Virial expansion of a harmonically trapped Fermi gas across a narrow Feshbach resonance

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We theoretically investigate the high-temperature thermodynamics of a harmonically trapped Fermi gas across a narrow Feshbach resonance by using the second-order quantum virial expansion, and point out some new features compared to the broad resonance. The interatomic interaction is modeled by the pseudopotential with an additional parameter, i.e., the effective range, to characterize the narrow-resonance width. Deep inside the width of a narrow Feshbach resonance, we find the second virial coefficient evolves with the effective range from the well-known universal value $1/4$ in the broad-resonance limit to one another value $1/2$ in the narrow-resonance limit. This means the Fermi gas interacts more strongly at the narrow resonance. In addition, far beyond the resonance width, we find the harmonically trapped Fermi gas still manifests an appreciable interaction effect across a narrow Feshbach resonance, which is contrary to our knowledge of the broad Feshbach resonance. All our results can be directly tested in current narrow Feshbach resonance experiments, which are generally carried out in a harmonic trap.

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I. INTRODUCTION

Recently, the accurate measurements of ^{6}Li atoms across the narrow Feshbach resonance at $B_0 = 534.3$G with the width $\Delta = 0.1$G [1] has raised a great deal of interest on narrow resonances. Ho *et al*. have shown that for narrow resonances, the system interacts more strongly, and the interaction energy is highly asymmetric [2]. Cui finds very different thermodynamic properties between broad and narrow resonances in quasi-one-dimensional geometry [3]. In addition, Nishida points out that a three-component Fermi gas near a narrow Feshbach resonance should have a universal ground state, which is absent for a broad resonance due to the Thomas collapse [4]. Therefore, the accurate manipulation of ultracold atoms across a narrow Feshbach resonance provides another experimental platform for studying fundamental problems in condensed matter and the strongly correlated many-body physics.

The quantum virial expansion method is a natural bridge between few-body and many-body physics [5–8], and the latter is always a challenge [9,10]. The biggest advantage of the virial expansion is that the thermodynamics of a profound many-body system may be evaluated perturbatively from the simple few-body solutions. For broad resonances, the second virial coefficient for a homogeneous two-component Fermi gas has been calculated [11], while the second and third virial coefficients of a strongly interacting Fermi gas in a harmonic trap were also obtained [6,7]. Recently, these theoretical results were confirmed experimentally [12].

However, for narrow Feshbach resonances, one additional parameter, namely the effective range, should be required to characterize the energy-dependent interaction between atoms, besides the scattering length [13–15]. This energy-dependent interaction may apparently affect the thermodynamic universality of the system, which should be quite different from that of the broad-resonance system [2]. All the previous works only considered the homogeneous systems across the narrow resonance [2,3], while the real experiments are generally carried out in a harmonic trap. In this paper, we aim to investigate how the resonance width, or the effective range, changes the high-temperature thermodynamics of a harmonically trapped Fermi gas, by using the second-order virial expansion. The second virial coefficient is obtained from the two-body solution, in which the interatomic interaction is modeled by the pseudopotential with an energy-dependent scattering length [16], or including an additional effective range [8,17]. We find, deep inside the resonance width, the second virial coefficient continuously evolves from the well-known universal value $1/4$ in the broad-resonance limit to one another value $1/2$ in the narrow-resonance limit. This means the Fermi gas is more strongly interacting at the narrow resonance, compared to the situation of the broad resonance. Interestingly, far beyond the resonance width, the harmonically trapped Fermi gas still manifests appreciable interaction effect across a narrow Feshbach resonance, which is contrary to our knowledge of the broad Feshbach resonance. All our results can be directly tested in the current experimental platform of narrow Feshbach resonances.

This paper is arranged as follows. We first summarize the crucial calculation methods of the virial expansion used in this paper in Sec. II. Subsequently, in Sec. III, the second virial coefficient for a harmonically trapped Fermi gas is calculated deep inside the narrow-resonance width. Based on this, the thermodynamics of the system is also discussed in detail. In Sec. IV, we investigate the thermodynamics of a harmonically trapped Fermi gas far beyond the width of a narrow Feshbach resonance. Then we present a simple toy model in Sec. V, which is helpful for understanding the origin of the energy-dependent interaction. Finally, our main results are summarized in Sec. VI.

II. VIRIAL EXPANSION METHOD

Virial expansion is a perturbation method to explore the high-temperature thermodynamics of strongly interacting

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Fermi gases based on the knowledge of few-body solutions. In this section, we will summarize the crucial calculation methods of virial expansion used in this paper, although virial expansion has been studied in depth [6,7].

The basic idea of virial expansion is that at high temperature all the thermodynamic quantities can be expanded in series of the fugacity $z \equiv e^{\mu/(k_B T)}$, which is small since the chemical potential μ is large and negative at high temperature. Here, k_B is the Boltzmann constant. For example, the thermodynamic potential may be written as

$$\Omega = -k_B T Q_1 (z + b_2 z^2 + \cdots + b_n z^n + \cdots), \tag{1}$$

where $Q_n \equiv \mathrm{Tr}[e^{-\mathcal{H}_n/(k_B T)}]$ is the n-particle partition function, and $\mathcal{H}_n$ is the total Hamiltonian of these n particles. The expansion coefficients b_n are the so-called virial coefficients. The nth virial coefficient b_n is related to the solutions of up to n-body problems. In this way, the complicated strongly correlated many-body problem is converted to a set of relatively simple few-body problems. For example, if we solve a two-body problem, we can obtain the second virial coefficient $b_2 = (Q_2 - Q_1^2/2)/Q_1$, and then we have the information about this many-body problem up to the second order of the fugacity. The more we can solve the few-body problems, the more accurate description of the many-body problem we will acquire. All the other thermodynamic quantities can then be derived from Ω via the standard thermodynamic relations, i.e., the particle number $N = -\partial\Omega/\partial\mu$, the entropy $S = -\partial\Omega/\partial T$, and the energy $E = \Omega + TS + \mu N$ [18].

Throughout this paper, we investigate the high-temperature thermodynamics of a two-component (two hyperfine states, or, two spin states) harmonically trapped Fermi gas only up to the second order of the fugacity. Generally, we are mostly interested in the contribution arising from the interactions. Thus to this end, let us consider the difference

$$\Delta b_2 = b_2 - b_2^{(1)} = \frac{Q_2 - Q_2^{(1)}}{Q_1}, \tag{2}$$

where the superscript 1 denotes the quantities of an ideal gas. For a two-component Fermi gas, we easily find

$$\Delta b_2 = \frac{1}{2}\sum_{\alpha}\left[e^{-E_\alpha^{\mathrm{rel}}/(k_B T)} - e^{-E_\alpha^{(1),\mathrm{rel}}/(k_B T)}\right], \tag{3}$$

where the summation runs over all possible states of the relative motion of two fermions with different spin states. Therefore, the spectrum of the relative motion determines the second virial coefficient. The average energy per atom in unit of the Fermi energy $E_F = (3N)^{1/3}\hbar\omega$ (ω is the trap frequency, and N is the total atom number) may be written as

$$\frac{E}{NE_F} = 3\left(\frac{T}{T_F}\right)^4\left[3\int_0^\infty t^2 \ln(1 + ze^{-t})dt + 6\Delta b_2 z^2 + 2z^2\ T\frac{\partial \Delta b_2}{\partial T}\right], \tag{4}$$

where $T_F = E_F/k_B$ is the Fermi temperature. The fugacity z (or the chemical potential μ) is determined by the total particle number N, and at a given temperature, can be solved from

$$\left(\frac{T}{T_F}\right)^3\left[z\int_0^\infty \frac{t^2 e^{-t}}{1 + ze^{-t}}dt + 4\Delta b_2 z^2\right] = \frac{1}{3}. \tag{5}$$

Subsequently, with the second virial coefficient Δb_2 and the fugacity z in hand, the average energy per atom can easily be obtained from Eq. (4). In addition, the other thermodynamic quantities can also be acquired in the same way.

III. THERMODYNAMICS DEEP INSIDE THE RESONANCE WIDTH

As we know, strongly interacting degenerate Fermi gases manifest universality in the vicinity of the resonances [9,10]. However, for narrow Feshbach resonances, the appreciable effective range becomes essential in this strongly interacting region. In this section, we are going to study how the universality of a strongly interacting Fermi gas is affected by the large effective range deep inside the resonance width.

In order to identify the effective range near the Feshbach resonance, we may use the effective-range expansion of the scattering phase shift ϕ_0 in the low-energy limit [1,2]. We find the scattering length a_0 is expressed as

$$a_0 = a_{bg}\left(1 - \frac{\Delta}{B - B_0}\right), \tag{6}$$

and the effective range has a general form

$$r_0 = -\frac{2\hbar^2}{m}\frac{\Delta}{a_{bg}\gamma(B - B_0 - \Delta)^2}, \tag{7}$$

where a_{bg} is the background scattering length, B_0 is the magnetic field strength at the resonance, Δ is the width of the resonance, and γ is the magnetic moment difference between two atoms in the open channel and the molecule in the closed channel. Deep inside the resonance width, i.e., $B - B_0 \ll \Delta$, the B dependence of the effective range is absent. The effective range becomes a constant, i.e., $r_0 \approx -2\hbar^2/(m a_{bg}\gamma\Delta)$, and is determined only by the intrinsic properties of the resonance.

In this case, it is quite convenient to use the modified pseudopotential introduced in Refs. [8,17] to describe the two-body interaction,

$$V_0(\mathbf{r}) = -\frac{4\pi\hbar^2}{m}\left(-\frac{1}{a_0} + \frac{1}{2}r_0 k^2\right)^{-1}\delta(\mathbf{r})\frac{\partial}{\partial r}r, \tag{8}$$

in which the *constant* effective range is included besides the scattering length. Here, $\mathbf{r}$ is the relative coordinate of two atoms. After some straightforward and conventional algebra, the relative-motion Schrödinger equation of two atoms is reduced to the following equation [8],

$$\frac{2\Gamma\left(-\frac{E}{2\hbar\omega} + \frac{3}{4}\right)}{\Gamma\left(-\frac{E}{2\hbar\omega} + \frac{1}{4}\right)} = \frac{d}{a_0} - \frac{r_0}{d}\frac{E}{\hbar\omega}, \tag{9}$$

where $\Gamma(\cdot)$ is the Γ function. We may easily obtain the two-body spectrum of the relative motion from Eq. (9) as presented in Fig. 1. The effective range of the narrow Feshbach resonance for ^{6}Li at $B_0 = 543.3$G in the experiment [1] is $r_0 = -7 \times 10^4 a_B$ (a_B is the Bohr's radius), and the trap frequency is around $\omega = 2\pi \times 1.3 \sim 3.6$ kHz, which determines the ratio of the effective range r_0 to the trap characteristic length $d = \sqrt{2\hbar/(m\omega)}$, i.e., $r_0/d \approx -2 \sim -4$. In our calculations, we choose $r_0/d = -3$ without loss of generality. As a comparison, we also plot the relative-motion spectrum of two atoms across a broad resonance, where the effective range is set to be $r_0/d = 0$

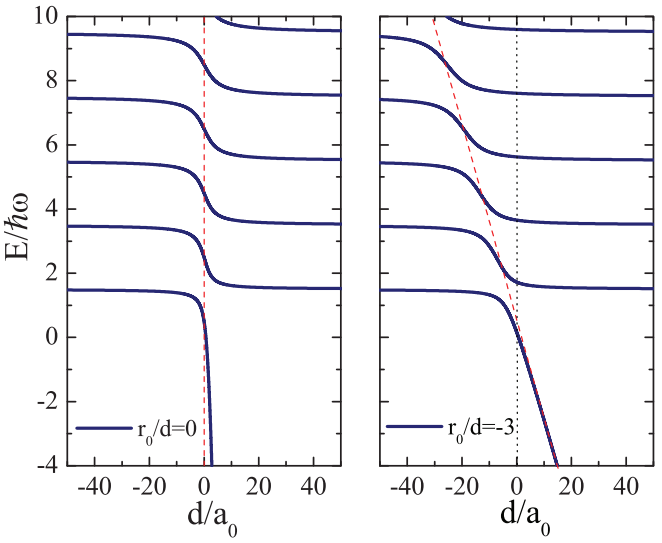

FIG. 1. (Color online) The relative-motion spectrums of two atoms in a harmonic trap for broad (left) and narrow (right) resonances, respectively. The red dashed lines are the eye guidance for the evolution between two adjacent energy levels.

in the broad-resonance limit. Obviously, the properties of the narrow-resonance spectrum are quite different from those of the broad resonances. For the narrow Feshbach resonance, the energy-level transitions occur on the BCS side. The higher the energy is, the more deeply in the BCS side the transitions are located. However, all the energy-level transitions are located in the vicinity of the broad resonance, and then such systems present the universality at the unitarity limit.

With the relative-motion spectrum of two atoms in hand, we can easily obtain the second virial coefficient according to Eq. (3). In order to demonstrate how the universality of a strongly interacting Fermi gas is affected by the effective range, we plot in Fig. 2 the evolution of the second virial

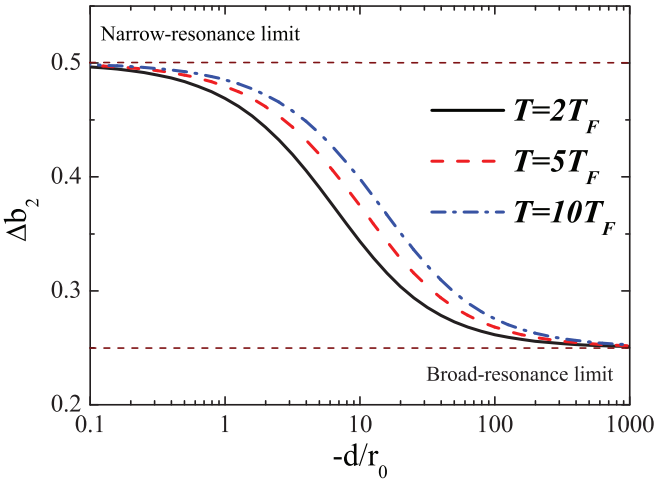

FIG. 2. (Color online) The second virial coefficients Δb_2 as functions of the inverse effective range $-d/r_0$ at different temperatures. Here, we have chosen the total atom number $N = 1 \times 10^5$. The two horizontal dashed lines indicate the narrow- and broad-resonance limits, respectively.

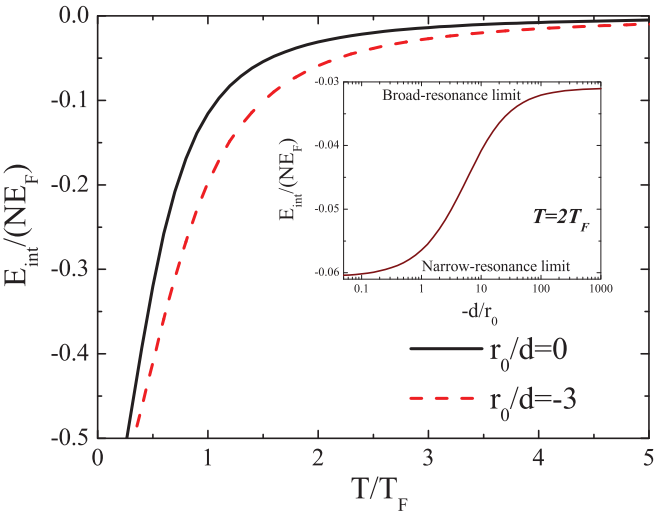

FIG. 3. (Color online) The temperature dependence of the interaction energy of a strongly interacting harmonically trapped Fermi gas for a broad resonance ($r_0/d = 0$) and a narrow resonance ($r_0/d = -3$). The insert is the evolution of the interaction energy with the effective range from the broad-resonance limit to the narrow-resonance limit at the temperature $T = 2T_F$. Here, we have chosen the atom number $N = 1 \times 10^5$ in our calculation.

coefficient from the broad-resonance limit to the narrow-resonance limit at different temperatures, as the effective range increases. In the broad-resonance limit, it is well known that the second virial coefficient has a universal value 1/4 for a strongly interacting harmonically trapped Fermi gas [6]. Interestingly, we find that this second virial coefficient will continuously evolve to a larger universal value 1/2 in the narrow-resonance limit, which means the large effective range will result in a stronger interaction between atoms at the resonance. Consequently, for a homogeneous Fermi gas at the resonance, we find the second virial coefficient $\Delta b_2^{\rm hom} = 2\sqrt{2}\Delta b_2 = \sqrt{2}$ [6]. This result is consistent with that of Ref. [2] (note that there is a $\sqrt{2}$ factor difference in the definition of the second virial coefficient).

According to Eq. (4), we can easily calculate the energy of a strongly interacting harmonically trapped Fermi gas as well as that of an ideal gas at a given temperature, and the difference gives the interaction effect as shown in Fig. 3. At the resonance, the interaction energy of a narrow resonance with appreciable effective range is larger than that of the broad resonance. As the temperature increases, the Fermi gas may approach to a classical ideal gas, and the interaction effect vanishes. The evolution of the interaction energy with the effective range from the broad-resonance limit to the narrow-resonance limit is also illustrated in the insert of Fig. 3 at a specific temperature $T = 2T_F$. We find the Fermi gas becomes more strongly interacting as the effective range increases at the resonance.

IV. THERMODYNAMICS FAR BEYOND THE RESONANCE WIDTH

Unlike the broad Feshbach resonance, it is relatively difficult to experimentally explore the properties of a strongly interacting Fermi gas quite deep inside a narrow Feshbach

resonance, due to the small resonance width. In the narrow-resonance experiment, it requires the controllability of the magnetic field with high stability and accuracy [1]. However, even outside the resonance width, the narrow-resonance system should also manifest unique properties, which are different from those of the broad resonance. In this section, we are going to study the thermodynamics of a harmonically trapped two-component Fermi gas across a narrow Feshbach resonance beyond the resonance width.

As we already find in Eqs. (6) and (7), both the scattering length and effective range are dependent on the magnetic field strength B across a narrow Feshbach resonance. In this case, it is convenient to use the pseudopotential with an energy-dependent scattering length $a_0(k)$ [16],

$$V_0(\mathbf{r}) = \frac{4\pi\hbar^2 a_0(k)}{m}\delta(\mathbf{r})\frac{\partial}{\partial r}r, \tag{10}$$

to describe the two-body interaction, where the energy-dependent scattering length $a_0(k)$ is defined from the scattering phase shift $\phi_0(k)$ as [1,2]

$$\begin{aligned} a_0(k) &\equiv -\frac{\tan\phi_0(k)}{k} \\ &= a_{bg}\frac{\hbar^2k^2/m - \gamma(B - B_0 - \Delta)}{\hbar^2k^2/m - \gamma(B - B_0)}. \end{aligned} \tag{11}$$

Then the relative-motion spectrum of two atoms is determined by the following equation,

$$B - B_0 = \frac{\left(E + \gamma\Delta\right)f(E) - E\frac{d}{a_{bg}}}{\left[f(E) - \frac{d}{a_{bg}}\right]\gamma}, \tag{12}$$

where

$$f(E) = \frac{2\Gamma\left(-\frac{E}{2\hbar\omega} + \frac{3}{4}\right)}{\Gamma\left(-\frac{E}{2\hbar\omega} + \frac{1}{4}\right)}, \tag{13}$$

and we have taken the approximation $k^2 = mE/\hbar^2$ [8,19,20].

At a given magnetic field strength, we can easily solve the relative-motion spectrum of two atoms, and subsequently evaluate the second virial coefficient according to Eq. (3). In Fig. 4, we plot the second virial coefficient in a real system of atoms ^{6}Li across a narrow Feshbach resonance at $B_0 = 543.25$G with the width $\Delta B = 0.1$G. At the resonance, i.e., $B = B_0$, we find the second virial coefficients at different temperatures almost cross in one point quite near the universal value $1/2$, which is consistent with the result of the last section. In addition, we interestingly find the second virial coefficient with nonzero value extends far beyond the resonance width to the deep BCS side, which means the Fermi gas is still strongly interacting even far away from the resonance.

The interaction energy of a harmonically trapped Fermi gas across a narrow Feshbach resonance at different temperatures is presented in Fig. 5. As we anticipate, there is indeed an appreciable interaction effect outside the resonance width. This is quite different from the broad-resonance case, in which we usually take the region within the resonance width as the strongly interacting area. For narrow resonances, due to large Fermi energy compared to the resonance width, there may be still scattering resonance even above the zero-energy-

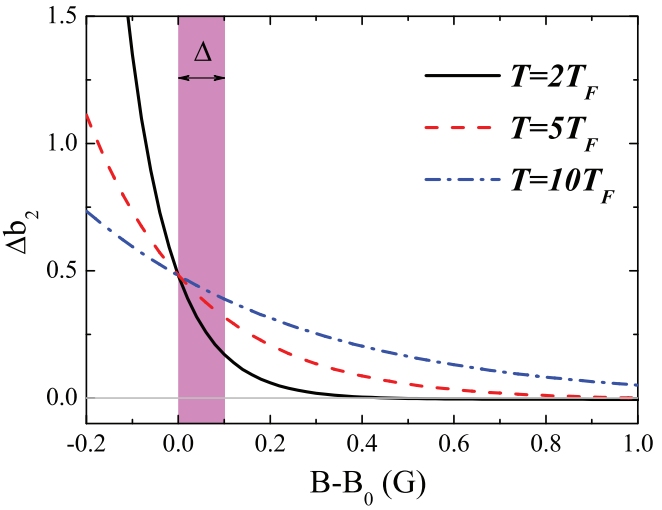

FIG. 4. (Color online) The second virial coefficient Δb_2 across a narrow Feshbach resonance at different temperatures. Here, we consider the narrow Feshbach resonance of a Fermi gas ^{6}Li at $B_0 = 543.25$G with the width $\Delta = 0.1$G, background scattering length $a_{bg} = 62a_B$, and the magnetic moment difference $\gamma = 2\mu_B$ (μ_B is the Bohr's magneton). We have chosen the trap frequency $\omega = 2\pi \times 2$ kHz, and the atom number $N = 1 \times 10^5$. The pink area is the conventional strongly interacting region within the resonance width.

resonance point, i.e., $B = B_0$ [2,14]. That is why the Fermi gas is still strongly interacting even deep in the BCS side.

V. ABOUT THE ENERGY-DEPENDENT INTERACTION

In our previous calculations, we just phenomenologically introduce an energy-dependent interaction in the pseudopotential model to characterize the narrow resonance. It is also very interesting to understand the origin of such energy-dependent interaction. We will see that if a metastable quasibound state with a positive energy [21] is supported by the interatomic

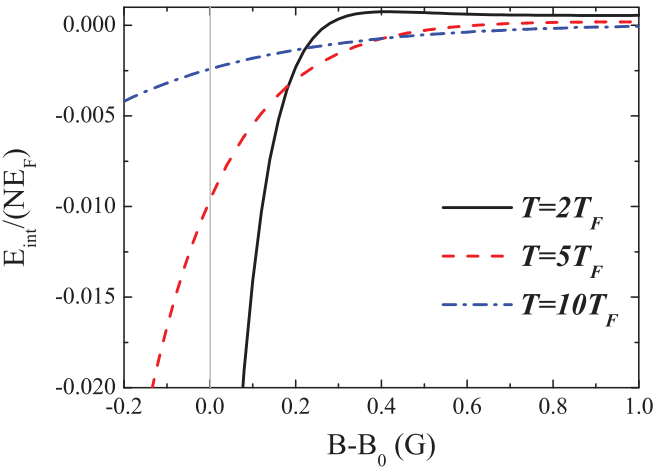

FIG. 5. (Color online) The interaction energy of a harmonically trapped Fermi gas across a narrow Feshbach resonance at different temperatures. We also consider the narrow Feshbach resonance of a Fermi gas ^{6}Li at $B_0 = 543.25$G with all parameters in Fig. 4.

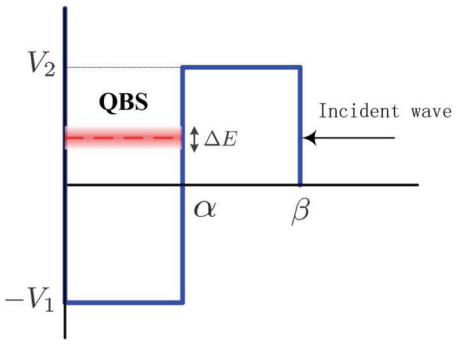

FIG. 6. (Color online) The square-well-barrier potential. Here, QBS is short for the quasibound state.

potential, it may result in a narrow scattering resonance with a large effective range.

To this end, let us consider a square-barrier-well potential, in which the interaction potential between atoms takes the form,

$$V(r) = \begin{cases} -V_1, & r < \alpha, \\ V_2, & \alpha < r < \beta, \\ 0, & r > \beta. \end{cases} \tag{14}$$

as illustrated in Fig. 6. Although the real Feshbach resonance is usually characterized by a two-channel model theory, the freedom of the choice of the interaction potential between ultracold atoms enables us to extract the key information from this simple single-channel model. This toy model is effectively equivalent to the two-channel model, and is already sufficient to realistically mimic the narrow Feshbach resonance [22].

We may easily solve the scattering problem within this interatomic potential, in presence and absence of the barrier, respectively. The scattering length a_0 and effective range r_0 can be evaluated from the scattering phase shift ϕ_0,

$$k \cot \phi_0 = -\frac{1}{a_0} + \frac{1}{2} r_0 k^2. \tag{15}$$

From Fig. 7, we find the presence of the barrier raises a much larger effective range near the resonance compared to the case without the barrier, which means this square-well-barrier model indeed causes an energy-dependent interaction. This is because, in presence of the barrier, a quasibound state with a positive energy may have a finite lifetime, and results in a relatively small energy broadening due to the uncertainty principle, compared to the case without the barrier. In this case, when the incident atoms energetically approach this bound state, a narrow scattering resonance occurs. Similarly, in the real two-channel Feshbach resonance, the lifetime of the bound state in the closed channel is prolonged due to the large Fermi energy of atoms in the open channel [14,23], and thus induces a relatively narrow Feshbach resonance.

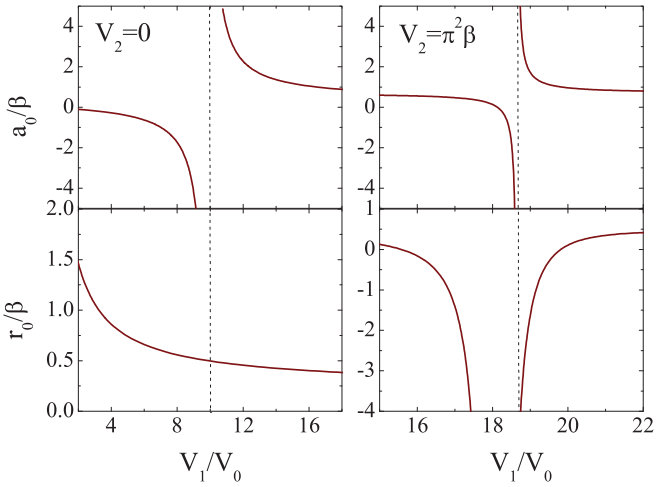

FIG. 7. (Color online) The scattering length a_0/β and the effective range r_0/β as functions of the square-well depth V_1/V_0 in absence (left panel) and in presence (right panel) of a barrier, where $V_0 = \sqrt{\hbar^2/m\beta^2}$ and m is the atomic mass. Here, we have chosen $\alpha/\beta = 0.5$.

VI. CONCLUSIONS

In summary, we have presented the virial expansion in studying the high-temperature thermodynamics of a harmonically trapped Fermi gas across a narrow Feshbach resonance. Deep inside the width of a narrow resonance, the second virial coefficient is obtained based on the two-body spectrum in a harmonic trap. We find the second virial coefficient undergoes a continuous evolution from $1/4$ in the broad-resonance limit to $1/2$ in the narrow-resonance limit, as the effective range increases. This results in a larger interaction energy for a narrow resonance compared to that of a broad resonance. Besides, contrary to our knowledge of a broad resonance, there is still a considerable interaction effect far beyond the width of a narrow resonance. Finally, we present a simple toy model for helping us understand the origin of the energy-dependent interaction in narrow Feshbach resonances. All our results can be directly tested in current narrow Feshbach resonance experiments, which are generally carried out in a harmonic trap.

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