Phase diagram and binding energy of interacting Bose gases

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(Received 16 April 2008; revised manuscript received 11 June 2008; published 12 August 2008)

From the many-body T matrix, the condition for a medium-dependent bound state and its binding energy is derived for a homogeneous interacting Bose gas. This condition provides the critical line in the phase diagram in terms of the medium-dependent scattering length. Separating the Bose pole from the distribution function, the influence of a Bose condensate is discussed and a thermal minimum of the critical scattering length is found.

DOI: 10.1103/PhysRevB.78.054508 PACS number(s): 05.30.Jp, 03.75.Hh, 64.60.F−

I. INTRODUCTION

The discovery of Feshbach resonances in gases of ultracold bosons in 1998 (Refs. 1–3) has provided an important tool to analyze interacting Bose systems. Near these resonances, it is possible to tune the interaction and especially the free scattering length a_0 with an external magnetic field B. In the vicinity of the resonance at $B=B_0$, the scattering length is[4]

$$a_0 = a_{\rm nr}\left(1+\frac{\Delta B}{B-B_0}\right), \tag{1}$$

as shown in Fig. 1. Here $a_{\rm nr}$ is the scattering length far away from the resonance and $\Delta B \propto 1/a_{\rm nr}$ describes the width of the resonance. A Fermi gas near a Feshbach resonance can be driven through a transition from a Bose-Einstein condensate (BEC) of two-particle bound states for $a_0>0$ to a BCS state of Cooper pairs for $a_0<0$ (Ref. 5). For bosons, the influence of the interaction on the Bose condensation is of main interest. Interacting Bose gases at ultralow temperatures are expected to consist of unbound, bound, and condensed bosons. Furthermore, one expects an influence of the interaction on the critical temperature and density of Bose condensation (see citations in Ref. 6). Here we focus on the formation of bound states in the presence or absence of a Bose condensate. We will derive the condition for bound states in terms of the medium-dependent scattering length to discuss the phase diagram and the binding energy.

II. THE MEDIUM-DEPENDENT T MATRIX

The two-particle scattering is described with the many-body T matrix in the ladder and quasiparticle approximation,[6]

$$\mathcal{T}_{p\bar{p}}(Q,\omega) = V_{p\bar{p}} + \int \frac{d^3q}{(2\pi)^3}\mathcal{T}_{pq}(Q,\omega)\frac{1+f_{Q/2-q}+f_{Q/2+q}}{\omega-\frac{\hbar^2Q^2}{4m}-\frac{\hbar^2q^2}{m}+i\eta}V_{q\bar{p}}. \tag{2}$$

The influence of the surrounding particles is represented by the distribution function f_p. The total momentum Q reflects the center-of-mass motion of the scattering particles relative to the medium, while q is their relative momentum. The medium is assumed to be a homogeneous ideal Bose gas with a distribution[7]

$$f_p = \frac{1}{e^{(\hbar^2p^2/2m-\mu)/T}-1} + \frac{(2\pi)^3 n_0}{2F+1}\delta(p), \tag{3}$$

and a density

$$n = (2F+1)\int \frac{d^3p}{(2\pi)^3}\frac{1}{e^{(\hbar^2p^2/2m-\mu)/T}-1} + n_0, \tag{4}$$

where n_0 is the condensate density and F is the total spin. Since we assume that the interaction does not change the spin, there are no degradation factors in the T-matrix (2). In the normal state, $n_0=0$ and Eq. (4) yields the chemical potential μ as a function of the temperature and density. In the superfluid state, $\mu=0$ and Eq. (4) determines the condensate density n_0. At the critical point, $\mu=0$ and $n_0=0$ and from Eq. (4), the critical temperature T_c and the critical density n_c follow. The dependence of the critical properties on the interaction will be neglected.

III. THE BOUND STATE FOR CONTACT INTERACTION

At low temperatures, only s-wave scattering at small momenta is important. Furthermore, we want to concentrate on bound states near the continuum edge. Therefore, and for the

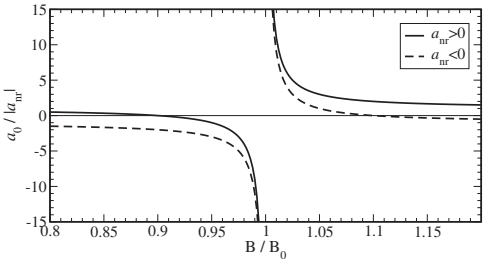

FIG. 1. Scattering length in the vicinity of a Feshbach resonance.

sake of simplicity, we neglect the range of the interaction and assume the interaction to be a contact interaction for which the potential is independent of the relative momenta $V_{pq}=V$. Accordingly, the T matrix is also independent of the relative momenta $\mathcal{T}_{pq}(Q,\omega)=\mathcal{T}(Q,\omega)$ and Eq. (2) simplifies to the algebraic relation $\mathcal{T}=V/(1-GV)$ with the two-particle propagator,

$$G(Q,\omega)=\int \frac{d^3q}{(2\pi)^3}\frac{1+f_{Q/2-q}+f_{Q/2+q}}{\omega-\frac{\hbar^2Q^2}{4m}-\frac{\hbar^2q^2}{m}+i\eta}. \tag{5}$$

Obviously we can split G into the free propagator G_0 resulting in the $f\to 0$ limit and the medium correction $G_m\propto f$. The free propagator diverges and a cutoff is necessary. To circumvent this cutoff, we introduce the vacuum T matrix $\mathcal{T}_0=V/(1-G_0V)$, which determines the free scattering length,

$$a_0=\frac{m}{4\pi\hbar^2}\mathcal{T}_0\left(Q,\frac{\hbar^2Q^2}{4m}\right). \tag{6}$$

The strength of the interaction is now described by the free scattering length, which is interpreted as the relevant physical quantity tunable near the Feshbach resonance.

Solving Eq. (6) yields,

$$a_0=\frac{m}{4\pi\hbar^2}\lim_{q_0\to\infty}\frac{V}{1+\frac{m}{2\pi^2\hbar^2}V\int_0^{q_0}dq}. \tag{7}$$

The inverse of the cutoff q_0 is proportional to the range of the interaction, i.e., contact interaction means $q_0\to\infty$. Postulating a finite a_0, it is necessary to renormalize the interaction strength,[6,8–10] such that

$$V=\lim_{q_0\to\infty}\left(-\frac{2\pi^2\hbar^2}{mq_0}\frac{1}{1-\frac{\pi}{2a_0q_0}}\right), \tag{8}$$

which follows from Eq. (7). Frequently, the pseudopotential[4,11]

$$\bar{V}=\frac{4\pi\hbar^2a_0}{m} \tag{9}$$

is used to describe the dependence of the interaction strength on the scattering length for contact interaction.[12,13] The difference of Eq. (9) to Eq. (8) is that the leading term of Eq. (8) with respect to a large cutoff q_0 is always negative and independent of a_0, i.e., the contact interaction is always attractive, while the pseudopotential is attractive for $a_0<0$ and repulsive for $a_0>0$. The reason for this difference is that the pseudopotential is only valid up to first-order Born approximation.[11] Within this approximation, one neglects G, i.e., $\mathcal{T}=V$, such that the diverging terms in the denominators of Eqs. (7) and (8) vanish.

The in-medium T matrix can be expressed by the free one $\mathcal{T}=\mathcal{T}_0/(1-G_m\mathcal{T}_0)$. Accordingly, the in-medium scattering length is

$$a=\frac{m}{4\pi\hbar^2}\mathcal{T}\left(Q,\frac{\hbar^2Q^2}{4m}\right)=\frac{a_0}{1-\frac{4\pi\hbar^2a_0}{m}G_m\left(Q,\frac{\hbar^2Q^2}{4m}\right)}=\frac{a_0}{1+\frac{a_0}{a_c}}, \tag{10}$$

with $a_c\geq 0$. We use here the definition of the many-body scattering length from Ref. 14 instead of the definition used in Refs. 6 and 8. Instead of a divergence, the many-body scattering length for $Q=0$ therefore has a zero at the critical point of Bose condensation, i.e., $a_c=0$. Splitting Eq. (5) in another way,

$$G(Q,\omega)=G\left(Q,\frac{\hbar^2Q^2}{4m}\right)+\frac{m}{4\pi\hbar^2}J(Q,\omega), \tag{11}$$

with

$$J\left(Q,\omega+\frac{\hbar^2Q^2}{4m}\right)=\int\frac{d^3q}{(2\pi)^3}\frac{4\pi\omega}{q^2}\frac{1+f_{Q/2-q}+f_{Q/2+q}}{\omega-\frac{\hbar^2q^2}{m}+i\eta}, \tag{12}$$

one obtains for the in-medium T matrix,

$$\mathcal{T}(Q,\omega)=\frac{4\pi\hbar^2a}{m}\frac{1}{1-aJ(Q,\omega)}. \tag{13}$$

A bound state, i.e., a pole of the T matrix, is therefore possible if

$$0<J\left(Q,\omega_B+\frac{\hbar^2Q^2}{4m}\right)=\frac{1}{a}, \tag{14}$$

where the corresponding binding energy $\omega_B<0$ is measured relative to the continuum edge, i.e., $\hbar^2Q^2/4m$. The binding energy is shown in Fig. 2. The fixed parameters in the plots define the corresponding length scale s, i.e., $Q=p_s=1/s$, $T=\varepsilon_s=\hbar^2/2\ ms^2$, or $n=0.05\ s^{-3}$, respectively. According to Eq. (10), the condition for the bound state $a>0$ is satisfied in two situations. In the first case $a_0>0$, the interaction is strong enough to form the bound state already in the vacuum. In the second case $a_0<-a_c$, the bound state is induced by the medium. For $-a_c<a_0<0$, the interaction is attractive but insufficient to form a bound state. For bosons near a Feshbach resonance, this means that in addition to the bound state in the $a_0>0$ region, a bound state is also possible on the other side of the resonance for $a_0<-a_c$. The appearance of the medium-induced bound state is also signaled by the divergence of the medium-dependent scattering length [Eq. (10)] at $a_0=-a_c$ (Ref. 15). From these three cases, the dependence of the bound-state region on the density, temperature, total momentum, scattering length, and spin follows as shown in Fig. 3.

IV. DISCUSSION OF THE PHASE DIAGRAM AND THE BINDING ENERGY

For large $|a_0|$, the binding energy converges toward a finite value ω_c as seen in Fig. 2(e), which follows from $J(Q,\omega_c+\hbar^2Q^2/4m)=1/a_c$. This convergence can be explained by the convergence of the medium-dependent scattering length [Eq. (10)] and also by the convergence of the

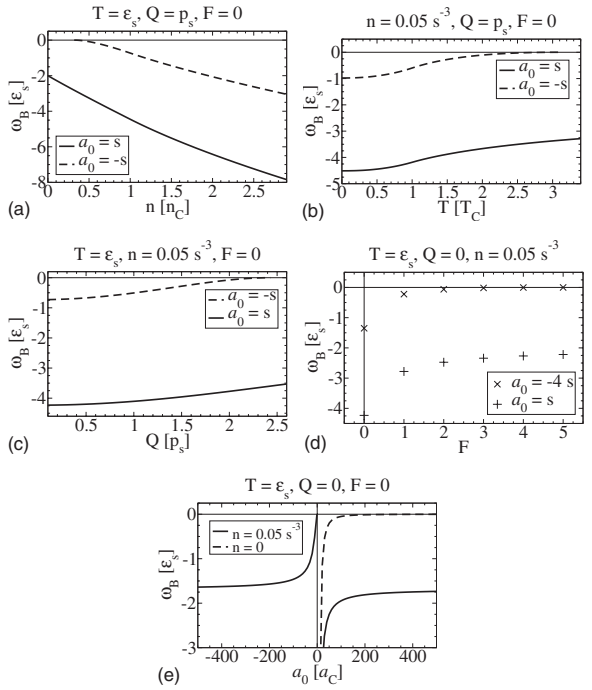

FIG. 2. Binding energy for the bound state of a homogeneous Bose gas with contact interaction. Fixed parameters are given above the plots. $n_c=0.06\ s^{-3}$, $T_c=0.90\ \varepsilon_s$, and $a_c=0.06\ s$.

interaction strength [Eq. (8)] for large $|a_0|$. The interaction strength [Eq. (8)] also shows that the interaction is stronger for positive a_0 and, therefore, $|\omega_B|$ is larger in this case. The region where a bound state is possible spreads with increasing density, as can be seen in Fig. 3(a). Figure 2(a) shows that for increasing density, $|\omega_B|$ increases too. This behavior can be explained by the increasing influence of many-body effects with increasing density. Due to the Bose enhancement, the formation of bound states is supported. On the other hand, thermal fluctuations hinder the formation of bound states, which is shown by the shrinkage of the bound-

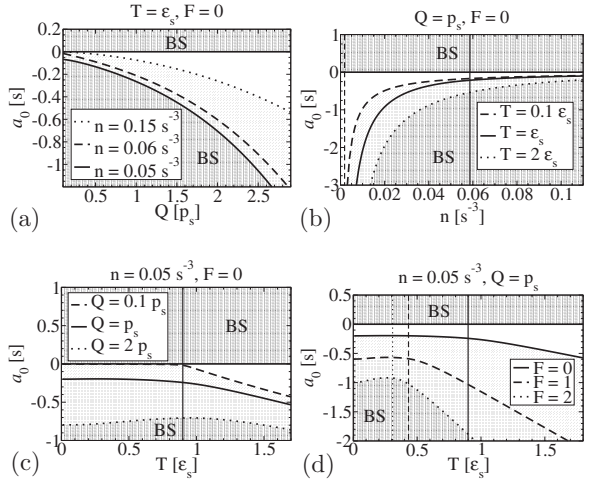

FIG. 3. Phase diagram for the appearance of the bound state (BS) of a homogeneous Bose gas with contact interaction. The vertical lines mark the onset of Bose condensation for the corresponding parameters.

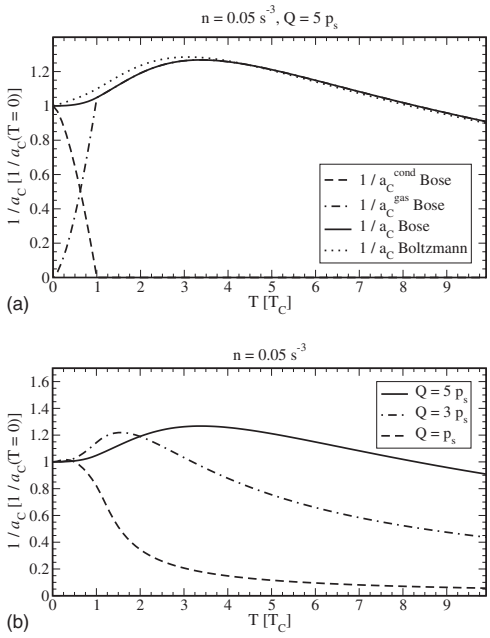

FIG. 4. Inverse critical scattering length versus temperature for different approximations (upper plot) and for different total momenta for a Bose gas with condensate (lower plot).

state region in Fig. 3(b) and the decrease in $|\omega_B|$ in Fig. 2(b) with increasing temperature. The motion of the scattered particles relative to the medium has a similar effect as Figs. 2(c) and 3(c) show. In the limit of vanishing density, the bound-state condition is $a_0>0$ and the binding energy is $\omega_{B0}=-\hbar^2/ma_0^2$. This simple result can only be explained by the potential (8). If one would follow the philosophy of pseudopotentials instead, one would have repulsion for $a_0>0$ and no bound states. In Figs. 2(d) and 3(d), one sees that with increasing total spin, $|\omega_B|$ decreases and the bound-state region shrinks. The reason is that with increasing total spin, the density of states also increases and, therefore, the occupation of states for a given density decreases. The effect is therefore similar to that of a decrease in density.

A remarkable feature in Figs. 3(c) and 3(d) is that a maximum of the critical line appears at some temperature T_{ex}. This means that in these cases, the region of bound states becomes smaller if the temperature is decreased further, which is in contrast to the behavior above T_{ex}. To understand this effect, we observe from Eqs. (3) and (10) that in the superfluid state, $1/a_c$ can be split into two parts $1/a_c=1/a_c^{\mathrm{cond}}+1/a_c^{\mathrm{gas}}$. The first part $1/a_c^{\mathrm{cond}}\propto n_0/Q^2$ bears the contribution from the condensate. The second part $1/a_c^{\mathrm{gas}}\propto f$ represents the uncondensed Bose gas vanishing as the temperature approaches zero. While a_c^{gas} diverges at $T=0$ and a_c^{cond} diverges at $T=T_c$, the scattering length a_c remains finite as Figs. 3(c) and 3(d) show. If the momentum Q is large enough, the extremum appears already above the critical temperature as seen in Fig. 4. The condensate part vanishes at T_c and the gas part is the only contribution above. For a large total momentum, the Bose distribution is well approximated by the Boltzmann distribution. This allows us to calculate G_m explicitly, which yields that the extremum appears at $T_{\mathrm{ex}}\approx 0.22\hbar^2Q^2/4m$. In other words, we have a

TABLE I. Binding energies for different species. The singlet (s) and triplet (t) scattering lengths a_0 are from Ref. 4, if not marked differently. The length scale s is chosen so that $T=\varepsilon_s=0.5\ \mu\mathrm{K}\ k_B\approx 43$ peV. The binding energy ω_B, as follows from Eq. (14) for $Q=0$ and $n=0.85n_c$, is compared to its vacuum value $\omega_{B0}=-\hbar^2/ma_0^2$ and $a_c\approx 64\times 10^{-3}$ s. The total spin F is that of the hyperfine state with lowest energy.

	s (nm)	F	n (cm^{-3})		a_0 (10^{-3} s)	ω_B (neV)	ω_{B0} (neV)
^{7}Li	263	1	8.2×10^{12}	t	-5.55 ± 0.11	No bound state	
^{85}Rb	76	2	5.8×10^{14}	t	-258 ± 12	$-(52\pm 5)\times 10^{-4}$	No bound state
^{133}Cs	60	3	1.6×10^{15}	t	2100 ± 90	$-(112.2\pm 2.2)\times 10^{-3}$	$-(19.6\pm 1.7)\times 10^{-3}$
^{85}Rb	76	2	5.8×10^{14}	s	1700 ± 500	-0.133 ± 0.023	-0.039 ± 0.022
^{133}Cs	60	3	1.6×10^{15}	s	245 ± 9	-1.49 ± 0.11	-1.44 ± 0.11
^{87}Rb	75	1	3.6×10^{14}	t	75.1 ± 2.9	-15.4 ± 1.2	-15.3 ± 1.2
				s	63.8 ± 0.8	-21.2 ± 0.6	-21.2 ± 0.6
^{4}He	348	0	1.2×10^{12}	s	30 ± 6 (Ref. 16)	-110 ± 50	
^{23}Na	145	1	4.9×10^{13}	t	23.8 ± 0.4	-152 ± 6	
				s	7.0 ± 0.8	-1800 ± 500	
^{7}Li	263	1	8.2×10^{12}	s	6.6 ± 0.5	-2000 ± 400	
^{1}H	696	0	1.5×10^{11}	t	9.1×10^{-2}	-1.04×10^7	
				s	3.1×10^{-2}	-8.97×10^7	

mere thermal effect. When the mean motion characterized by the total momentum comes in resonance with the thermal motion, we observe an extremum in the critical scattering length.

The ladder and quasiparticle approximation proposed in this paper cannot describe the dynamic formation or breaking of bound states. This is due to the fact that for the formation or destruction of a bound state, an exchange of energy and momentum, either with a third particle or with the medium, has to be allowed. Therefore, either more diagrams or a self-consistent spectral function would have to be included in the T matrix. This is the reason why the pole of Eq. (13) lies on the real axis, i.e., has no imaginary part and, therefore, the bound state has an infinite lifetime. On the other hand, Figs. 2(a), 2(b), and 2(e) show that in the normal state, $|\omega_B|$ is of the order of the thermal energy for $a_0<-a_c$ and for $a_0\gg a_c$, i.e., near the resonance. This makes the bound states very unstable toward collisions with medium particles and, therefore, limits their lifetime. However, experimental experience shows that bound-state and cluster formation has even to be suppressed by decreasing the density to be able to directly investigate Bose condensation.[17] If Bose condensation shall be reached by decreasing the temperature, then bound states are always possible before T_c is reached for any interaction, as Fig. 3(c) shows. The only exception is the ideal-gas case, i.e., $a_0=0$.

The binding energies at typical conditions for some elements used for Bose-condensation experiments are compiled in Table I. These data show that the scattering length can be positive and its absolute value can be of the magnitude or even less than a_c. In these cases, the binding energy is more than two orders of magnitude higher than the thermal energy, i.e., the bound state is stable, although $|\omega_B|$ is too small compared with experimental values of bound states near the continuum edge. For example, the energy of the last vibrational state below the continuum edge for sodium is (-13100 ± 900)neV (Ref. 18). The reason for that difference is that the contact interaction is a low energy approximation. One would expect an increase in the binding energy for an increasing potential range. Table I shows further that for stable bound states, i.e., $|\omega_B|\gg T$, the influence of the medium on the binding energy is negligible. On the other hand, since a finite-range potential would stabilize the bound states, a medium influence on them may be measurable.

V. SUMMARY

To summarize, it was shown that the contact interaction always produces attractive forces if one postulates a finite scattering length. A bound state appears as soon as the interaction is strong enough. Due to the Bose enhancement, many-body effects support the formation of bound states, while thermal fluctuations and the motion relative to the medium hinder this formation. The model describes the experimental experience that bound states and cluster formation appear before the Bose condensation. The calculations show

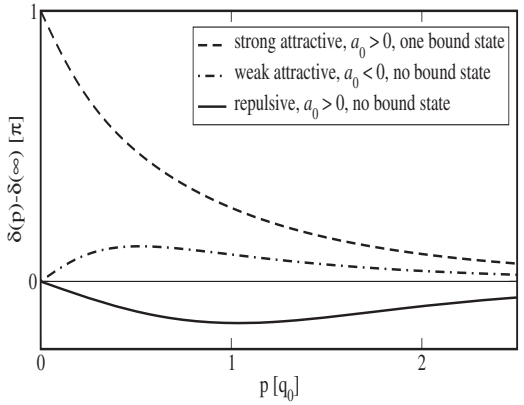

FIG. 5. Scattering phase versus momentum for a finite-range two-particle interaction with one possible bound state.

that for bosons at finite density, bound states are possible on both sides of a Feshbach resonance but they are quite unstable near the resonance too. To find better agreement with the experiment and to make predictions for future experiments, the model has to be improved to describe an interaction with finite range and bound states with finite lifetime. Our T-matrix approximation shows that in contrast to the pseudopotential ansatz, the scattering length is not necessarily proportional to the interaction strength and that whether the interaction is attractive or repulsive does not follow inevitably from the sign of the scattering length. Whether an interaction is repulsive or attractive can be found from the sign of the scattering phase, the slope of which for small momenta is related to the scattering length, as shown in Fig. 5. The contact interaction can only describe the strong and weak attractive cases, while the pseudopotential can only describe the weak attractive and repulsive cases. Therefore, the sign of the scattering length alone is not decisive whether the interaction is attractive or repulsive. Otherwise, one would have to face the paradoxical situation that bound states also appear for a repulsive interaction. Though the contact interaction can describe the BEC-BCS transition,[19] it seems that one has to include inevitably the effect of a finite potential range in order to be able to describe bound states, pairing, and BEC correctly at the same time.

ACKNOWLEDGMENTS

The discussions with R. Zimmermann are gratefully acknowledged. This work was supported by the German DAAD and Czech Research Plan under Contract No. MSM 0021620834, by DFG Priority Program 1157 via Contract No. GE1202/06, by the BMBF, and by European ESF program NES.

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