Modeling atom–atom interactions at low energy by Jost–Kohn potentials

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Abstract
More than 65 years ago, Jost and Kohn (1952 Phys. Rev. 87, 977) derived an explicit expression for a class of short-range model potentials from a given effective range expansion with the s-wave scattering length $a_s$ being negative. For $a_s > 0$, they calculated another class of short-range model potentials (Jost and Kohn 1953 Dan. Mat. Fys. Medd 27, no. 9) using a method based on an adaptation from Gel’fand–Levitan theory (Gel’fand and Levitan 1951 Dokl. Akad. Nauk. USSR 77, 557-60) of inverse scattering. We here revisit the methods of Jost and Kohn in order to explore the possibility of modeling resonant finite-range interactions at low energy. We show that the Jost–Kohn potentials can account for zero-energy resonances. The s-wave phase shift for positive scattering length is expressed in an analytical form as a function of the binding energy of a bound state. We show that, for small binding energy, both the scattering length and the effective range are strongly influenced by the binding energy; below a critical binding energy the effective range becomes negative provided the scattering length is large. As a consistency check we carry out some simple calculations to show that Jost–Kohn potentials can reproduce the standard results of contact interaction in the limit of the effective range going to zero.

Keywords: atom–atom interaction, Feshbach resonance, finite-range interaction

(Some figures may appear in colour only in the online journal)

1. Introduction

The purpose of this paper is to develop a description of s-wave resonant interactions between neutral particles at low energy in terms of the finite-range model interaction potentials derived in the early 1950s by Jost and Kohn [1, 2]. Though there is a multitude of model potentials to describe the physics of interacting particles at low energy at different length scales [3], there exists no unique or standard method to construct a model potential for the particles interacting through a scattering resonance with a finite range. Such a model potential for resonant interactions would be particularly important for many-body physics of ultracold atoms [4] with magnetically tunable Feshbach resonances [5, 6] that make the atoms interact strongly. The well-known contact-type pseudo-potential approximation [7, 8] does not hold good in the case of resonant interactions with a large effective range. The strength of the contact potential is proportional to the s-wave scattering length $a_s$. At a resonance, $a_s$ diverges, but this does not necessarily mean that mean-field interaction should diverge. The low density approximation $n|a_s|^3 \ll 1$ used in the case of a contact potential may break down for resonant interactions for which the effective range of interaction becomes important. In recent times, several theoretical [9] and experimental works [10–12] have demonstrated that the effective range at or near a Feshbach resonance becomes finite or large and even negative. The effective range is shown to be quite important for three-body Efimov states [12–16]. The finite-range and finite energy effects of s-wave interaction have been shown to be incorporated in a contact-type pseudo-potential approach with an energy-dependent scattering length or phase shift [17].

Jost and Kohn constructed two classes of model potentials that include, among other parameters, the effective range $r_0$ of interaction. One class is for negative $a_s$ [1] and the other class is for positive $a_s$ [2]. The model potential $V_{\text{s}}(r)$ ($r$ being...
the inter-particle separation) for negative $a_s$ was derived by a perturbative inverse scattering method using the effective range expansion of the $s$-wave scattering phase shift. For positive $a_s$, the actual two-body interaction potential may support one or many bound states. Jost and Kohn derived a class of 'equivalent' potentials $V_b(r)$ for positive $a_s$ from an analytical form of s-wave phase shift that includes the parameter $\kappa$ related to the binding energy $E_b = -\hbar^2 \kappa^2 / 2\mu$ ($\mu$ is the reduced mass of the two particles and $\hbar$ is the Planck’s constant divided by $2\pi$). It is important to note that $V_b(r)$ does not support any bound state, but another 'equivalent' potential $V_d(r)$ can support the bound state with the same binding energy. $V_d(r)$ is a three-parameter potential; the other two parameters are the $a_s$ and $r_0$ which are the same as corresponds to $V_b(r)$. It is a consequence of the theorem of Gel’fand–Faddeev and Levitan [18] that it is possible to construct a class of ‘equivalent’ potentials with the same phase shift but with or without a bound state, showing the independence of phase shifts from the bound states. However, from low-energy scattering theory it follows that the positive $a_s$ may be related to the binding energy of a near-zero-energy bound state. According to Gel’fand–Levitan theory, in order to construct $V_d(r)$ by an appropriate modification of $V_b(r)$, one has to include the normalization constant of the bound state that may be extracted from the asymptotic analysis of the scattering state through analytic continuation into the complex energy. Nevertheless, since both $V_s(r)$ and $V_d(r)$ are ‘equivalent’ yielding the same scattering properties, one can work with $V_s(r)$ as far as elastic scattering properties of the system are concerned.

Here we show that the Jost–Kohn potentials $V_+(r)$ and $V_s(r)$ are applicable to describe resonant interactions under certain physical conditions. They can naturally take into account the effective range effects of the interactions. We demonstrate that, in the limits $\alpha_s \to \pm \infty$ and $\kappa \to 0$, both the potentials yield zero-energy resonance [19, 20]. We analyze in some detail how the tuning of the parameter $\kappa$ can control the value of the effective range. $V_s(r)$ is derived from an analytical form of the s-wave phase shift which is a function of $\kappa$. Note that the parameter $r_0$ and $a_s$ used to construct $V_s(r)$ correspond to the effective range and the scattering length only in the limit $\kappa \to \infty$. On the other hand, in the limit $\kappa \to 0$, the scattering length and the effective range become drastically modified due to the proximity of zero-energy resonance. As a result, the modified effective range may become large and negative. The Jost–Kohn potentials do not readily reduce to contact-type potentials in the limits $r_0 \to 0$ for small $|a_s|$. However, as a consistency check, we carry out numerical scattering calculations with Jost–Kohn potentials and show that in the limits $r_0 \to 0$, $\kappa \to \infty$ and for small $a_s$, the calculated results qualitatively reproduce the standard results that can be obtained from a contact interaction. Finally, we discuss in some detail how to fit Jost–Kohn potentials to describe Feshbach resonances under certain physical situations. In this context, it is worth mentioning that recently several theoretical works [21] have explored different procedures with a wide variety of model potentials to study the finite-range effects of low-energy atom–atom interactions. For instance, Schneider et al [22] have used the Born–Oppenheimer potential with an adjustable parameter to correspond to the experimental value of $a_s$, and Lange et al [23] have used a pair of square-well potentials with several adjustable parameters like binding energy and van der Waals length scale. Flambaum et al [24] have used a model Bennard–Jones potential to explore finite-range effects near a Feshbach resonance. Veksler et al [25] have developed a modified inter-particle interaction to calculate corrections in the ground state solution to the Gross–Pitaevskii equation. The most widely used model is the two-channel model [26] with a pair of potentials which depend on several experimental parameters of a particular system for which the Feshbach resonance is sought. Gao [27] has given a prescription, based on his angular-momentum-insensitive quantum defect approach [28], on how to construct model potentials of hard sphere and Bennard–Jones type with a $1/r^6$ asymptote.

The paper is organized in the following way. In section 2, we analyze the method of construction of Jost–Kohn potentials. In section 3, we present and discuss our result showing the limits of zero-energy resonance and zero-range effects of Jost–Kohn potentials. We show that multi-channel Feshbach resonances may be described by the Jost–Kohn potentials in some regimes. In the end, we conclude in section 4.

2. Jost–Kohn method

Here we discuss the inverse scattering method of Jost and Kohn. Let us consider that a pair of particles interact via a spherically symmetric potential $V(r)$ satisfying the condition $\int_0^{\infty} |V(r)|rdr < \infty$. The problem one addresses here is, given the phase shift $\eta(k)$ as a function of the wave number $k$ for a particular partial wave $\ell$, whether it is possible to derive a model potential $V(r)$ that can reproduce the same $\eta(k)$. A treatise on this problem was originally developed by Gel’fand and Levitan [18], and also by Jost and Kohn [1, 2], who formulated a perturbative inverse scattering method. It was first shown by Bargmann [29] and later corroborated by Jost and Kohn that one can derive a class of equivalent potentials corresponding to the same phase shift. However, if there exists no bound state, then it is possible to derive a unique potential from the given function $\eta(k)$. Jost and Kohn obtained an explicit expression for a class of model potentials from the effective range expansion of $\eta(k)$ when there is no bound state and the s-wave scattering length $a_s$ is negative. Here we first discuss the method of derivation of the negative $a_s$ potential. Then we discuss the method to derive an equivalent potential for positive $a_s$ [1, 2].

The Schrödinger equation of relative motion for s-wave is

$$\frac{d^2 \phi}{dr^2} + k^2 \phi = U\phi \quad (1)$$

where $U = 2\mu V(r)/\hbar^2$, $k$ is related to the collision energy $E = \hbar^2 k^2 / 2\mu$ and $\mu$ is the reduced mass. Let $f(\pm k, r)$ be the two linearly independent solutions of equation (1) with asymptotic
boundary conditions
\[ \lim_{r \to \infty} e^{ikr} f(\pm k, r) = 1 \]  
(2)

A general solution \(\phi(r)\) then asymptotically behaves as
\[ \phi(r) \to f(-k)e^{-ikr} + f(k)e^{ikr} \]  
(3)

where \(f(\pm k) = f(\pm k, 0)\) are called Jost functions. The scattering phase shift \(\eta(k) = \eta_f(k)\) and S-matrix is given by
\[ S(k) = e^{2i\eta(k)} = \frac{f(k)}{f(-k)} \]  
(4)

and the Jost functions have the property \(f(-k, 0) = f^*(k, 0)\). Therefore, one obtains
\[ \eta(k) = \text{Im} \left[ \log f(k) \right] \]  
(5)

From equation (4), one finds \(\eta(k) + \eta(-k) = 2n\pi\). If \(n = 0\) then \(\eta(k) = -\eta(-k)\).

Using the Green function, the solution \(f(k, r)\) of equation (1) can be expressed as an integral Volterra equation
\[ f(k, r) = e^{ikr} - \int_r^\infty k^{-1} \sin k(r' - r) U(r')f(k, r')dr' \]  
(6)

In order to explore the analyticity of the scattering problem, let \(z = 2ik\), \(g(z, r) = g(2ik, r) = e^{-ikr} f(k, r)\). So, \(g(z) = g(0)\) and \(\eta(k) = \text{Im} \left[ \log g(z) \right]\). By multiplying both sides of equation (6) by \(e^{-ikr}\) and replacing \(2ik\) by \(z\), one obtains
\[ g(z, r) = 1 + \int_r^\infty \frac{1}{z} [1 - e^{-izr'}] U(r')g(z, r')dr' \]  
(7)

This equation can be solved by iteration with the assumption \(\text{Re}[z] \geq 0\). The function \(g(z)\) is regular in \(\text{Re}[z] > 0\) and continuous in \(\text{Re}[z] \geq 0\). After the successive iteration of equation (7), we have
\[ g(z) - 1 = \frac{1}{z} \int_0^\infty dr_1 \int_r^\infty dr_2 \int_{r_2}^\infty dr_3 \cdots \int_{r_n}^\infty \frac{1}{z} \left(1 - e^{-izr'}\right) U(r')g(z, r')dr' \]  
(8)

Under the approximation of small \(U(r)\) this equation reduces to
\[ g(z) - 1 \approx \frac{1}{z} \int_0^\infty dr(1 - e^{-izr})U(r) \]  
(9)

To the first approximation, \(U(r)\) is replaced by an auxiliary potential \(U_1(r)\) defined by
\[ g(z) - 1 = \frac{1}{z} \int_0^\infty dr(1 - e^{-izr})U_1(r) \]  
(10)

which can be recast into the form
\[ \frac{1}{z} \left[ \frac{d}{dz} g(z) - 1 \right] = \int_0^\infty dre^{-izr}U_1(r) \]  
(11)

So, \(U_1(r)\) is given by the inverse Laplace transform of the function
\[ \Phi_1(z) = \frac{1}{z} \left[ \frac{d}{dz} g(z) - 1 \right] \]  
(12)

Thus equation (8) can be reformulated in the following form
\[ \int_0^\infty (1 - e^{-2zr})[U_1(r) - U(r)]dr = \sum_{l=2}^{\infty} \int_0^\infty dr_1 \int_0^\infty dr_2 \frac{1}{z} \left(1 - e^{-2zr_2}\right) \cdots \left(1 - e^{-2zr_{l-1}}\right) U(r_1)U(r_2) \cdots U(r_l) \int_0^\infty dr l \]  
(13)

The right-hand side (RHS) of the above equation approaches zero as \(z \to \infty\). This implies
\[ \int_0^\infty [U_1(r) - U(r)]dr = 0 \]  
(14)

Thus \((U(r) - U_1(r))\) is given by the inverse Laplace transform of the RHS equation (13) in \(z\). We can therefore write
\[ U(r) = U_1(r) + \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{iz} \Phi_1(z)dz \]  
(15)

where
\[ \Phi_1(z) = \int_0^\infty dr_1 \int_0^\infty dr_2 \cdots \left(1 - e^{-2zr_{l-1}}\right) \cdots U(r_1)U(r_2) \cdots U(r_l) \]  
(16)

Equation (15) can be solved perturbatively. We next follow the [1, 2] to elucidate how Jost and Kohn obtained model finite-ranged potentials using effective range expansion.

2.1. Negative a* potential

In the absence of any bound state, \(\log g(z)\) becomes regular for \(\text{Re}[z] > 0\) for \(g(0) \not= 0\) and continuous for \(\text{Re}[z] \geq 0\), its imaginary part being equal to the phase shift as given by \(\eta(k) = \text{Im} \left[ \log g(z) \right]\). Now, one can represent \(\log g(z)\) in \(\text{Re}[z] \geq 0\) in terms of phase shift \(\eta(k)\) by Poisson’s integral
\[ \log g(z) = -\frac{2k}{\pi} \int_{-\infty}^{\infty} \frac{\eta(k')}{2ik' - z}dk' \]  
(17)

Suppose \(\eta(k)\) admits an effective range expansion
\[ k \cot \eta(k) = -\frac{1}{a_*} + \frac{1}{2}\eta k^2 + \ldots \]  
(18)

where it is assumed that \(a_* < 0\). Using the relation \(\tan^{-1} x = (i/2) \log[(1 - ix)/(1 + ix)]\), one can express \(\eta(k)\) in the form
\[ \eta(k) = \frac{i}{2} \log \frac{(z + a)(z - b)}{(z - a)(z + b)} \]  
(19)

where \(a = \frac{2}{\alpha} \left[1 + \sqrt{1 - \frac{2\alpha}{\sqrt{a_*}}}\right], b = \frac{2}{\alpha} \left[-1 + \sqrt{1 - \frac{2\alpha}{\sqrt{a_*}}}\right]\).
Substituting equation (19) in equation (17), one obtains

\[ g(z) = \frac{(z + b)}{(z + a)} = 1 + \frac{2a\lambda}{(z + a)} \]  

(20)

where \( \lambda = \frac{ib - a}{2a} \) is a small parameter (\(|\lambda| < 1\)). Expanding the potential \( U(r) \) in polynomial form

\[ U(r) = \sum_{m} \lambda^{m} U_{m}(r) \]  

(21)

each of the terms \( U_{m}(r) \) can be calculated by inverse Laplace transform of \( \Phi_{m}(z) \) as discussed above. The detailed derivation is given in appendix A. The resulting series can be expressed in compact form, giving an explicit expression

\[ U_{r}(r) = \frac{2a^{2}\lambda(1 + \lambda)e^{-ar}}{1 + \lambda(1 - e^{-ar})^{2}} \]  

(22)

for negative \( a_{r} \). From here onward, for the sake of simplicity, we consider \( r_{0} \) as the unit of length, and the quantity \( E_{0} = \hbar^{2}/(2\mu_{r_{0}}^{2}) \) as the unit of energy, unless otherwise specified. Hence,

\[ V_{r}(r) = \frac{8\beta^{2}\lambda(1 + \lambda)e^{-2\beta r}}{[1 + \lambda(1 - e^{-2\beta r})]} \]  

(23)

where \( \beta = \left(1 + \sqrt{1 - \frac{2\alpha}{\alpha}}\right) \).

2.2. Positive \( a_{p} \) potential

For positive scattering length, the potential may support bound states. The binding energies of the bound states given by the zeros \( \xi_{i} \) of \( g(z) \) in \( \text{Re}[z] > 0 \) lie on the real axis for the \( z \)-plane. Therefore, in presence of bound states, the function \( g(z) \) needs to be modified. Suppose

\[ g(z) = g(z)\prod_{i} \frac{(z + \xi_{i})}{(z - \xi_{i})} \]  

(24)

which is non-zero for \( \text{Re}[z] > 0 \) and follows the same asymptotic properties of \( g(z) \). The modified equation (17) has the form of

\[ \log g(z) = -\frac{2i}{\pi} \int_{-\infty}^{\infty} \frac{\tilde{h}(k')}{2k' - z} dk' \]  

(25)

Let the binding energy of the \( i \) th bound state energy be

\[ E_{i} = -\hbar^{2}\kappa_{i}^{2}/2\mu \]  

(26)

In deriving a potential that can support only one bound state and give positive \( a_{p} \), Jost and Kohn first calculated an auxiliary potential \( V_{b}(r) \) which may yield the same low-energy scattering cross section but no bound state. The Jost function corresponding to \( V_{b}(r) \) is assumed to have the form

\[ \tilde{f}(k) = \frac{(2k - 2i\lambda)^{2}}{(2k + ib)(2k - ia)} \]  

(27)

which obviously does not have a proper zero for the bound state. \( V_{r}(x) \) is derived by iteration as above. This is expressed in terms of the three parameters which are \( r_{0} \), \( a_{s} \) and where \( d \) is a dimensionless parameter \( \Lambda \) related to the binding energy \( E_{b} = -\hbar^{2}\kappa^{2}/2\mu \) of the bound state. The detailed method of derivation is discussed in appendix B. Explicitly,

\[ V(x) = 8e^{-2(1 - \alpha)x} \left\{ \left[1 + (1 + \lambda\Lambda)(\alpha + \lambda)(1 - \alpha) - (1 - \lambda^{2})e^{-2\beta x}\right]^{2} - \frac{8\beta^{2}}{1 + \lambda(1 - e^{-2\beta x})} \right\} \]  

where \( x = \frac{r}{r_{0}} \), \( \alpha = \sqrt{1 - \frac{2\alpha}{\alpha}} \) and

\[ \Lambda = \frac{\kappa r_{0} - (1 + \alpha)}{\kappa r_{0} + (1 + \alpha)} \]  

(28)

is a parameter with \(-1 < \Lambda < 1\) and determined by \( \kappa \).

3. Results and discussion

We calculate low-energy elastic collisions for Jost–Kohn potentials using the well-known Numerov–Cooley algorithm [30] to verify whether these potentials yield the same scattering length and the asymptotic states. The numerical results obtained for \( V_{r}(r) \) agree absolutely well with any set of chosen parameters \( a_{s} \) and \( r_{0} \) used to construct \( V_{r}(r) \). For \( V_{e}(r) \), the low-energy scattering properties depend on the parameter \( \kappa \) as we discuss below. We further show that, in the limits of \( a_{s} \rightarrow \pm \infty \) and \( \kappa \rightarrow 0 \) or equivalently \( \Lambda ightarrow -1 \), the scattering solutions of Jost–Kohn potentials yield zero-energy resonances. On the other hand, in the limit \( r_{0} \rightarrow 0 \), \( \kappa \rightarrow \infty \) or equivalently \( \Lambda \rightarrow 1 \) and for \( |a_{s}| < \infty \), the solutions of the potentials can reproduce the standard results of zero-range or weak interaction.

3.1. Low-energy expansion of the phase shift yielded by \( V_{r}(r) \)

Though \( V_{e}(r) \) does not support any bound state, it explicitly depends on the parameter \( \kappa \) which determines binding energy \( E_{b} \) of a bound state that is supported by an ‘equivalent’ potential, say \( V_{b}(r) \). The \( S \)-matrix for \( V_{e}(r) \) is \( S = e^{2i\eta} = \tilde{f}(k)/\tilde{f}(-k) \), where \( \eta \) is the phase shift and \( \tilde{f}(k) \) is given by equation (27). It is easy to deduce that in the limit \( \kappa \rightarrow \infty \), \( \eta \) becomes independent of \( \kappa \) and so the phase shift in the low-energy limit will be determined only by \( a_{s} \) and \( r_{0} \). On the
other hand, for small $\kappa$, $\eta$ will depend on all the three parameters $\alpha_s$, $r_0$ and $\kappa$. As given by equation (24), we have

$$\eta(k) = \eta(k) - 2\tan^{-1}\left(\frac{\kappa}{k}\right)$$

(29)

where $\eta(k)$ corresponds to $V_0(r)$ and is assumed to have an effective range expansion in terms of $\alpha_s$ and $r_0$ as in equation (18) but for $\alpha_s > 0$. The expression (29) shows that, for $\kappa \rightarrow 0$ and $k \rightarrow 0$, $\eta = \eta - \pi$. So, both the potentials $V_0(r)$ and $V_{\kappa}(r)$ will yield the same s-wave scattering cross section at low energy. The question here is how $\kappa$ affects the effective range expansion.

From equation (29), we obtain

$$k \cot\eta(k) = \frac{1}{\alpha_s} + \frac{1}{2} \bar{r}_0 k^2 + ...$$

(31)

where

$$\bar{r}_0 = \frac{a_s}{\alpha_s} \left(\frac{1}{\kappa}\right) \left[\kappa r_0 - 4 + \frac{1}{2\kappa a_s} + \frac{1 - 2r_0\kappa}{4 - 4\kappa a_s}\right]$$

(33)

where $\bar{r}_0$ is the modified range. From this formula, it is clear that $\bar{r}_0$ is negative but $\bar{a}_s > 0$ for $\kappa r_0 \ll 1$ and $\alpha_s > 2$. On the other hand, $\bar{a}_s < 0$ for $\kappa a_s < 2$. So, for $\kappa a_s < 1$, $\bar{r}_0$ may vary from positive to negative values as $\kappa r_0$ changes from small ($< 1$) to large values ($> 1$). The negativity of $\bar{r}_0$ may be interpreted as resulting from the breakdown of the standard effective range expansion due to the proximity of a zero-energy resonance as we describe in the next subsection. In the

In this subsection we first calculate the scattering phase shift and cross section as a function of collision energy $E$ or wave number $k$ for Jost–Kohn potentials. Zero-energy resonance occurs when $\eta(0) = \pi/2$, that is, the s-wave phase shift at $k = 0$ is $\pi/2$. This happens if $f(0) = 0$, physically this implies that the potential is about to support a bound state at an energy given by $f(k = 0) = 0$ if the potential is slightly modified. This follows from the fact that there exists no bound state at zero energy for s-wave unlike that at higher partial waves. A bound state for s-wave can exist only at finite energy, in which case $f(0) \neq 0$ and $\eta(0) = \pi$ [19].

From the effective range expansion, it follows that for $\alpha_s \rightarrow -\infty$, we have $\eta(0) \rightarrow \pi/2$. Since $V_{\kappa}(r)$ is derived based solely on the effective range expansion, one would expect that numerically calculated phase shift for $V_{\kappa}(r)$ should reproduce this result. In fact, the calculated phase shift as plotted in figure 1 shows this expected behavior.

The Jost function corresponding to the potential $V_{\kappa}(r)$ is given by $\tilde{f}(k)$ of equation (27). One can notice that $f(0) = 0$ if $\kappa \neq 0$. In this case, in the limit $k \rightarrow 0$, the S-matrix $S(k) = f(k)/\tilde{f}(-k)$ approaches infinity and so the phase shift $\eta(0) \rightarrow \pi$. On the other hand, for $\kappa = 0$, $\alpha_s = \infty$, we have $S(k \rightarrow 0) \rightarrow -1$. The expression equation (31) shows that for $\kappa a_s < 2$, $k \rightarrow 0$, $\alpha_s \rightarrow \infty$ with $ka_s > 1$, we have $\cot\eta(k) \rightarrow 0$, implying that $\eta(k \rightarrow 0) = \pi/2$. Therefore the system exhibits zero-energy resonance. In figure 2, we have plotted the s-wave scattering cross sections $\sigma_0(E)$ as a function of dimensionless energy $E/E_0$ in the resonance limit. Consequently $\sigma_0(E)$, shows a divergent signature in the limit $E \rightarrow 0$ as in figure 2. From the inset of figure 2, it is clear that the phase shift goes to $+\pi/2$ as $\kappa \rightarrow 0$. In this context, it is
different values of $\kappa$ are shown in the inset. The corresponding phase shifts are shown as a function of $k/\kappa_0$ for different values of $\kappa$. This low-energy behavior of $\eta(E)$ is consistent with that of a contact or weak interaction potential.

Having shown that the Jost–Kohn potentials can describe the standard low-energy scattering properties of a pair of ultracold atoms in free space, we now discuss whether these potentials are good enough to model the interaction between a pair of trapped atoms. There exists an exact solution for a pair of ultracold atoms interacting via a regularized contact potential in a 3D isotropic harmonic oscillator [38]. Several theoretical studies [39] have shown that this exact solution is good enough so long as $|a_s|$ is much smaller than the characteristic length scale or more specifically the size of the ground state of the isotropic harmonic oscillator. In a previous study [40], it has been demonstrated that the bound state solutions of a pair of ultracold atoms interacting via Jost–Kohn potentials in an isotropic harmonic oscillator can qualitatively reproduce the results of [38] when $r_0$ is much smaller than the harmonic oscillator length scale provided $a_s$ is small enough. Also, for a quasi-one-dimensional trap, Jost–Kohn potentials are shown to agree qualitatively with the results of a contact interaction only when $r_0$ is much smaller than the length scale of the transverse 2D harmonic oscillator and small $a_s$ [40].

3.3. Zero-range limit of Jost–Kohn potentials

Jost–Kohn potentials do not explicitly reduce to a delta-function like zero-range contact potential in the limit $r_0 \to 0$. The derivation of $V_+(r)$ makes use of the assumption $a_s > 2r_0$.

Here we numerically verify whether the Jost–Kohn potentials reproduce the known results of weak interaction regime (small $|a_s|$) in the limit $r_0 \to 0$. In figure 3, we show the variation of scattering cross section as a function of energy, for large $\kappa$. Here, the quantity $\sigma_0(E)/4\pi a_s^2$ nearly equals unity at a very low energy limit. We have verified this limit for different values of $\kappa$ and scattering lengths. The inset of figure 3 exhibits the behavior of the phase shift at the limit $E \to 0$. We note that $\eta(E \to 0) \propto \pm \sqrt{E}$, where $\pm$ corresponds to negative(positive) $a_s$. This low-energy behavior of $\eta(E)$ is consistent with that of a contact or weak interaction potential.

3.4. Feshbach resonances

Here we discuss to what extent and under what physical conditions it may be possible to describe Feshbach-resonant interactions between ultracold atoms by Jost–Kohn potentials. Feshbach resonance is a multi-channel scattering problem where a quasi-bound state supported by one or multiple closed channels is made degenerate or quasi-degenerate with the bare scattering state of at least one open channel by means of an external magnetic or optical field. As a consequence, a Feshbach resonance occurs due to an admixture of bound and
continuum states leading to a dressed continuum which can also be dealt with by Fano’s method [41, 42]. If there is only one open channel, then the physical S-matrix derived upon elimination of all the closed channels corresponds to the open channel only. If the experimentally determined phase shift corresponding to this effective single-channel physical S-matrix element admits an effective range expansion with the effective range \( r_f \) (we use different notation for the effective range of the Feshbach resonance to distinguish it from \( r_0 \) that corresponds to Jost–Kohn potentials) then the method of Jost and Kohn will be definitely applicable to this effective single-channel problem. The pertinent question here is how to reduce a multi-channel scattering problem into an effective single-channel one describable by the Jost–Kohn potentials.

In the current literature on magnetic Feshbach resonances [5, 6] of ultracold atoms, the resonances are mainly categorized into two types depending on the width of the resonance: narrow or open channel dominated and broad or open channel dominated. The width of a Feshbach resonance is quantified by the dimensionless strength parameter defined by

\[
\delta \mu = \frac{\delta \mu \Delta a_{bg}}{E} \quad \text{where } \delta \mu \text{ is the difference between the magnetic moments of the bare quasi-bound state and the two separated atoms, } a_{bg} \text{ is the background scattering length and } \Delta \text{ in units of magnetic field strength is the width of the resonance.}
\]

For a potential behaving asymptotically as \(-\frac{C_6}{r^6}\), with \( C_6 \) being the van der Waals’ coefficient, Gribakin and Flambaum [43] defined a length called the mean scattering length \( a = \frac{2 \pi}{\Gamma_{rf} \sqrt{2}} \left( \frac{2 a_{bg}}{\Delta} \right)^{1/4} \), and corresponding energy scale \( E = \frac{\hbar^2}{2 a^2} \). A narrow or closed-channel-dominated resonance occurs when \( s_{res} < 1 \) while for a broad or entrance-channel-dominated resonance, \( s_{res} > 1 \). Gao [44] and Flambaum et al [24] have defined an effective range \( R_e \) for asymptotic van der Waals potential by

\[
R_e \approx \frac{\left( \frac{\Gamma_{rf}}{\hbar \Gamma_{rf}} \right)}{2 \pi a_{bg}} \left( 1 - 2 \left( \frac{a}{a_{bg}} \right)^2 \right) \tag{1}
\]

The \( r_f \) dependence of a narrow Feshbach resonance has been shown to be quite different from that of a broad Feshbach resonance [45]. It has been further demonstrated, both theoretically [9] and experimentally [11, 12], that \( r_f \) near a narrow Feshbach resonance may become quite large, negative and magnetic field dependent. The experimental observation [12] shows that near the narrow Feshbach resonance (\( B_0 = 58.9 \text{G} \) of \(^{6}\text{Li} \)) the effective range sharply changes with scattering length (or magnetic field) and the effective range is found to be large negative in the vicinity of this Feshbach resonance. For the case of \(^{6}\text{Li} \) NFR near 543.3G, similar results are found [11]. In contrast, \( r_f \) near a broad Feshbach resonance is usually positive, small and close to \( R_e \). In the case of an intermediate-range Feshbach resonance (\( s_{res} \sim 1 \)), quite interesting field dependence of \( r_f \) has been experimentally demonstrated [11]. From the analysis made in section 3.2, we understand that the effective range of the resonant interaction with \( a_0 > 0 \) may be controlled by the parameter \( \kappa \) of the potential \( V_f \).

In the case of \( a_0 < 0 \), the model Jost–Kohn potential \( V_f(r) \) has only two parameters, \( r_0 \) and \( a_e \), and so it is straightforward to model a Feshbach resonance by using these two parameters as fitting parameters provided the Feshbach resonance phase shift \( \eta_f \) admits an effective range expansion with \( r_f > 0 \). Then \( r_0 = r_f \) and the Feshbach-resonant scattering length is the same as in \( V_f(r) \). In fact, even in the case of a narrow Feshbach resonance, \( r_f \) is found to be positive in the regime of negative \( a_e \) in many ultracold atomic species [11]. However, in the case \( a_e > 0 \), we need three parameters: the third parameter \( \kappa \) determines the binding energy of the bound state of an equivalent potential. In order to discuss how to model Feshbach-resonant interaction with \( V_f(r) \), it may be instructive to recall the salient features of two-channel model of Feshbach resonances [26] which has found considerable applications in modeling magnetic Feshbach resonances (MFRs) of ultracold atoms [5].

In the two-channel model, the lower channel is open and the upper channel is closed, meaning that the asymptotic collision energy is above the threshold of the open channel but below the threshold of the closed channel. The closed channel is assumed to support a bound state \( \psi_b(r) \) with binding energy \( E_b \). There is a coupling \( W(r) \) between the two channels. The S-matrix for the open channel is given by

\[
S(k) = \exp[2i\eta_{bg}(k)] \frac{E - E_f - E_{\text{shift}} - i \hbar \Gamma_f/2}{E - E_f - E_{\text{shift}} + i \hbar \Gamma_f/2} \tag{34}
\]

where \( \eta_{bg} \) is a non-resonant background phase shift, \( E_{\text{shift}} \) is a shift of the closed-channel bound state due to its coupling with the bare scattering state of the open channel and \( \Gamma_f \) is the Feshbach resonance width defined by

\[
\Gamma_f = 2\pi \int |\psi_E(r)W(r)\psi_E(r)|^2 dr \tag{25}
\]

where \( \psi_E(r) \) is the bare scattering state of the open channel at collision energy \( E \). The resonance phase shift \( \eta_f \) is given by

\[
\cot \eta_f = \frac{E - \dot{E}_c}{\hbar \Gamma_f/2} \tag{35}
\]

where \( \dot{E}_c = E_c + E_{\text{shift}} \). The total phase shift is \( \eta = \eta_{bg} + \eta_f \). Therefore, we have

\[
\cot \eta = \frac{\cot \eta_{bg} \cot \eta_f - 1}{\cot \eta_{bg} + \cot \eta_f} \tag{36}
\]

Considering \( \eta_{bg} \) to be small, one may approximate \( \cot \eta_{bg} \sim -1/\kappa a_{bg} \) where \( a_{bg} \) is the background scattering length. This approximation is particularly good for a narrow resonance. At low energy, \( \Gamma_f \) may be proportional to \( k \), because the energy-normalized scattering wave function asymptotically behaves as \( \psi_E(r) \sim \sqrt{k} r \). This will happen if \( W(r) \) is most prominent beyond the range of the open channel potential. Under these conditions, we may write

\[
\frac{1}{a_r} = -\lim_{k \to 0} \frac{2\kappa \dot{E}_c}{\hbar \Gamma_f} \tag{37}
\]

and

\[
r_f = -\lim_{k \to 0} \frac{2/k}{\mu \Gamma_f} \tag{38}
\]
In an MFR, the energy \( E_r \) of the quasi-bound state is magnetically tuned across the threshold of the open channel. The resonant scattering length \( a_s \) is negative (positive) if \( E_r \) is positive (negative). The resonance at zero energy occurs when \( E_r \) is zero, in which case \( a_s \to \infty \).

From equation (36), we can obtain \( k \cot \eta \simeq -1/a_s + (1/2) rf k^2 \) where \( \frac{1}{a_s} = \frac{1}{a} \left( 1 - \frac{a_{bg}}{a} \right) \) and

\[
r_f = 2a_{bg} \left( 1 + \frac{r_s}{r_s} - \frac{a_{bg}}{a_s} \right) + r_s.
\]

Close to resonance, \( |a_{bg}| \ll |a_s| \). Writing \( \Gamma_f \simeq kG \), where \( G \) is a constant, we note that the parameter \( r_f \) is inversely proportional to \( G \). Therefore, \( r_f \) will be large for small \( G \) or for a narrow resonance. Let us now assume that \( a_{bg} > 0 \) and consider the case \( a_s > 0 \). For a broad resonance, usually \( r_f \) is positive and small. This means that for a broad resonance \( \kappa \) should be large and we may set \( r_s \approx r = r_f \). In the case of a far-off resonance, we may set \( \kappa \to \infty \) and \( r_0 = R_e \). In the case of a narrow resonance, the parameter \( \kappa \) can be used to control the deviation of \( r_f \) from \( R_e \). For a magnetic field very close to a resonant magnetic field at which \( a_s \to +\infty \), we can safely assume that \( \kappa a_s \gg 2 \) so that \( a_s \approx a_s \) as follows from equation (32). Then the value of \( \kappa \) can be set by equating equation (33) with the experimentally observed \( r_f \) assuming \( r_0 = R_e \). The negative effective range can be mimicked by making \( \kappa a_s < 4 \). In the universality regime [5], \( a_s = 1/\kappa \), implying that for \( a_{bg} > 0 \) and \( a_{bg} \ll a_s \), \( \Gamma_f \propto k \kappa \) which will happen if the bound state behaves as \( e^{-k} \). This means that inter-channel coupling should predominantly occur in the asymptotic limit of the bound state. Then \( r_f \approx \frac{1}{\kappa} \); therefore in the limit \( \kappa \to 0 \), \( r_f \) will be large and the effective range \( r_f \) as given by equation (39) will be negatively large, indicating the breakdown of the effective range expansion. A universality regime is found to occur mostly in broad Feshbach resonances for which it has been shown that nonlinear energy dependence of the phase shift even very close to zero energy becomes important, suggesting that effective range expansion may fail at the universality regime [9].

To illustrate quantitatively how the effective range of equation (39) can be fixed from a two-channel Feshbach resonance model, and thereby energy or magnetic field dependence of the scattering \( T \)-matrix element \( T(k) = 1 - S(k) \) (where \( S(k) \) is the \( S \)-matrix element) can be described by an effective one-channel Jost–Kohn potential, we consider magnetic Feshbach resonance of ultracold \(^{40}\)K atoms near magnetic field \( B = B_0 = 202.1 \) G as experimentally observed by Regal et al [46]. The modeling of this MFR by a two-channel model has been discussed in detail by Nygaard, Schneider and Julienne [47]. The parameter \( r_s \) can be determined from equation (38) by replacing \( \Gamma_f \) by \( 2\Delta(b_0^s)ka_{bg} \) [47] where \( \Delta = 7.788 \) G is the width of zero crossing, \( a_{bg} = 172.06a_0 \) and \( b_0^s = 1.68\mu_B \left( a_0 \right) \), \( \mu_B \) being Bohr radius and Bohr magneton, respectively) [5, 46] is the difference between the magnetic moments of the quasi-bound state and the two free atoms. We thus find \( r_s = -32.15a_0 \). Taking \( a_s \) to be very large corresponding to \( E_r \approx 0 \), we have \( r_0 = r_f \approx 2a_{bg} + r_s = 283.7a_0 \). We show in figure 4 the energy dependence of the square of the absolute value of the \( T \)-matrix and the phase shift, which qualitatively agree well with those obtained by R-matrix method in [47].

4. Conclusions

The foregoing analysis on the Jost–Kohn potentials reveal that these potentials can account for collision physics near-zero-energy resonances with finite-range effects as can be exhibited by Feshbach resonances of ultracold atoms in certain physical situations. We have shown that the finite-range effects displayed by the phase shift corresponding to the potential \( V_s(r) \) critically depends on the relative strength of the parameters \( \kappa a_s \) and \( \kappa a_s \), where \( r_0 > 0 \) and \( a_s \) correspond to an equivalent potential with \( \kappa \to \infty \). However, in the limit \( \kappa \to 0 \) the effective range and the scattering length obtained by effective range expansion of the phase shift are drastically modified. We have shown that the physical origin of the modification can be identified with a zero-energy resonance. A zero-energy resonance for \( s \)-wave occurs when the potential is about to support a bound state. By construction, \( V_s(r) \) does not support any bound state but has parametric dependence on the bound state energy. For \( \kappa a_s < 1 \) and \( \kappa a_s > 2 \), the modified effective range \( \tilde{r}_0 \) is found to be negative although the modified scattering length \( a_s \) remains positive. On the other hand, \( \tilde{r}_0 \) is positive for \( \kappa a_s < 1 \). In both cases \( \tilde{r}_0 \) can become quite large if \( \kappa a_s \ll 1 \). Thus, according to the theory of Jost and Kohn, it is possible to construct a model potential which has no bound state but can provide the resonant scattering effects which may be induced by bringing a bound state close to the threshold of the potential as in the case of Feshbach resonances. We have also shown that \( V_s(r) \) can describe a universality regime where \( a_s = 1/\kappa \) but then \( \tilde{r}_0 \) becomes negative and large.
Under appropriate limiting conditions, as mentioned earlier, Jost–Kohn potentials reduce to the Pöschl–Teller form, which has been extensively used for quantum Monte Carlo simulation of many-body effects of a Fermi gas of atoms for \( a_i \to -\infty \) \[33–37\]. Therefore, the use of Jost–Kohn potentials in quantum simulation will open a broad perspective of \( s \)-wave many-body physics of atomic gases. For a homogeneous many-particle system, many-body theories are conveniently developed in momentum-space under a second quantization formalism where a model pseudo-potential with an energy- or momentum-dependent phase shift may be applicable in order to explore effective range effects. However, for inhomogeneous systems like tightly confined atomic gases, such momentum-dependent description is not appropriate. So, Jost–Kohn potentials discussed in this paper will be particularly useful for developing many-body physics of trapped atomic gases. Finally, we like to note that the Jost–Kohn potentials may also describe low-energy \( s \)-wave collisional physics of a charged particle interacting with a neutral polarizable particle such as ion-atom cold collisions for which the interaction potential asymptotically goes as \(-1/r^4\). This is because such potentials also admit \( s \)-wave effective range expansion, though the method of expansion is different from that of the usual short-range or long-range potentials that go as \( \sim 1/r^n \) with \( n > 5 \) as shown by O’Malley, Spruch and Rosenberg more than 50 years ago \[48\].

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Appendix A. Derivation of negative \( a_s \) potential

Now the first-order potential \( U_1(r) \) is evaluated as

\[
\chi r U_1(r) = \frac{1}{2i} \int_{-\infty}^{\infty} e^{iz} \frac{d}{dz} [g(z) - 1] dz = 2a^2 \chi e^{-ar} \tag{A.1}
\]

or

\[
U_1(r) = 2a^2 e^{-ar} \tag{A.2}
\]

\[
\int_{0}^{\infty} e^{-ar} U_2(r) dr = 2a^2 \int_{0}^{\infty} \left( \frac{1}{z + a} + \frac{1}{z + 2a} \right) \tag{A.4}
\]

so that after the inverse Laplace transformation

\[
U_2(r) = 2a^2 (-e^{-ar} + 2e^{-2ar}) \tag{A.5}
\]

similarly

\[
U_3(r) = 2a^2 (e^{-ar} - 4e^{-2ar} + 3e^{-3ar}) \tag{A.6}
\]

Finally, the whole potential is given by equation (21)

\[
U_\infty(r) = \chi U_1(r) + \chi^2 U_2(r) + \chi^3 U_3(r) + \ldots
\]

where, \( \chi \) may be applicable in order to explore effective range effects.

Appendix B. Derivation of positive \( a_s \) potential

Based on the Gel’fand–Levitan theory \[18\], Jost and Kohn derived a four-parameter potential \( V(r) \) for \( a_i > 0 \), where the four parameters are \( a_s, m, \kappa \) and the normalization constant \( C \) of a single bound state assuming that the potential is capable of supporting only one bound state. The Jost function for \( V(r) \) is

\[
f(k) = \frac{4(k^2 + \kappa^2)}{(2k + ib)(2k - ia)} \tag{B.1}
\]

so that the bound state is given by \( k = -i\kappa \), which is a zero of \( f(k) \).

\[
\sum_{l=1}^{m} \int_{r_1}^{\infty} dr_1 \int_{r_1}^{\infty} dr_2 \ldots \int_{r_{n-1}}^{\infty} dr_{n-1} \frac{1}{z} \times (1 - e^{-iz}) (1 - e^{-z(r_2 - r_1)}) \ldots (1 - e^{-z(r_n - r_1)}) V(r_1) \times V(r_2) \ldots V(r_n) \tag{B.2}
\]

The function \( g(z) \) is given from equation (25)

\[
\log g(z) = \log \frac{(z + \xi_0)^2}{(z - b)(z + a)} \tag{B.3}
\]

We consider \( \xi_\pm = \kappa \pm i\kappa \), then

\[
g(z) = \frac{(z + \xi_+)(z + \xi_-)}{(z + a)(z - b)} = \frac{(z + \kappa)^2 + k^2}{(z + a)(z - b)} \tag{B.4}
\]
The explicit form of $V_+(r)$ is given by

$$rV_1(r) = \frac{1}{2\pi i} \int_{i\infty}^{i\infty} e^z \frac{d}{dz} \left[\bar{g}(z) - 1\right] dz \quad (B.5)$$

Now substitute $\bar{g}(z)$ in the above equation and we get

$$V_1(r) = C_1 e^{-ar} + C_2 e^{br} \quad (B.6)$$

where $C_1 = -\frac{(\kappa - a^2 + k^2)}{1 + \frac{\kappa}{r}}$ and $C_2 = -\frac{(\kappa + b^2 + k^2)}{1 + \frac{\kappa}{r}}$. With the reference of equation (A.3), next higher-order potential is given by

$$V_2(r) = \left( \frac{C_1 e^{-ar}}{a} - \frac{C_2 e^{br}}{b} \right)^2 - \frac{C_1^2 e^{-2ar}}{2a^2} - \frac{C_2^2 e^{2br}}{2b^2}$$

$$+ \frac{C_1 C_2}{ab(a-b)}(ae^{-ar} - be^{br}) \quad (B.7)$$

Similarly, higher-order terms can be calculated.

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