwise no particular significance.

The T matrix may be expanded [22] as $t_{pg}^{-1}(\Omega,\mathbf{q})=a_0\Omega+a_1\Omega^2-\xi^2q^2$, after analytic continuation $(i\Omega_l\to\Omega+i0^+)$, where we have neglected the small imaginary part Γ_Q. The coefficients can be derived from the pair susceptibility: $a_0=(\partial\chi/\partial\Omega)|_{\Omega=0,q=0}$, $a_1=(1/2)(\partial^2\chi/\partial\Omega^2)|_{\Omega=0,q=0}$, and $\xi^2=(1/6)(\partial^2\chi/\partial q^2)|_{\Omega=0,q=0}$. Following this expansion, the pseudogap contribution can be written as

$$\Delta_{pg}^2 = \sum_{\mathbf{q}} \frac{b(\tilde\Omega_{\mathbf{q}})}{\sqrt{a_0^2+4a_1\xi^2q^2}}. \tag{5}$$

Here $b(x)$ is the Bose distribution function and $\tilde\Omega_{\mathbf{q}}=(\sqrt{a_0^2+4a_1\xi^2q^2}-a_0)/2a_1$. In the BEC limit, it can be shown that $a_1/a_0\to 0$ and $\Omega_{\mathbf{q}}\to q^2/2M^*$, where $M^*=a_0/2\xi^2$ is the effective pair mass. Importantly, in this limit M^* approaches the total mass of the two constituent fermions, and T_c approaches the BEC temperature of ideal bosons of density $\min(n_\uparrow,n_\downarrow)/2$ and mass M^*.

The gap equation [Eq. (4)] is equivalent to an extremal condition on the thermodynamic potential $\partial\Omega_{MF}/\partial\Delta=0$, where

$$\Omega_{MF} = -\frac{\Delta^2}{g} + \sum_{\mathbf{k}} (\xi_k^+ - E_k) - T\sum_{\mathbf{k},\sigma} \ln(1+e^{-E_{k\sigma}/T}). \tag{6}$$

Superfluid stability requires that the number susceptibility matrix $\partial n_\sigma/\partial\mu_{\sigma'}$ should be positive definite [21]. This can be shown to coincide with the condition that $\partial^2\Omega_{MF}/\partial\Delta^2>0$. When this condition is violated, phase separated states may occur.

We arrive at a reasonable estimate of the pairing onset temperature T^* from Eqs. (2)–(4), which is plotted in Fig. 1 as a function of $1/(k_Fa)$. Two different signs of the polarization p are indicated in the right and left panels. We will see that throughout the Rapid Communication a superfluid phase with $p<0$ (where the lighter species is the majority) appears

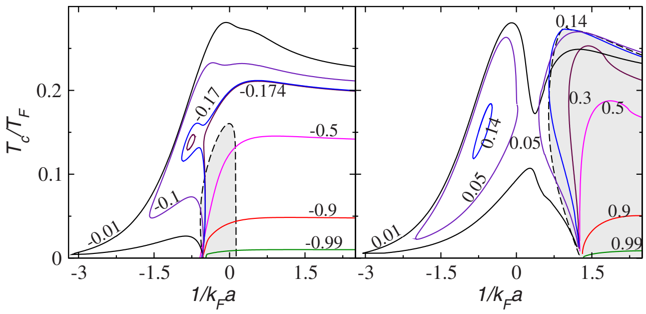

FIG. 2. (Color online) T_c as a function of $1/(k_F a)$ for selected values of p. Here $p<0$ when the lighter species is the majority (left panel) and $p>0$ otherwise. The polarized superfluid solution is unstable in the shaded regions.

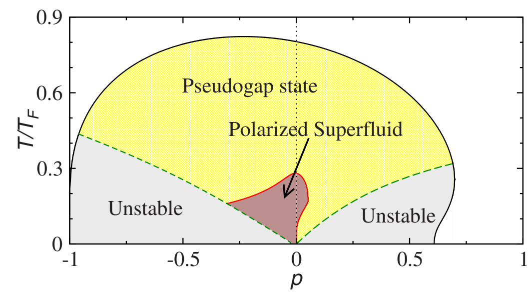

FIG. 3. (Color online) Phase diagrams for mixtures of ^{6}Li and ^{40}K atoms at unitarity. Here $p<0$ when ^{6}Li is the majority species and $p>0$ otherwise. The black solid, red solid, and green dashed lines are T^*, T_c, and the boundary of stable phases, respectively. Labeled are polarized superfluid (brown), pseudogap state (yellow) and unstable Sarma (gray) phases. The white open space is a polarized normal Fermi gas.

to be more readily obtainable than the one with $p>0$. The arguments behind this asymmetry in p are subtle and involve both energetic comparisons as well as mechanical stability (in the sense of $\partial^2\Omega_{MF}/\partial\Delta^2>0$). It can be analytically shown that at $T=0$ when polarization is small in the BEC regime, a superfluid phase with $p<0$ is more energetically favorable than one with $p>0$.

The figure shows that T^* vanishes when the attraction is sufficiently weak and near its vanishing point it displays nonmonotonic behavior. Similar behavior has been observed previously for population imbalanced Fermi gases of equal masses [21]. The insets of Fig. 1 indicate the unstable regimes for $p=\pm 0.5$. The unstable regimes are asymmetric in the sign of p, and at $T=0$ the behavior is consistent with phase diagrams obtained earlier [8,9]. This instability can be associated with the existence of a phase separated state [6].

We turn next to the superfluid transition temperature, T_c, which is plotted in Fig. 2 as a function of $1/(k_F a)$, for both $p<0$ (left panel) and $p>0$ (right panel). The shaded regions indicate where this form of (Sarma state) superfluidity is unstable against phase separated states. Note that there is a rather pronounced asymmetry between the $p<0$ and $p>0$ cases. Indeed, when $p>0$, a stable superfluid cannot be found in the shallow BEC near $1/k_F a=1.5$ although it will emerge again the deep BEC. An "intermediate temperature superfluid" phase exists in the BCS through unitary regimes, which is stabilized only away from the ground state. This is an unusual phase corresponding to a polarized superfluid enclosed by both a lower and an upper critical temperature, as previously found for population imbalanced equal mass Fermi gases both theoretically [21] and experimentally [4], albeit in a trap. As the polarization increases, in order to establish continuous behavior, isolated islands of this intermediate temperature superfluid develop on the BCS side of resonance, until at sufficiently high p, a homogeneously polarized superfluid is no longer stable for negative scattering lengths.

In Fig. 3 we present the phase diagram at unitarity as a function of T and p. A uniformly polarized superfluid exists at low $|p|$ and low but finite T (the dark shaded region). At higher T and higher $|p|$, the unusual normal state emerges in which there is a finite excitation (pseudo)gap. At still higher T, (above T^*) the system is expected to be in a more conventional Fermi gas state.

Note that at low T and relatively high $|p|$, the Sarma superfluid phase (in the light shaded region) is found to be unstable to phase separated states. There is a clear asymmetry in the phase diagram so that for $p>0$ both the pseudogap phase and the superfluid phases occupy a relatively smaller region of phase space. One might be concerned that upon a vertical (temperature) sweep at fixed $p>0$ superconductivity appears to be re-entrant. That is, the pseudogap phase exists at both low and high Ts. This is presumably an artifact of the fact that we have not included phase separated states; indeed, similar behavior was seen for the equal mass case as well [21].

In a strict mean-field calculation [9] the pseudogap state would be indistinguishable from the superfluid phase. It is clear, then, that pair fluctuation effects are extremely important for they greatly reduce the regime of superfluidity. In a similar vein, one can see in both panels of Fig. 3 that while mean-field theory predicts large values of the upper critical polarization p_c (beyond which the superfluid phase cannot exist), our calculations reveal a much smaller range for superfluidity. In the equal mass homogeneous case, where there is an opportunity to compare with experiments [10], both p_c and T_c were found [20] to be in reasonable agreement with the data [10].

Another notable feature of the figure is that when the heavier species is the majority, a stable homogeneously polarized superfluid only exists in a very narrow regime of extremely low polarization. This should serve as an important guide to future experiments for it suggests one has to be very careful in order not to miss the (homogeneously) polarized superfluid in this case. It might seem as though the transition temperatures are much higher in the case of unequal masses than in the equal mass case. We stress that it is more meaningful to compare quantities such as T_c/T^* than T_c/T_F because, unlike in the equal mass case, here the energy unit T_F does not correspond to the Fermi energy of either species of the atoms. For the equal-mass case $T_c/T^*\approx 0.5$ while $T_c/T^*\approx 0.3$ for a mixture of ^{6}Li and ^{40}K atoms at $p=0$.

To address how the phase diagram evolves from unitarity to the BEC side of the Feshbach resonance, we present in Fig. 4 the counterpart phase diagrams at $1/k_F a=0.5$ for the

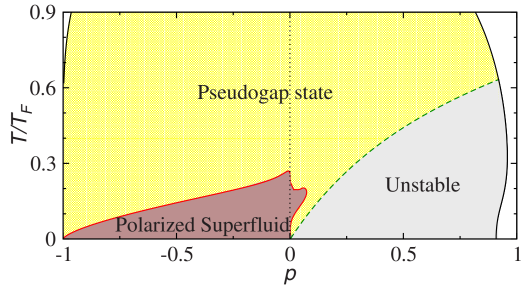

FIG. 4. (Color online) Phase diagrams for mixtures of ^{6}Li and ^{40}K atoms at $1/k_Fa=0.5$. The convention follows that in Fig. 3.

interspecies superfluid. It should be clear from the figure that, just as in the previous case, pair fluctuation effects that allow us [via Eq. (1)] to distinguish between the gap Δ and the order parameter Δ_{sc} are extremely important as they greatly reduce the regime of stable homogeneous superfluidity.

When the heavier species is the majority ($p>0$), there is virtually no stable polarized superfluid. While a vertical (temperature) sweep at constant $p>0$ would seem to suggest a (re-entrant) low T pseudogap phase, this is an artifact of our neglect of phase separation effects. When $p<0$, there is no longer an intermediate temperature superfluid phase. Rather a stable superfluid can be found for all polarizations and temperatures below the (single) critical temperature T_c. This behavior can be contrasted with the equal mass case where, for, e.g., $p=0.5$ at $T=0$, a stable superfluid cannot be found until deep in the BEC regime (when $1/k_Fa>2$). Importantly, for a moderate polarization, say $p=-0.5$, this transition temperature $T_c \approx 0.18T_F$, which should be accessible in future.

We end by noting that, although we have considered a homogeneous rather than trapped situation, there are now experimental capabilities for addressing the associated phase diagrams using tomography [23]. Moreover, our earlier work [20] characterizing the changes in the phase diagram (for the equal mass case) upon going from the homogeneous to the trapped situation can be used to argue that the characteristic values of T_c are not significantly altered. This comparison [20] also reveals that the homogeneously polarized or Sarma phase considered here has a greatly expanded range of stability in the presence of a trap.

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[1] M. W. Zwierlein, A. Schirotzek, C. H. Schunck, and W. Ketterle, Science **311**, 492 (2006).
[2] Y. I. Shin, M. W. Zwierlein, C. H. Schunck, A. Schirotzek, and W. Ketterle, Phys. Rev. Lett. **97**, 030401 (2006).
[3] G. B. Partridge, W. Li, R. I. Kamar, Y. A. Liao, and R. G. Hulet, Science **311**, 503 (2006).
[4] G. B. Partridge, W. Li, Y. A. Liao, R. G. Hulet, M. Haque, and H. T. C. Stoof, Phys. Rev. Lett. **97**, 190407 (2006).
[5] C. H. Schunck, Y. I. Shin, A. Schirotzek, M. W. Zwierlein, and W. Ketterle, Science **316**, 867 (2007).
[6] D. E. Sheehy and L. Radzihovsky, Phys. Rev. Lett. **96**, 060401 (2006).
[7] E. Wille *et al.*, Phys. Rev. Lett. **100**, 053201 (2008).
[8] M. Iskin and C. A. R. Sa de Melo, Phys. Rev. Lett. **97**, 100404 (2006); Phys. Rev. A **76**, 013601 (2007); **77**, 013625 (2008).
[9] M. M. Parish, F. M. Marchetti, A. Lamacraft, and B. D. Simons, Phys. Rev. Lett. **98**, 160402 (2007).
[10] Y. I. Shin, C. H. Schunck, A. Schirotzek, and W. Ketterle, Nature (London) **451**, 689 (2008).
[11] P. F. Bedaque, H. Caldas, and G. Rupak, Phys. Rev. Lett. **91**, 247002 (2003); H. Caldas, Phys. Rev. A **69**, 063602 (2004).
[12] S. Pilati and S. Giorgini, Phys. Rev. Lett. **100**, 030401 (2008).
[13] T. K. Koponen, T. Paananen, J.-P. Martikainen, M. R. Bakhtiari, and P. Törmä, New J. Phys. **10**, 045014 (2008); G. G. Batrouni, M. J. Wolak, F. Hebert, and V. G. Rousseau, EPL **86**, 47006 (2009).
[14] M. Casula, D. M. Ceperley, and E. J. Mueller, Phys. Rev. A **78**, 033607 (2008); M. Tezuka and M. Ueda, Phys. Rev. Lett. **100**, 110403 (2008).
[15] Y. He, C.-C. Chien, Q. J. Chen, and K. Levin, Phys. Rev. A **75**, 021602(R) (2007).
[16] S. T. Wu, C. H. Pao, and S. K. Yip, Phys. Rev. B **74**, 224504 (2006); C. H. Pao, S. T. Wu, and S. K. Yip, Phys. Rev. A **76**, 053621 (2007).
[17] W. Yi and L. M. Duan, Phys. Rev. A **73**, 031604(R) (2006).
[18] A. Gezerlis, S. Gandolfi, K. E. Schmidt, and J. Carlson, e-print arXiv:0901.3148.
[19] Q. J. Chen, J. Stajic, S. N. Tan, and K. Levin, Phys. Rep. **412**, 1 (2005).
[20] Q. J. Chen, Y. He, C. C. Chien, and K. Levin, e-print arXiv:0810.1940.
[21] C. C. Chien, Q. J. Chen, Y. He, and K. Levin, Phys. Rev. Lett. **97**, 090402 (2006); Q. J. Chen, Y. He, C. C. Chien, and K. Levin, Phys. Rev. A **74**, 063603 (2006).
[22] In contrast to previous work we take higher terms ($a_1\Omega^2$) in the T-matrix expansion to avoid numerical complications from vanishing a_0.
[23] A. Schirotzek, Y. I. Shin, C. H. Schunck, and W. Ketterle, Phys. Rev. Lett. **101**, 140403 (2008).