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Cold Bose gases near Feshbach resonances

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Abstract

The lowest order constrained variational method [Phys. Rev. Lett. 88 (2002) 210403] has been generalized for a dilute (in the sense that the range of interatomic potential, R, is small compared with inter-particle spacing r_0) uniform gas of bosons near the Feshbach resonance using the multi-channel zero-range potential model. The method has been applied to $Na(F = 1, m_F = 1)$ atoms near the $B_0 = 907$ G Feshbach resonance. It is shown that at high densities $na^3 \gg 1$, there are significant differences between our results for the real part of energy per particle and the one-channel zero-range potential approximation. We point out the possibility of stabilization of the uniform condensate for the case of negative scattering length.

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1. Introduction

The newly created Bose–Einstein condensates (BEC) of weakly interacting alkali-metal atoms [1] stimulated a large number of theoretical investigations (see recent reviews [2]). Most of these works are based on the assumption that the properties of BEC are well described by the Gross–Pitaevskii (GP) mean-field theory [3].

Recently, it has become possible to tune atomic scattering length to essentially any value, by exploiting Feshbach resonances (FR) [4,5]. A fundamental open problem is how to describe the physics of dilute BEC near FR (dilute in the sense that the range of interatomic potential, R, is small compared with inter-particle spacing r_0) in the regime of a large scattering length, a, which we take to be positive. The GP approach fails in the regime of a large gas parameter, $n|a|^3$, where n is the particle density.

The dilute BEC for a large gas parameter regime in one-channel approximation has been considered previously in Ref. [6] (for the corresponding problem for a Fermi gas see Ref. [7]).

In this Letter we consider the ground state properties of the dilute homogeneous Bose gas near the FR using a multi-channel zero-range potential (ZRP) model of FR.

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In Section 2 we describe the lowest order constrained variational (LOCV) method [6,8] for the one-channel N-body problem. The calculations for model interaction potentials used by Ref. [9] are presented. The description of the multi-channel ZRP model is given in Section 3. Section 4 develops the LOCV method for the dilute Bose gas near FR. We conclude the Letter in Section 5 with a brief summary.

2. Lowest order constrained variational method

In a dilute many-body problem in the large gas parameter regime correlations between particles are very important.

The LOCV method [6,8] for the homogeneous N-body system is to assume a Jastrow many-body wave function, of the form

$$\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \prod_{i<j} f(\vec{r}_i - \vec{r}_j), \tag{1}$$

where at short distances, f is solution of the two-particle Schrödinger equation

$$\left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} + V(r)\right) rf(r) = \lambda r f(r), \tag{2}$$

while at large distances f must approach a constant.

In the LOCV method [6,8] the boundary conditions for $f(r)$ are

$$f(d) = 1, \qquad f'(d) = 0, \tag{3}$$

the expectation value of the energy is given by

$$E/N = 2\pi n\lambda \int_0^d f^2(r) r^2\, dr, \tag{4}$$

and d is defined by the normalization

$$4\pi n \int_0^d f^2(r) r^2\, dr = 1. \tag{5}$$

In Ref. [6] for the dilute case ($R \ll r_0$, where the inter-particle spacing $r_0 = (3/(4\pi n))^{1/3}$) inter-atomic interaction was replaced by the zero-range potential (ZRP) model [9]

$$\left.\frac{(rf)'}{rf}\right|_{r=0} = -\frac{1}{a}. \tag{6}$$

In this case

$$f(r < d) = \frac{d}{r}\frac{\sin(kr + \delta)}{\sin(kd + \delta)}, \tag{7}$$

with $k\cot\delta = -1/a$, $kd\cot(kd + \delta) = 1$, where $k = \sqrt{m\lambda/\hbar^2}$.

In the small a/r_0 limit, $\delta = -ka$, $d = r_0$ and the LOCV result for E/N [6] is given by

$$\frac{E}{N} = 2\pi\frac{\hbar^2 a}{m} n \tag{8}$$

and is same as that first found by Lenz [10].

The ground state energy per particle, E/N, in the low-density regime, $na^3 \ll 1$, can be calculated using an expansion in power of $\sqrt{na^3}$

$$\frac{E}{N} = \frac{2\pi\hbar^2}{m}an\left[1 + \frac{128}{15\sqrt{\pi}}\left(na^3\right)^{1/2} + 8\left(\frac{4\pi}{3} - \sqrt{3}\right)na^3\left[\ln\left(na^3\right) + C\right] + \cdots\right]. \tag{9}$$

The coefficient of the $(na^3)^{3/2}$ term (the second term) was first calculated by Lee, Huang, and Yang [11], while the coefficient of the last term was first obtained by Wu [12]. The constant C after the logarithm was considered in Ref. [13].

The expansion (9) is asymptotic, and it was shown in Ref. [14] that the Lee–Huang–Yang (LHY) correction (second term in Eq. (9)) represents a significant improvement on the mean field prediction (the first term in Eq. (9)).

In Refs. [15–19] the Lenz–Lee–Huang–Yang (LLHY) expansion (first two terms in expansion (9)) has been used to study effects beyond the mean field approximation. In Ref. [18], it was found that the correction to the GP results may be as large as 30% in the ground state properties of the condensate, when the conditions of the JILA experiment for ^{85}Rb are considered [5].

In the large a/r_0 limit, $\delta = \pi/2$, $kd\tan(kd) = -1$, and the energy is given by [6]

$$\frac{E}{N} = 13.33\hbar^2\frac{n^{2/3}}{m} = 10.2597\frac{\hbar^2}{2mr_0^2}, \tag{10}$$

which is very close to the Legett's unpublished variational result

$$\frac{E}{N} = \frac{3\pi^2}{2}\frac{\hbar^2 n^{2/3}}{m} \tag{11}$$

(this was quoted by Baym [20]).

To study the validity of the ZRP model we consider an example of the square-well (SW) potential with $a/r_0 \to \infty$. The calculated energies per particle, E/N, are presented in Table 1. The ratio R/r_0 is typically of the order of 10^{-2}. From Table 1, we can see that even for $a/r_0 \to \infty$ the ZRP model is a very good approximation (the difference for E/N between the ZPR and the SW is less than 1% if $R/r_0 \approx 10^{-2}$). In this case the LOCV results for E/N have universal properties that depend on the interatomic potential only through the single low-energy parameter a, even for large gas-parameter regime.

We note that for an attractive potential the atomic BEC is metastable and energy per particle can be written as $E/N - i\Gamma/2$. Therefore, the real part of energy in LOCV method would be reliable if $E/N > \Gamma/2$ [6].

In Ref. [14], the authors have used a diffusion Monte Carlo method to calculate the lowest-energy state of uniform gas of bosons interacting through four different model potentials that have all the same scattering length a.

(i) The hard-sphere potential

$$V^{(\mathrm{HS})}(r) = \begin{cases} \infty & (r < a), \\ 0 & (r > a), \end{cases} \tag{12}$$

where the diameter of the hard-sphere is equal to the scattering length.

Table 1
Energy per particle, E/N, in units of $\hbar^2/(2mr_0^2)$ vs. R/r_0 for the square-well attractive potential with $a = \infty$. The ZRP model for this case gives $E/N = 10.2597\hbar^2/(2mr_0^2)$ [6]

R/r_0	E/N
10^{-1}	11.1906
5×10^{-2}	10.7143
10^{-2}	10.3502
5×10^{-3}	10.3057
10^{-3}	10.2703

Table 2
Energy per particle, E/N, in units of $2\pi\hbar^2 na/m$, as a function of R/r_0 for soft-sphere potentials. R is the range of potential and $r_0 = (3/(4\pi n))^{1/3}$ is the atomic separation

R/r_0	E/N	E/N [14]	R
0.081	1.01961	1.00427	$5a$
0.161	1.01951	1.00427	$10a$
0.174	1.04292	1.01382	$5a$
0.347	1.04288	1.01302	$10a$
0.374	1.09599	1.04167	$5a$
0.748	1.0973	1.03689	$10a$
0.806	1.23315	1.11011	$5a$

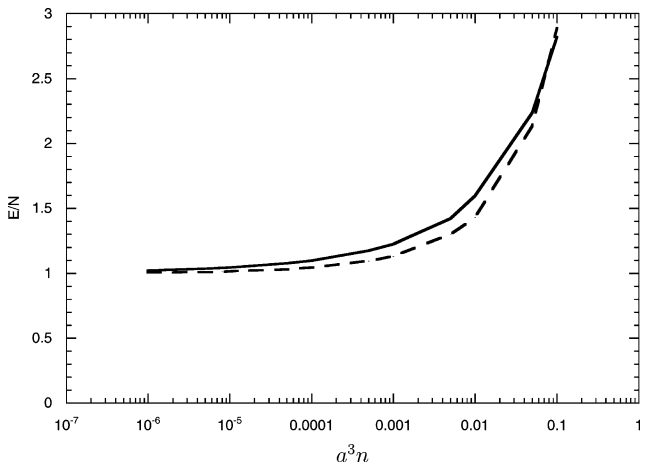

Fig. 1. Ground-state energy per particles, E/N, in units of $2\pi\hbar^2 na/m$, vs. a^3n for hard-sphere interactions. The LOCV results are shown by full line. The diffusion Monte Carlo calculations [14] are shown as dashed line.

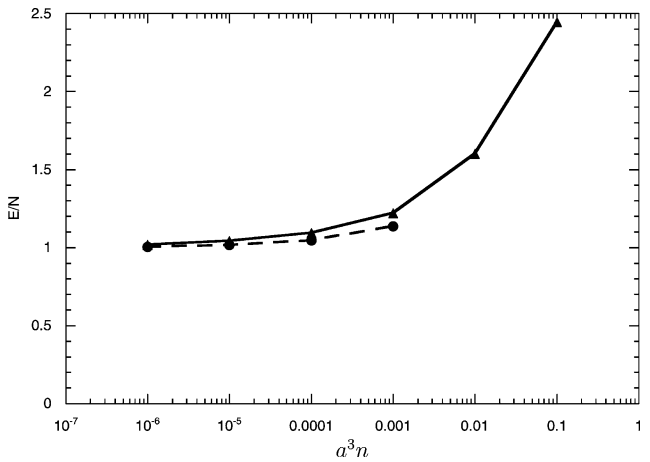

Fig. 2. Ground-state energy per particles, E/N, in units of $2\pi\hbar^2 na/m$, vs. a^3n for hard-core square-well potential (HCSW). Triangles and circles correspond to the LOCV and the diffusion Monte Carlo [14] results, respectively. Lines are drawn to guide the eyes.

(ii) Two soft-sphere (SS) potentials

$$V^{(\mathrm{SS})}(r) = \begin{cases} V_0 & (r < R_0), \\ 0 & (r > R_0), \end{cases} \tag{13}$$

with $R_0 = 5a$, $V_0 = 0.031543\hbar^2/(ma^2)$ and $R_0 = 10a$, $V_0 = 0.003408\hbar^2/(ma^2)$.

(iii) The hard-core square-well (HCSW) potential

$$V^{(\mathrm{HCSW})}(r) = \begin{cases} +\infty & (r < R_c), \\ -V_0 & (R_c < r < R_0), \\ 0 & (r > R_0). \end{cases} \tag{14}$$

The parameters of the HCSW potential are $R_c = a/50$, $R_0 = a/10$ and $V_0 = 412.815\hbar^2/(ma^2)$. The HCSW potential has a two-body bound state with energy $-1.13249\hbar^2/(ma^2)$ [21].

Comparison the LOCV results for potentials (12)–(14) with the available diffusion Monte Carlo (DMC) calculations (Table 2, Figs. 1 and 2) shows that the LOCV energies in the case of $R/r_0 \approx 10^{-2}$ are in very good agreement with the DMC results.

3. Zero-range potential model of Feshbach resonance

We start from the coupling channel equation

$$\begin{aligned} &\left(-\frac{\hbar^2}{m}\nabla^2 + V^P(r)\right)\psi^P(\vec{r}) + g(r)\psi^Q(\vec{r}) = E\psi^P(\vec{r}), \\ &\left(-\frac{\hbar^2}{m}\nabla^2 + V^Q(r) + \mathcal{E}\right)\psi^Q(\vec{r}) + g^*(r)\psi^P(\vec{r}) = E\psi^Q(\vec{r}), \end{aligned} \tag{15}$$

where $\mathcal{E}$ is the energy shift of the closed channel Q with respect to the collision continuum. Since potentials $V^P(r)$, $V^Q(r)$ and $g(r)$ have a range typically of the order of interatomic potential range or less, we can replace Eq. (15) by

$$\begin{aligned} &\left(-\frac{\hbar^2}{m}\nabla^2 + V_{11}\right)\psi^P(\vec{r}) + V_{12}\psi^Q(\vec{r}) = E\psi^P(\vec{r}), \\ &\left(-\frac{\hbar^2}{m}\nabla^2 + V_{22} + \mathcal{E}\right)\psi^Q(\vec{r}) + V_{21}\psi^P(\vec{r}) = E\psi^Q(\vec{r}), \end{aligned} \tag{16}$$

where

$$V_{ik}(\vec{r}) = -\frac{4\pi\hbar^2}{m}M_{ik}^{-1}\delta(\vec{r})\frac{\partial}{\partial r}r \tag{17}$$

is a multi-channel generalization of the Huang pseudo-potential [22].

Eq. (16) can be rewritten as free equations

$$-\frac{\hbar^2}{m}\nabla^2\psi^P(\vec{r}) = E\psi^P(\vec{r}), \qquad \left(-\frac{\hbar^2}{m}\nabla^2 + \mathcal{E}\right)\psi^Q(\vec{r}) = E\psi^Q(\vec{r}), \tag{18}$$

with boundary conditions

$$\begin{aligned} \left.\frac{d(r\psi^P)}{dr}\right|_{r=0} &= \left(M_{11}r\psi^P + M_{12}r\psi^Q\right)\big|_{r=0}, \\ \left.\frac{d(r\psi^Q)}{dr}\right|_{r=0} &= \left(M_{21}r\psi^P + M_{22}r\psi^Q\right)\big|_{r=0}, \end{aligned} \tag{19}$$

which is a multi-channel ZRP model [23].

It is easy to show that the Hamiltonian of the particle moving in the field of multi-channel ZPR is Hermitian, that is, the condition

$$\int \left[\left(\phi_1^P\right)^* \nabla^2 \phi_2^P + \left(\phi_1^Q\right)^* \nabla^2 \phi_2^Q\right] d^3r = \int \left[\left(\nabla^2 \phi_1^P\right)^* \phi_2^P + \left(\nabla^2 \phi_1^Q\right)^* \phi_2^Q\right] d^3r \tag{20}$$

is valid for any ϕ_1^P, ϕ_1^Q and ϕ_2^P, ϕ_2^Q which satisfy the boundary conditions (19) with energy independent constant Hermitian matrix M.

We shall use the following parameterization for the matrix M

$$M_{11} = -\frac{1}{a_{\mathrm{bg}}}, \qquad M_{12} = M_{21} = -\frac{\beta}{a_{\mathrm{bg}}}, \qquad M_{22} = -\frac{\gamma}{a_{\mathrm{bg}}}, \tag{21}$$

where a_{bg} is the background value of the scattering length. The model (21) with $\gamma = 1$ was considered in [23].

Solutions of Eqs. (18), (19) can be written as

$$\psi^P(\vec{r}) \propto \sin(kr + \delta), \qquad \psi^Q(\vec{r}) \propto e^{-\sqrt{\widetilde{\mathcal{E}} - k^2}\, r}, \tag{22}$$

with $\widetilde{\mathcal{E}} = m\mathcal{E}/\hbar^2$, $k^2 = mE/\hbar^2$.

Since the energy shift $\mathcal{E}$ can be converted into an external magnetic field B by $\mathcal{E} \propto B$, the scattering length a depends on the external magnetic field by the dispersive law [24]

$$a = a_{\mathrm{bg}}\left(1 + \frac{\Delta(B)}{B_0 - B}\right), \tag{23}$$

where

$$\Delta(B) = \frac{(1 - \sqrt{\alpha B_0})(\sqrt{\alpha B} + \sqrt{\alpha B_0})}{\alpha}, \tag{24}$$

$$\alpha = \frac{4B_0}{(2B_0 + \Delta)^2}, \qquad \frac{\beta}{\gamma} = \sqrt{\frac{\Delta}{\Delta + 2B_0}}, \tag{25}$$

and $\Delta = \Delta(B_0)$ characterizes the resonance width.

Two parameters of our model Eq. (21), a_{bg} and β/γ, are completely determined from the external magnetic field dependence of the scattering length. For example, in the sodium case [25] the width Δ of the Feshbach resonance ($B_0 = 907$ G) is 1 G, therefore $\alpha = 1.1013210^{-3}$ 1/ G, $\beta/\gamma = 2.3472610^{-2}$, and $a_{\mathrm{bg}} = 53$ au.

As for parameter γ, it can be determined from the energy dependence of the scattering phase shift, δ

$$k \cot\delta = \frac{1}{a_{\mathrm{bg}}}\left(-1 + \frac{\Delta}{\Delta + 2B_0 - \sqrt{4B_0 B - (k a_{\mathrm{bg}}(\Delta + 2B_0)/\gamma)^2}}\right). \tag{26}$$

We note that the multi-channel ZRP model gives the same results for the scattering phase shift as obtained in the contact potential model of Ref. [26], which uses a cutoff regularization in the momentum representation.

4. Dilute Bose gas near Feshbach resonance

For a generalization of the LOCV method for a dilute uniform gas of bosons interacting through the two-channel ZRP, Eqs. (18), (19), (21), we assume

$$\Psi^P(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \prod_{i<j} f^P(\vec{r}_i - \vec{r}_j), \tag{27}$$

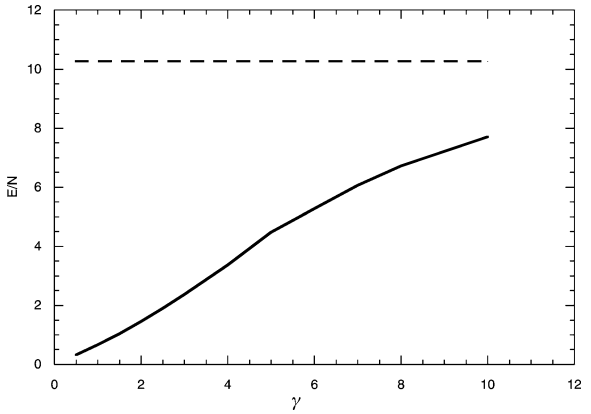

Fig. 3. Ground-state energy per particles, E/N, of $Na(F=1, m_F=+1)$ atoms at 907 G in units of $10^4 2ma_{\rm bg}^2/\hbar^2$, as a function of parameter γ, (solid line). Dashed line represent approximation of Ref. [6], Eq. (10). ($r_0 = 10^2 a_{\rm bg}$).

where $\Psi^P(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)$ is the Jastrow wave function, index P denotes the projection onto the Hilbert subspace of the incident (atomic) channel, and f^P at short distance is solution of the Schrödinger equation

$$-\frac{\hbar^2}{m}\frac{d^2}{dr^2} r f^P(r) = \lambda r f^P(r), \tag{28}$$

with boundary conditions

$$\left.\frac{d(rf^P)}{dr}\right|_{r=0} = -\frac{1}{a_{\rm eff}} r f^P, \qquad f^P(d) = 1, \qquad \left.\frac{df^P}{dr}\right|_{r=d} = 0, \tag{29}$$

where

$$a_{\rm eff} = a_{\rm bg}\left(1 + \frac{\Delta}{2B_0 - \sqrt{4B_0 B - (\kappa a_{\rm bg}(\Delta + 2B_0)/\gamma)^2}}\right), \tag{30}$$

and $\kappa = \sqrt{m\lambda}/\hbar$. The real part of ground-state energy per particle is given by

$$E/N = 2\pi n\lambda \int_0^d \left(f^P(r)\right)^2 r^2\, dr, \tag{31}$$

and d is defined by the normalization

$$4\pi n \int_0^d \left(f^P(r)\right)^2 r^2\, dr = 1. \tag{32}$$

We note that the effective scattering length, $a_{\rm eff}$ is a many-body parameter (it depends on E/N), and, for $B = B_0$, $a_{\rm eff}$ does not tend to infinity.

The calculated energies per particle, E/N, of $Na(F=1, m_F=1)$ atoms at resonance magnetic field ($B = B_0 =$ 907 G) for $r_0 = 10^2 a_{\rm bg}$ are compared with the one-channel approximation, Eq. (10), in Fig. 3. These comparisons show that for finite values of γ there are significant differences between our results and the approximation of Ref. [6]. Our results are much smaller than the Legett's variational estimate [20].

Table 3
Energy per particle of $Na(F=1,m_F=1)$ atoms, E/N, multiplied by $10^6 2ma_{\rm bg}^2/\hbar^2$ as a function of γ and B near the $B=907$ G Feshbach resonance

γ	$B=906$ G	$B=906.5$ G	$B=906.8$ G	$B=906.9$ G	$B=906.98$ G	$B=908.5$ G
0.1	5.147	6.008	6.835	7.185	7.498	0.889
0.5	6.078	8.939	15.59	21.51	29.58	0.998
1.0	6.128	9.225	18.06	29.69	55.30	1.002
2.0	6.141	9.304	19.00	34.94	100.3	1.003
3.0	6.144	9.319	19.20	36.41	137.9	1.003
4.0	6.144	9.319	19.27	36.41	168.2	1.003
5.0	6.145	9.327	19.30	37.27	197.5	1.003
6.0	6.145	9.328	19.32	37.42	215.5	1.003
7.0	6.145	9.329	19.33	37.52	231.4	1.003
8.0	6.145	9.330	19.34	37.58	243.0	1.003
9.0	6.145	9.330	19.34	37.62	254.5	1.003

Table 4
Ratio $(\Gamma/2)/(E/N)$ of $Na(F=1,m_F=1)$ atoms vs. γ and B near the $B=907$ G Feshbach resonance

γ	$B=906$ G	$B=906.5$ G	$B=908.5$ G
0.1	2.1×10^{-3}	1.8×10^{-2}	1.2×10^{-3}
0.5	1.8×10^{-3}	1.2×10^{-2}	1.1×10^{-3}
9.0	1.8×10^{-3}	1.2×10^{-2}	1.1×10^{-3}

Table 5
Energy per particle of $Na(F=1,m_F=1)$ atoms, E/N, multiplied by $10^6 2ma_{\rm bg}^2/\hbar^2$, effective scattering length, $a_{\rm eff}$ in units of $a_{\rm bg}$, as a function of γ at $B=907.1$ G with $a(B)=-9a_{\rm bg}$

γ	E/N	$a_{\rm eff}$
0.1	8.02	2.59
0.5	49.1	13.8
1.0	146	31.8
1.5	299	49.5
2.0	502	72.6

To consider, so-called, nonuniversal effects [21], i.e., the sensitivity to the parameters of the interatomic interactions other than the scattering length, we calculate E/N as a function of γ. Table 3 shows a strong γ dependence of E/N near the FR.

However, near the FR the atomic BEC is metastable, and the LOCV E/N would be reliable if $E/N > \Gamma/2$ [6]. We have extracted the values of $\Gamma/2$ from experimental data of Ref. [25]. Using these values of $\Gamma/2$ we have calculated the ratio $(\Gamma/2)/(E/N)$ (see Table 4). From Table 4 we can see that the LOCV results for the real part energy, E/N, is valid for the experimental conditions of Ref. [25], since $(\Gamma/2)/(E/N)\approx 10^{-2}$.

Now suppose that a, Eq. (23), near the FR is negative ($a_{\rm bg}$ for the $Na(F=1,m_F=1)$ atoms is positive). In one-channel case the uniform condensate for negative a is always mechanically unstable. But the two-channel consideration can lead to stable uniform solution, since the many-body parameter $a_{\rm eff}$ can be positive. Table 5 illustrates this stabilization effect. Although the three-body recombination processes [23,25,27–29] can make it difficult to observe this effect experimentally, we note that Ref. [30] considered the possibility of suppressing three-body recombinations in a trap. There is a similar case [31] of uniform 1D gas of N bosons on a ring for which inelastic decay processes, such as the three-body recombination, are suppressed in the strongly interacting and intermediate regimes.

5. Summary and conclusion

In summary we have considered the LOCV method for a dilute uniform gas of bosons.

Comparison of the LOCV results for potentials Eqs. (12)–(14) with the available diffusion Monte Carlo (DMC) calculations shows that the LOCV energies in the case of $R/r_0 \approx 10^{-2}$ are in very good agreement with the DMC results.

We have generalized the LOCV method [6,8] for dilute uniform gas of bosons near the FR, using the multi-channel ZRP model. As an example of application, we have considered $Na(F = 1, m_F = 1)$ atoms near the $B_0 = 907$ G FR.

At high density $na^3 \gg 1$, there are significant differences between our results and one-channel ZRP [6] for the real part of energy per particle. For the case of negative scattering length, we point out the possibility of stabilization of the uniform condensate.

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