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2005 J. Phys. A: Math. Gen. 38 4469

(http://iopscience.iop.org/0305-4470/38/20/013)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **38** (2005) 4469–4481 doi:10.1088/0305-4470/38/20/013

Scattering properties for a solvable model with a three-dimensional separable potential of rank 2

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Received 2 November 2004, in final form 30 March 2005
Published 3 May 2005
Online at stacks.iop.org/JPhysA/38/4469

Abstract

The scattering by a three-dimensional separable potential of rank 2 is described analytically. The model potential is chosen so that the Lippmann–Schwinger equation can be exactly solved and all calculations are carried out analytically. The explicit expressions for a number of scattering properties, such as phase shifts, cross sections, T- and S-matrices, resonances and poles of the resolvent are calculated. The second virial coefficient is also evaluated in terms of phase shifts and bound state energies for the particular potential model presented.

PACS number: 03.65.Nk

1. Introduction

Exactly solvable models have played an important role in understanding many anomalous aspects of scattering theory, and in the investigations of the reliability of hypothesis therein. A convenient description of collision of a wavepacket, initially a Lorentzian-like function in momentum representation, with a Dirac delta function potential is given by Elberfeld and Kleber [1]. Scattering by a separable potential of rank 1 in one dimension was also studied in previous works [2, 3]. In order to find an explicit wavefunction and resonance scattering, the time-dependent collision of an initial Lorentzian-type state with a one-dimensional separable potential model has recently been solved analytically in terms of wavepackets [4]. Some applications of separable potentials to the solution of various problems have been studied by other investigators [5–12]. In this paper, we use a solvable model of three-dimensional separable potential of rank 2 to obtain explicit analytical results which may provide a better starting point for more realistic treatments.

2. Separable potential

The nonlocal separable potentials are used more widely in the areas of nuclear and condensed matter than in other fields of physics. These potentials have proven to be useful in the study

of few-nucleon problems, particularly in the determination of the three-body binding energy using a two-body separable potential model. A separable potential model can generally be written as [13, 14]

$$\hat{V} = \sum_{i=1}^{n} |\chi_i\rangle v_i \langle\chi_i| \tag{2.1}$$

where n is the rank of the potential operator $\hat{V}$, $|\chi_i\rangle$ is the state of the system, which is compatible with the domain of Hamiltonian and v_i is the potential strength, which is a real number in the unitary case. General properties of separable potential have been examined by Ghirardi and Rimini [15]. Such a potential has some advantages, which are briefly discussed here: (i) it can be shown that the Schrödinger equation, $\hat{H}|\Psi_E\rangle = E|\Psi_E\rangle$, reduces to an algebraic equation in momentum space; (ii) the scattering matrix is diagonal for any symmetric and antisymmetric combinations of plane waves; (iii) the transmission, reflection and absorption coefficients can be written in terms of phase shifts; (iv) the potential allows all quantities of interest, such as resonance energy, life time, phase shift, etc, to be expressed in a completely analytical form. It can also serve as a checking point for scattering formulae. (v) It is well known that almost all short-range potential models can be accurately approximated by separable ones of a certain rank [16].

In this work, we consider the separable potential model of rank 2 ($n = 2$)

$$\hat{V} = |\chi_1\rangle v_1 \langle\chi_1| + |\chi_2\rangle v_2 \langle\chi_2|. \tag{2.2}$$

For a particular choice of $|\chi_i\rangle$, we use a three-dimensional Lorentzian-like function in momentum representation as follows:

$$\chi_i(\boldsymbol{p}) \equiv \langle \boldsymbol{p}|\chi_i\rangle = \frac{a_i^{1/2}}{\pi} \frac{1}{a_i^2 + p^2} \qquad (i = 1, 2) \tag{2.3}$$

where the momentum parameters a_1 and a_2 play the role of scale factors. This interaction model acts in the s-waves only. It was shown that the rank-2 potential with Yamaguchi form factor leads to algebraic expressions for most quantities of interest [17]. In configuration space, $|\chi_i\rangle$ has the Yukawa form as

$$\chi_i(\boldsymbol{r}) \equiv \langle \boldsymbol{r}|\chi_i\rangle = \frac{a_i^{1/2}}{2h^{1/2}} \frac{\mathrm{e}^{-a_i r/\hbar}}{r} \qquad (i = 1, 2) \tag{2.4}$$

which depends only on $r \equiv |\boldsymbol{r}|$ and is independent of direction of $\boldsymbol{r}$. Therefore, due to the use of a Lorentzian-like potential model (2.3), the problem becomes restricted to the s-wave separable potentials. The angular contribution to the integral is a factor of 4π.

3. The scattering states

The Lippmann–Schwinger equation for the scattering state associated with the incident plane wave $|\varphi\rangle$ is as follows:

$$|\psi_z\rangle = |\varphi\rangle + \frac{1}{z - \hat{H}_0} \hat{V} |\psi_z\rangle \tag{3.1}$$

where $\hat{H}_0$ is, generally, the reference Hamiltonian in the absence of the separable potential and $z \equiv E + \mathrm{i}\varepsilon$ is the complex energy parameter, wherein the energy E is the eigenvalue of $\hat{H}_0$, $\hat{H}_0|E\rangle = E|E\rangle$. In our present work, the reference Hamiltonian $\hat{H}_0$ is the free kinetic energy operator.

The components of the scattering wavefunction in the χ_1 and χ_2 directions can be obtained from the following system of equations:

$$\begin{cases} \big(v_1 Q_{11}^0 - 1\big)\langle\chi_1|\psi_z\rangle + v_2 Q_{12}^0\langle\chi_2|\psi_z\rangle + C_1 = 0 \\ v_1 Q_{21}^0\langle\chi_1|\psi_z\rangle + \big(v_2 Q_{22}^0 - 1\big)\langle\chi_2|\psi_z\rangle + C_2 = 0 \end{cases} \tag{3.2}$$

where C_i $(i = 1, 2)$ is the inner product $\langle\chi_i|\varphi\rangle$ and the matrix elements of free motion resolvent are defined for any complex z as

$$Q_{ij}^0(z) \equiv \langle\chi_i|\frac{1}{z - \hat{H}_0}|\chi_j\rangle \qquad (i, j = 1, 2). \tag{3.3}$$

Solution of equation (3.2) leads to

$$B_j \equiv \langle\chi_j|\psi_z\rangle = C_j + \sum_l v_l Q_{jl}^0 B_l \tag{3.4}$$

or in matrix form

$$\begin{pmatrix} B_1 \\ B_2 \end{pmatrix} = \frac{1}{D}\begin{pmatrix} 1 - v_2 Q_{22}^0 & v_2 Q_{12}^0 \\ v_1 Q_{21}^0 & 1 - v_1 Q_{11}^0 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} \tag{3.5}$$

where

$$B = (1 - Q^0 v)^{-1} C, \tag{3.6}$$

$$C = \begin{pmatrix} \langle\chi_1|\varphi\rangle \\ \langle\chi_2|\varphi\rangle \end{pmatrix}, \tag{3.7}$$

$$v = \begin{pmatrix} v_1 & 0 \\ 0 & v_2 \end{pmatrix}, \tag{3.8}$$

and

$$D = \big(1 - v_1 Q_{11}^0\big)\big(1 - v_2 Q_{22}^0\big) - v_1 v_2 Q_{12}^{0^2}. \tag{3.9}$$

The matrix elements $Q_{ij}^0(z)$ of the free motion resolvent of equation (3.3) can be obtained in the upper half q-plane as

$$Q_{ij}^0(q) = 2m\int_C \frac{\chi_i^*(\boldsymbol{p})\chi_j(\boldsymbol{p})}{(q^2 - p^2)}\,\mathrm{d}\boldsymbol{p} = \frac{4m(a_i a_j)^{1/2}}{(a_i + a_j)(q + ia_i)(q + ia_j)} \tag{3.10}$$

where $q \equiv \sqrt{2mz}$.

It is convenient to use the dimensionless variables (position, momentum and energy) denoted here with a tilde, which are related to the corresponding dimensional quantities, in the following expressions:

$$\tilde{q} = q/\bar{a}; \qquad \tilde{p} = p/\bar{a}; \qquad \tilde{a}_i = a_i/\bar{a}; \qquad \tilde{r} = \frac{\bar{a}}{\hbar}r; \qquad \tilde{v}_i = \frac{m v_i}{a_i^2}$$

where the parameter $\bar{a}$ is the average of a_1 and a_2, i.e. $\bar{a} \equiv \frac{a_1 + a_2}{2}$. The matrix elements of $Q_{ij}^0(q)$ and $B_i(q)$ in terms of dimensionless quantities are given by

$$Q_{ij}^0(\tilde{q}) = \frac{2m(\tilde{a}_i\tilde{a}_j)^{1/2}}{\bar{a}^2(\tilde{q} + i\tilde{a}_i)(\tilde{q} + i\tilde{a}_j)} \tag{3.11}$$

$$B_i(\tilde{q}) = D^{-1}\frac{1}{\pi\bar{a}^{3/2}}\left[(1 - w_j)\frac{\tilde{a}_i^{1/2}}{\big(\tilde{q}^2 + \tilde{a}_i^2\big)} + \frac{2\tilde{v}_j\tilde{a}_j^3\tilde{a}_i^{1/2}}{(\tilde{q} + i\tilde{a}_i)(\tilde{q} + i\tilde{a}_j)\big(\tilde{q}^2 + \tilde{a}_j^2\big)}\right] \qquad (j \neq i) \tag{3.12}$$

where

$$w_j = \frac{2\tilde{v}_j \tilde{a}_j^2 (\tilde{a}_i \tilde{a}_j)^{1/2}}{(\tilde{q} + i\tilde{a}_j)(\tilde{q} + i\tilde{a}_i)} \qquad (i \neq j) \tag{3.13}$$

$$D = (1 - w_1)(1 - w_2) - \tilde{a}_1 \tilde{a}_2 w_1 w_2. \tag{3.14}$$

In the momentum representation, the scattering wavefunction $\psi_z(\boldsymbol{p}) \equiv \langle \boldsymbol{p}|\psi_z\rangle$ can be evaluated by using the model potential (2.2) and equation (3.1) as

$$\begin{aligned}\psi_z(\boldsymbol{p}) &= \varphi(\boldsymbol{p}) + \sum_{i=1}^{2} v_i \int\int_c \langle \boldsymbol{p}| \frac{1}{\hat{z} - \hat{H}_0} |\boldsymbol{p}'\rangle \chi_i(\boldsymbol{p}') \chi_i^*(\boldsymbol{p}'') \psi_z(\boldsymbol{p}'')\, \mathrm{d}\boldsymbol{p}'\, \mathrm{d}\boldsymbol{p}'' \\ &= \varphi(\boldsymbol{p}) + \sum_{i=1}^{2} \frac{2\tilde{a}_i^{5/2}\tilde{v}_i}{\pi} \frac{B_i(\tilde{q})}{(\tilde{q}^2 - \tilde{p}^2)\left(\tilde{a}_i^2 + \tilde{p}^2\right)}\end{aligned} \tag{3.15}$$

where the q contour C goes from $-\infty$ to $+\infty$ passing above all the singularities of the resolvent. The scattering wavefunction $\psi_z(\boldsymbol{p})$ is clearly independent of any direction of incident beam, since the potential model acts on the s-wave only. Furthermore, the energy E, physically, should be the same as the energy of the incoming wave. This is satisfied if $\varphi(\boldsymbol{p}) \propto \delta(p - p')$, with p' the same as that associated with E, where $\delta(p - p')$ is the Dirac delta function and $p \equiv |\boldsymbol{p}|$. Hence, it may be written as

$$\psi_z(\tilde{p}) = \delta(\tilde{p} - \tilde{p}') + \sum_{i=1}^{2} \frac{2\tilde{a}_i^{5/2}\tilde{v}_i}{\pi} \frac{B_i(\tilde{q})}{(\tilde{q}^2 - \tilde{p}^2)\left(\tilde{a}_i^2 + \tilde{p}^2\right)}. \tag{3.16}$$

Thus, the corresponding coordinate representation can be obtained by a Fourier transformation, so we have

$$\psi_z(\tilde{r}) = \mathrm{e}^{\mathrm{i}\tilde{p}'\tilde{r}} - \frac{2\bar{a}^{3/2}}{D\pi} \sum_{i=1}^{2} \beta_i \left[\frac{\mathrm{e}^{\mathrm{i}\tilde{q}\tilde{r}}}{\tilde{r}} + \frac{\mathrm{e}^{-\tilde{a}_i\tilde{r}}}{\tilde{r}} \right] \tag{3.17}$$

where

$$\beta_i = \frac{(1 - w_j)\tilde{a}_i w_i}{(\tilde{q} - i\tilde{a}_i)^2} + \frac{\tilde{a}_i \tilde{a}_j w_i w_j}{(\tilde{q} - i\tilde{a}_i)(\tilde{q} - i\tilde{a}_j)} \qquad (j \neq i). \tag{3.18}$$

The asymptotic behaviour (large distance from the origin) of $\psi_z(\tilde{r})$ then reads

$$\psi_z(\tilde{r}) \to \mathrm{e}^{\mathrm{i}\tilde{p}'\tilde{r}} - \frac{2\bar{a}^{3/2}(\beta_1 + \beta_2)}{\pi D} \frac{\mathrm{e}^{\mathrm{i}\tilde{q}\tilde{r}}}{\tilde{r}} \qquad (r \to \infty). \tag{3.19}$$

Comparing equation (3.19) with the following equation:

$$\psi_z(\tilde{r}) \to \mathrm{e}^{\mathrm{i}\tilde{p}'\tilde{r}} - f(\tilde{q}) \frac{\mathrm{e}^{\mathrm{i}\tilde{q}\tilde{r}}}{\tilde{r}} \qquad (r \to \infty) \tag{3.20}$$

gives the scattering amplitude $f(\tilde{q})$ as

$$f(\tilde{q}) = -\frac{2\bar{a}^{3/2}(\beta_1 + \beta_2)}{\pi D}. \tag{3.21}$$

4. Transition and scattering matrices

We turn now to investigate the analytical properties of the transition and scattering matrices in the complex q-plane. The transition matrix $\hat{T}$ is connected to the Møller wave operator $\hat{\Omega}$ as

$$\hat{T} = \hat{V}\hat{\Omega} \tag{4.1}$$

where the Møller wave operator $\hat{\Omega}$ is an operator by which a free state changes into the scattering one

$$\hat{\Omega} = 1 - \mathrm{i}\int_{-\infty}^{0} \exp(\mathrm{i}\hat{H}t)\,\hat{V}\exp(-\mathrm{i}\hat{H}_0 t)\,\mathrm{d}t \tag{4.2}$$

where $\hat{H} = \hat{H}_0 + \hat{V}$ is the interacting Hamiltonian, in which $\hat{H}_0$ is the free Hamiltonian. By introducing the convergence factor $\mathrm{e}^{\mathrm{i}\varepsilon t}$ with positive real ε, the convergence of the infinite time appeared in equation (4.2) can be enhanced. For this purpose, the parametrized Møller operator can be defined as

$$\hat{\Omega}_\varepsilon = 1 - \mathrm{i}\int_{-\infty}^{0} \exp(\mathrm{i}\hat{H}t)\,\hat{V}\exp[-\mathrm{i}(\hat{H}_0 + \mathrm{i}\varepsilon)t]\,\mathrm{d}t. \tag{4.3}$$

Therefore, the operator has the domain of applicability that exceeds that of the abstract Møller operator. The parametrized form of the Møller operator is, for finite ε, well defined when acting on an eigenstate of $\hat{H}_0$; $\hat{H}_0|E\rangle = E|E\rangle$. Since the action of $\hat{H}_0$ reduces the scalar energy E, the parametrized Møller operator reduces to the complex number parametrized Møller operator $\hat{\Omega}(z)$ as

$$\hat{\Omega}_\varepsilon|E\rangle = \Omega(E + \mathrm{i}\varepsilon)|E\rangle. \tag{4.4}$$

Thus, the complex number parametrized Møller operator can be represented as

$$\hat{\Omega}(z) = 1 + (z - \hat{H})^{-1}\hat{V} = 1 + (z - \hat{H}_0)^{-1}\hat{V}\hat{\Omega}(z) \tag{4.5}$$

where $z \equiv E + \mathrm{i}\varepsilon$. The operator $\hat{\Omega}(z)$ converges to abstract Møller operator $\hat{\Omega}$ as ε goes to 0. Defining the interacting resolvent $\hat{Q} \equiv (z - \hat{H}^{-1})$ and free motion resolvent $Q^0 \equiv (z - \hat{H}_0)^{-1}$, it can be easily shown that the parametrized Møller operator can be rewritten as

$$\hat{\Omega}(z) = \hat{1} + (\hat{1} - \hat{Q}^0\hat{V})^{-1}\hat{Q}^0\hat{V}. \tag{4.6}$$

Therefore, the transition matrix elements in momentum representation may be written as

$$\begin{aligned}\langle \boldsymbol{p}|\hat{T}(z)|\boldsymbol{p}'\rangle &= \langle \boldsymbol{p}|\hat{V}[\hat{1} + (\hat{1} - \hat{Q}^0\hat{V})^{-1}\hat{Q}^0\hat{V}]|\boldsymbol{p}'\rangle \\ &= \langle \boldsymbol{p}|\hat{V}(\hat{1} - \hat{Q}^0\hat{V})^{-1}|\boldsymbol{p}'\rangle.\end{aligned} \tag{4.7}$$

Taking $z = E + \mathrm{i}0$ and inserting equations (2.2), (2.3) and (3.3) into equation (4.7), after some manipulations, it is found that

$$\langle \boldsymbol{p}|\hat{T}|\boldsymbol{p}'\rangle = \frac{1}{\pi^2 D}\sum_{i,j=1}^{2} \frac{\sqrt{a_i a_j}\lambda_{ij}}{\left(a_i^2 + p^2\right)\left(a_j^2 + p'^2\right)} \tag{4.8}$$

where D is given by equation (3.14) and λ_{ij} is the matrix element of λ, which is defined as

$$\lambda \equiv \begin{pmatrix} v_1\left(1 - Q_{22}^0 v_2\right) & Q_{12}^0 v_1 v_2 \\ Q_{21}^0 v_1 v_2 v_2 & v_2\left(1 - Q_{11}^0 v_1\right)\end{pmatrix} \tag{4.9}$$

where Q_{ij}^0 is given by equation (3.11). Equation (4.8) ensures that the matrix elements of T-matrix are independent of direction of momentum, due to the use of the Yamaguchi potential

model. The corresponding matrix elements of the S-matrix, which satisfies the equation

$$\langle p|S(E)|p'\rangle = \delta(p - p') - 2\pi \mathrm{i}\delta(E_p - E_{p'})T_{pp'}(E) \tag{4.10}$$

is diagonal in energy. Using equations (4.8)–(4.10), one obtains, after some simple manipulations, the s-wave scattering matrix of the potential model as

$$S(\tilde{q}) = \frac{X - \mathrm{i}Y}{X + \mathrm{i}Y} \tag{4.11}$$

where

$$X = \sum_{n=0}^{4} x_n \tilde{q}^{2n} \tag{4.12}$$

and

$$Y = 4\tilde{q} \sum_{n=0}^{2} y_n \tilde{q}^{2n} \tag{4.13}$$

in which

$$\begin{aligned}
x_0 &= \tilde{a}_1^4 \tilde{a}_2^4 [1 + 2(\tilde{v}_1 + \tilde{v}_2) + 4(1 - \tilde{a}_1\tilde{a}_2)\tilde{v}_1\tilde{v}_2] \\
x_1 &= 2\tilde{a}_1^2\tilde{a}_2^2 \left[\left(\tilde{a}_1^2 + \tilde{a}_2^2\right) + 2\left(\tilde{a}_1^2\tilde{v}_1 + \tilde{a}_2^2\tilde{v}_2\right) - \left(\tilde{a}_1^2\tilde{v}_2 + \tilde{a}_2^2\tilde{v}_1\right) - 4(1 - \tilde{a}_1\tilde{a}_2)(2 + \tilde{a}_1\tilde{a}_2)\tilde{v}_1\tilde{v}_2\right] \\
x_2 &= \left(\tilde{a}_1^2 + \tilde{a}_2^2\right)^2 + 2\tilde{a}_1^2\tilde{a}_2^2(1 - 2(\tilde{v}_1 + \tilde{v}_2)) + 2\left(\tilde{a}_1^4\tilde{v}_1 + \tilde{a}_2^4\tilde{v}_2\right) + 4\tilde{a}_1^2\tilde{a}_2^2(1 - \tilde{a}_1\tilde{a}_2)\tilde{v}_1\tilde{v}_2 \\
x_3 &= 2\left(\tilde{a}_1^2 + \tilde{a}_2^2\right) - 2\left(\tilde{a}_1^2\tilde{v}_1 + \tilde{a}_2^2\tilde{v}_2\right) \\
x_4 &= 1
\end{aligned} \tag{4.14}$$

and

$$\begin{aligned}
y_0 &= \tilde{a}_1^3\tilde{a}_2^3[(\tilde{a}_1\tilde{v}_2 + \tilde{a}_2\tilde{v}_1) + 4(1 - \tilde{a}_1\tilde{\tilde{a}}_2)\tilde{v}_1\tilde{v}_2] \\
y_1 &= 2\tilde{a}_1^2\tilde{a}_2^2[(\tilde{a}_1\tilde{v}_1 + \tilde{a}_2\tilde{v}_2) - 2(1 - \tilde{a}_1\tilde{a}_2)\tilde{v}_1\tilde{v}_2] \\
y_2 &= \tilde{a}_1^3\tilde{v}_1 + \tilde{a}_2^3\tilde{v}_2.
\end{aligned} \tag{4.15}$$

5. Second virial coefficient

The two-particle correlation in thermal equilibrium can be described by the second virial coefficient. Bethe and Uhlenbeck obtained the second virial coefficient in terms of phase shifts [18]. Some alternative expressions are calculated in terms of S- and T-matrices [19–22]. A pole expansion of the momentum matrix elements of the difference between the resolvents of the interacting and free Hamiltonians, and ultimately its trace, has also been presented by Wei and Snider to obtain an expression for the second virial coefficient [23]. In this paper, we evaluate an explicit expression for the second virial coefficient of a system interacting via a rank-2 separable potential in terms of scattering parameters, providing an alternative method to that of Wei and Snider. We contend that the advantage of this method lies in the way in which some general properties of the macroscopic quantities, such as $B(T)$, are almost uniquely related to the behaviour of the microscopic quantities.

The explicit expression for evaluating the second virial coefficient $B(T)$ is given by the difference between the interacting and free Hamiltonians for the relative motion of a pair of particles

$$B(T) = K\,\mathrm{Tr}(\mathrm{e}^{-\beta\hat{H}} - \mathrm{e}^{-\beta\hat{H}_0}) \tag{5.1}$$

where K is a constant depending on the dimensionality of the system, Tr is the trace over all states of the relative motion of pair of particles and $\beta \equiv 1/k_B T$ in which k_B is Boltzmann's

constant. The $B(T)$ can be expressed as an appropriate contour integral over the difference between the interacting and free resolvents

$$\begin{aligned} B(T) &= \frac{\mathrm{i}K}{2\pi}\int_{-\mathrm{i}\infty}^{\mathrm{i}\infty} \mathrm{d}z\,\mathrm{Tr}[\hat{R}(z)]\,\mathrm{e}^{-\beta z} \\ &= \frac{\mathrm{i}K}{2\pi m}\int_{-\infty+\mathrm{i}\varepsilon}^{\infty+\mathrm{i}\varepsilon} q\,\mathrm{d}q\,\mathrm{Tr}[\hat{R}(z)]\,\mathrm{e}^{-\beta z} \end{aligned} \tag{5.2}$$

where $\hat{R}(z)$ is the difference of the resolvents for interacting and free motion Hamiltonians:

$$\hat{R}(z) = \left(\frac{1}{z-\hat{H}} - \frac{1}{z-\hat{H}_0}\right). \tag{5.3}$$

The difference operator $\hat{R}(z)$ and transition operator $\hat{T}(z)$ are related to each other as the following:

$$\begin{aligned} \hat{R}(z) &= \frac{1}{z-\hat{H}} - \frac{1}{z-\hat{H}_0} = \frac{1}{z-\hat{H}_0}\hat{V}\frac{1}{z-\hat{H}} \\ &= \frac{1}{z-\hat{H}_0}\hat{V}\hat{\Omega}\frac{1}{z-\hat{H}_0} = \frac{1}{z-\hat{H}_0}\hat{T}(z)\frac{1}{z-\hat{H}_0}. \end{aligned} \tag{5.4}$$

Therefore, the diagonal matrix element of resolvent in the momentum space is given by

$$\langle \boldsymbol{p}|\hat{R}(z)|\boldsymbol{p}\rangle = \left(\frac{2m}{p^2-q^2}\right)^2 \langle \boldsymbol{p}|\hat{T}(z)|\boldsymbol{p}\rangle. \tag{5.5}$$

Using equation (5.2), one obtains

$$B(T) = \frac{2\mathrm{i}K}{\pi\bar{a}}\int_{-\infty+\mathrm{i}\varepsilon}^{\infty+\mathrm{i}\varepsilon} \tilde{q}\,\mathrm{d}\tilde{q}\,\frac{\mathcal{N}(\tilde{q})}{\mathcal{D}(\tilde{q})}\,\mathrm{e}^{-\beta z} \tag{5.6}$$

where $\mathcal{N}(\tilde{q})$ and $\mathcal{D}(\tilde{q})$ are given by the following relations:

$$\begin{aligned} \mathcal{N}(\tilde{q}) &= \sum_{k=0}^{3} c_k \tilde{q}^k \\ \mathcal{D}(\tilde{q}) &= (\tilde{q}+\mathrm{i}\tilde{a}_1)(\tilde{q}+\mathrm{i}\tilde{a}_2)\sum_{k=0}^{4} d_k \tilde{q}^k \end{aligned} \tag{5.7}$$

in which the coefficients c_k and d_k are independent of $\tilde{q}$:

$$\begin{aligned} c_0 &= -\mathrm{i}\tilde{a}_1^2\tilde{a}_2^2[\tilde{a}_2\tilde{v}_1 + \tilde{a}_1\tilde{v}_2 + 4\tilde{v}_1\tilde{v}_2(1-\tilde{a}_1\tilde{a}_2)] \\ c_1 &= -\tilde{a}_1^2\tilde{a}_2^2[3(\tilde{v}_1+\tilde{v}_2) + 4\tilde{v}_1\tilde{v}_2(1-\tilde{a}_1\tilde{a}_2)] \\ c_2 &= 3\mathrm{i}\tilde{a}_1\tilde{a}_2(\tilde{a}_1\tilde{v}_1 + \tilde{a}_2\tilde{v}_2) \\ c_3 &= \tilde{a}_1^2\tilde{v}_1 + \tilde{a}_2^2\tilde{v}_2 \end{aligned} \tag{5.8}$$

and

$$\begin{aligned} d_0 &= -\tilde{a}_1^2\tilde{a}_2^2[1 + 2(\tilde{v}_1+\tilde{v}_2) + 4\tilde{v}_1\tilde{v}_2(1-\tilde{a}_1\tilde{a}_2)] \\ d_1 &= -4\mathrm{i}\tilde{a}_1\tilde{a}_2(1 + \tilde{a}_1\tilde{v}_1 + \tilde{a}_2\tilde{v}_2) \\ d_2 &= -2\big(2 + \tilde{a}_1\tilde{a}_2 + \tilde{a}_1^2\tilde{v}_1 + \tilde{a}_2^2\tilde{v}_2\big) \\ d_3 &= 4\mathrm{i} \\ d_4 &= 1 \end{aligned} \tag{5.9}$$

Furthermore, we can write $\mathcal{D}(\tilde{q})$ as

$$\mathcal{D}(\tilde{q}) = (\tilde{q}+\mathrm{i}\tilde{a}_1)(\tilde{q}+\mathrm{i}\tilde{a}_2)\prod_{n=1}^{4}(\tilde{q}-\tilde{q}_n) \tag{5.10}$$

where $\tilde{q}_n$ is the poles of $\frac{\mathcal{N}(\tilde{q})}{\mathcal{D}(\tilde{q})}$. The integrand of equation (5.6), i.e. $\tilde{q}\frac{\mathcal{N}(\tilde{q})}{\mathcal{D}(\tilde{q})}$ with four poles at $\tilde{q}_n : n = 1,\ 2,\ 3,\ 4$, and two poles at $-\mathrm{i}\tilde{a}_1$ and $-\mathrm{i}\tilde{a}_2$, can then be written as a sum over all its poles, according to

$$\tilde{q}\frac{\mathcal{N}(\tilde{q})}{\mathcal{D}(\tilde{q})} = \frac{\alpha_1}{\tilde{q}+\mathrm{i}\tilde{a}_1} + \frac{\alpha_2}{\tilde{q}+\mathrm{i}\tilde{a}_2} + \sum_{n=1}^{4}\frac{\alpha(\tilde{q}_n)}{\tilde{q}-\tilde{q}_n} \tag{5.11}$$

where

$$\alpha_i = \lim_{\tilde{q}\to-\mathrm{i}\tilde{a}_i}\left[\frac{\mathcal{N}(\tilde{q})}{\mathrm{d}\mathcal{D}(\tilde{q})/\mathrm{d}\tilde{q}}\right] \qquad i = 1, 2 \tag{5.12}$$

in which

$$\begin{aligned}\alpha_1 &= -\frac{\tilde{v}_1\left[(\tilde{a}_1-\tilde{a}_2)^3 - 4\tilde{v}_2\tilde{a}_2^2(\tilde{a}_1-1)(\tilde{a}_1\tilde{a}_2-1)\right]}{4(\tilde{a}_1-\tilde{a}_2)\left[2\tilde{v}_1(\tilde{a}_1-\tilde{a}_2)^2 - 4\tilde{v}_1\tilde{v}_2\tilde{a}_2^2(\tilde{a}_1\tilde{a}_2-1)\right]}\\ \alpha_2 &= -\frac{\tilde{v}_2\left[(\tilde{a}_2-\tilde{a}_1)^3 - 4\tilde{v}_1\tilde{a}_1^2(\tilde{a}_1-1)(\tilde{a}_1\tilde{a}_2-1)\right]}{4(\tilde{a}_2-\tilde{a}_1)\left[2\tilde{v}_2(\tilde{a}_1-\tilde{a}_2)^2 - 4\tilde{v}_1\tilde{v}_2\tilde{a}_1^2(\tilde{a}_1\tilde{a}_2-1)\right]}.\end{aligned} \tag{5.13}$$

We have also defined

$$\alpha(\tilde{q}_n) = \lim_{\tilde{q}\to\tilde{q}_n}\left[\frac{\mathcal{N}(\tilde{q})}{\mathrm{d}\mathcal{D}(\tilde{q})/\mathrm{d}\tilde{q}}\right]. \tag{5.14}$$

Inserting of equation (5.11) into equation (5.6) leads to the following expression for the reduced second virial coefficient $B^*(T^*) \equiv B(T)/K$ in term of $\zeta(z)$ function:

$$B^*(T^*) = 8\left[\alpha_1\zeta\left(\frac{-\mathrm{i}\tilde{a}_1}{\sqrt{T^*}}\right) + \alpha_2\zeta\left(\frac{-\mathrm{i}\tilde{a}_2}{\sqrt{T^*}}\right) + \sum_{n=1}^{4}\alpha(\tilde{q}_n)\zeta(\tilde{q}_n/\sqrt{T^*})\right] \tag{5.15}$$

where $T^* \equiv \frac{2mk_BT}{\tilde{a}^2}$ is the reduced temperature and $\zeta(z)$ is defined as

$$\zeta(z) = \frac{\mathrm{i}}{\pi}\int_{-\infty}^{\infty}\frac{\mathrm{e}^{-t^2}}{z-t}\,\mathrm{d}t \qquad (\mathrm{Im}\, z > 0). \tag{5.16}$$

6. Results and discussion

The singularities of the scattering matrix located on the imaginary axis of the complex q-plane corresponding to the poles on the imaginary axis in the upper half-plane are considered bound states whose energies can be determined from the condition $S(\tilde{q}) \to \infty$. For every pole position at $\tilde{q}_k$, which arises from $X + \mathrm{i}Y = 0$, there is also an associated zero of S at $\tilde{q}_k^*$, which is complex conjugate of $\tilde{q}_k$. The qualitative features of the roots of $X + \mathrm{i}Y = 0$ depend on the values of three parameters $\tilde{a}_1$ (or $\tilde{a}_2 = 2 - \tilde{a}_1$), $\tilde{v}_1$ and $\tilde{v}_2$. In figure 1, the distribution of poles and zeros of the scattering matrix in the complex q-plane are shown for some cases, which have been chosen by varying the parameters defining the interaction and momentum parameters $\tilde{v}_i$ and $\tilde{a}_i$. For all cases, there are two double poles of S at $\tilde{q}_1 = \tilde{q}_2 = \mathrm{i}\tilde{a}_1$ and $\tilde{q}_3 = \tilde{q}_4 = \mathrm{i}\tilde{a}_2$. Furthermore, there exist two poles of S with opposite real parts symmetrically placed with respect to the imaginary axis located at $\tilde{q}_k = s_1 - \mathrm{i}s_2$ ($s_1, s_2 \geqslant 0$). Even further, each pole $\tilde{q}_k$ in the fourth quadrant goes with a twin pole $-\tilde{q}_k^*$ in the third quadrant. For cases with $\tilde{v}_1 \neq \tilde{v}_2$, however, one of the symmetric poles may be located on the imaginary axis. The poles of the S-matrix with opposite real parts on both sides of the negative imaginary axis, sometimes called 'resonance' and 'antiresonance' poles, although not all resonances can be associated with observable effects. The core singularities are resonance poles in the fourth

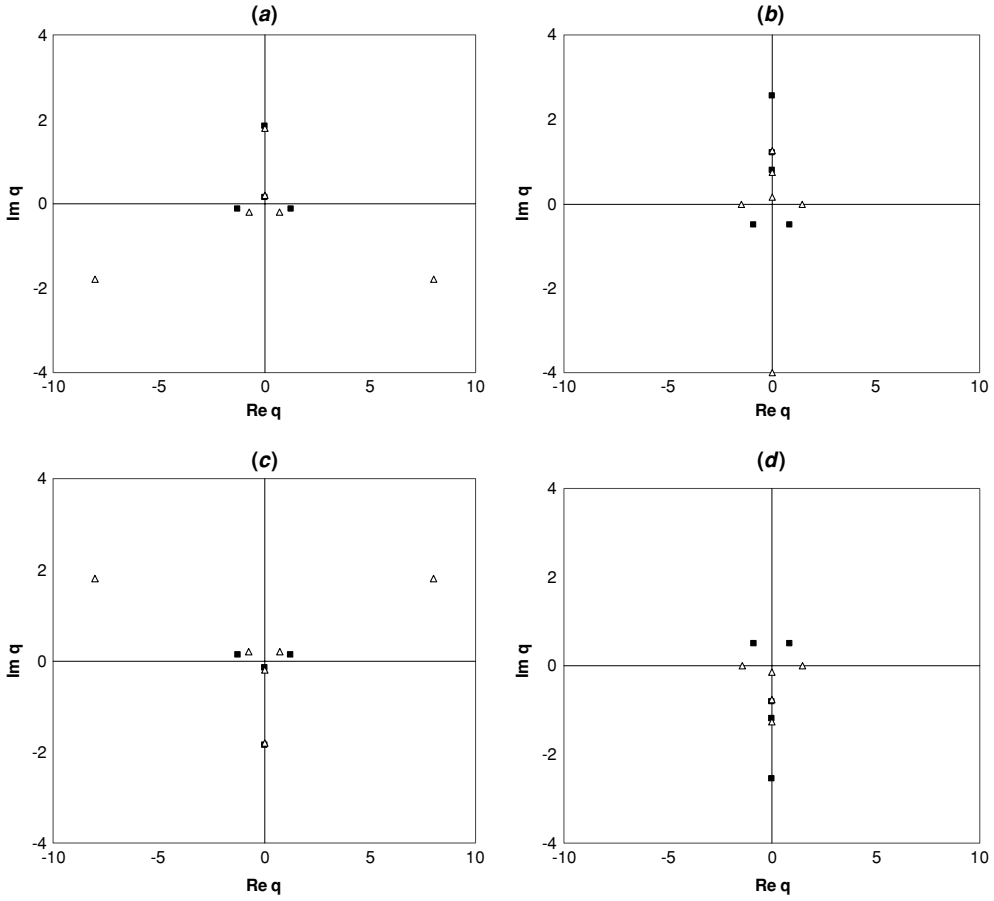

Figure 1. Poles and zeros of the scattering matrix for various momentum and potential parameters $\tilde{a}_i$ and $\tilde{v}_i$. (*a*) Poles for cases with (■) $\tilde{a}_1 = 0.15, \tilde{a}_2 = 1.85$, $\tilde{v}_1 = 50, \tilde{v}_2 = -10$; (Δ) $\tilde{a}_1 = 1.80, \tilde{a}_2 = 0.20$, $\tilde{v}_1 = 10, \tilde{v}_2 = 10$. (*b*) Poles for cases with (■) $\tilde{a}_1 = 0.80, \tilde{a}_2 = 1.20$, $\tilde{v}_1 = 10, \tilde{v}_2 = -10$; (Δ) $\tilde{a}_1 = 0.75, \tilde{a}_2 = 1.25$, $\tilde{v}_1 = 10, \tilde{v}_2 = -5$. (*c*) Same as (*a*) for zeros. (*d*) Same as (*b*) for zeros.

quadrant at $\tilde{q}_k = s_1 - \mathrm{i}s_2$ with s_1 and s_2 as positive real numbers, whereas the corresponding antiresonance poles are located at $-\tilde{q}_k^*$ in the third quadrant. Figures 1(*a*) and (*b*) show the distribution of poles for four cases: (i) $\tilde{a}_1 = 0.15, \tilde{a}_2 = 1.85$, $\tilde{v}_1 = 50$ and $\tilde{v}_2 = -10$ with large positive value of repulsive potential parameter $\tilde{v}_1$ and a small value for its corresponding momentum parameter $\tilde{a}_1$; (ii) $\tilde{a}_1 = 1.80, \tilde{a}_2 = 0.20$, $\tilde{v}_1 = 10$ and $\tilde{v}_2 = 10$, in which the interaction is assumed to be completely repulsive; (iii) $\tilde{a}_1 = 0.80, \tilde{a}_2 = 1.20$, $\tilde{v}_1 = 10$ and $\tilde{v}_2 = -10$ with similar strength of repulsive and attractive potential parameters, i.e., $\tilde{v}_1 = |\tilde{v}_2|$, but different momentum parameters, i.e., $\tilde{a}_1 \neq \tilde{a}_2$; (iv) $\tilde{a}_1 = 0.75$, $\tilde{a}_2 = 1.25$, $\tilde{v}_1 = 10$ and $\tilde{v}_2 = -5$.

The energies of the bound states are determined by the zeros of the scattering matrix positioned on the imaginary axis in the lower half-plane of $\tilde{q}$ or by the poles of the S-matrix positioned on the imaginary axis in the upper half-plane of $\tilde{q}$. The number of bound states in our potential model depends on three parameters $\tilde{v}_1$, $\tilde{v}_2$ and $\tilde{a}_1$ (or $\tilde{a}_2$). There are always two bound states located at $\mathrm{i}\tilde{a}_1$ and $\mathrm{i}\tilde{a}_2$, although an additional bound state may arise for negative

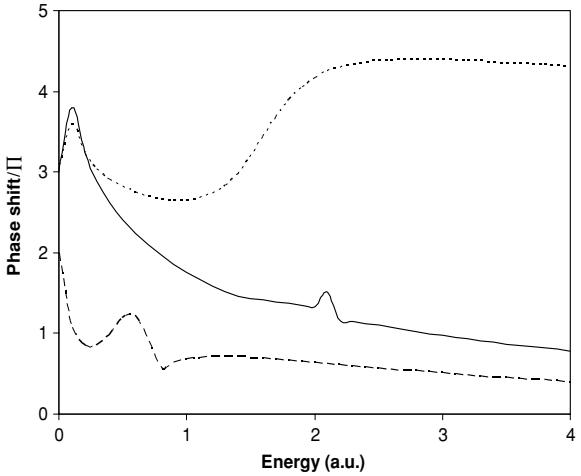

Figure 2. Scattering phase shift for a system with (——) $\tilde{a}_1 = 0.75, \tilde{a}_2 = 1.25$, $\tilde{v}_1 = 10$, $\tilde{v}_2 = -5$; (- - -) $\tilde{a}_1 = 1.8, \tilde{a}_2 = 0.2$, $\tilde{v}_1 = 10, \tilde{v}_2 = 10$; (· · ·) $\tilde{a}_1 = 0.15, \tilde{a}_2 = 1.85$, $\tilde{v}_1 = 50, \tilde{v}_2 = -10$.

values of $\tilde{v}_2$. Moreover, the virtual states lying on the negative imaginary axis may appear for cases with $\tilde{v}_1 \neq \tilde{v}_2$. The bound states move upward, as $\tilde{v}_2$ grows negative, while the virtual states move downward on the imaginary axis. Poles of the scattering matrix in the lower half-plane of $\tilde{q}$ which are not located on the imaginary axis correspond to quasi-stationary states, describing decay or capture in the system.

Furthermore, the scattering matrix elements can be written in terms of the phase shift

$$S(\tilde{q}) = \mathrm{e}^{2\mathrm{i}\delta(\tilde{q})}. \tag{6.1}$$

Comparing equations (4.11) and (6.1), the phase shift is given by [21]

$$\delta = -\mathrm{arc\,cot}\left(\frac{X}{Y}\right) \tag{6.2}$$

where X and Y are defined by equations (4.12) and (4.13). Therefore, the scattering phase shift associated with our separable potential model can be obtained analytically. Since the arccotangent is a multivalued function, it is necessary to choose a particular branch. The usual convention is to choose the branch that gives $\lim_{E\to\infty} \delta(E) = 0$ and makes δ continuous. The behaviour of the phase shift depends on the sign of X and Y, or alternatively, depends on the values of the potential model parameters. Three representative cases are depicted in figure 2. The distinctive feature of this plot to which we draw attention is that in the low-energy limit, $E \to 0$, the scattering phase shift is an integer number of π

$$\lim_{E\to 0} \delta(E) = N_B\pi \tag{6.3}$$

where N_B is the number of bound states. This behaviour may be understood by recalling Levinson's theorem, which connects the zero-energy scattering phase shift with the number of bound states. We have seen that a finite energy resonance leads to a smooth jump in the phase shift.

The resonance pole causes a rapid variation to the cross section, which is related to smooth jumps of the phase shift. To see this characteristic more explicitly, a dimensionless partial

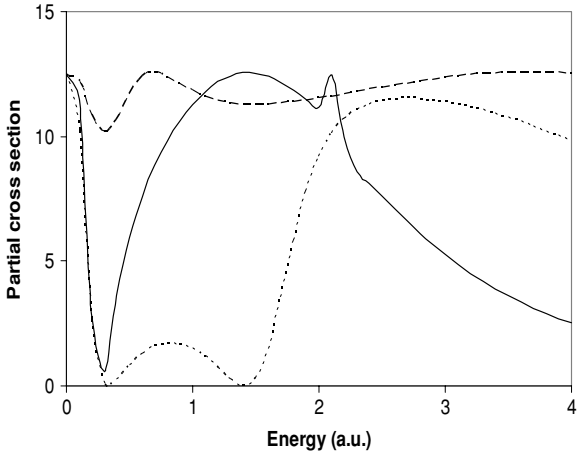

Figure 3. Scattering cross section for a system with (——) $\tilde{a}_1 = 0.75, \tilde{a}_2 = 1.25$, $\tilde{v}_1 = 10$, $\tilde{v}_2 = -5$; (- - -) $\tilde{a}_1 = 1.8, \tilde{a}_2 = 0.2$, $\tilde{v}_1 = 10, \tilde{v}_2 = 10$; $(\cdots)$ $\tilde{a}_1 = 0.15, \tilde{a}_2 = 1.85$, $\tilde{v}_1 = 50, \tilde{v}_2 = -10$.

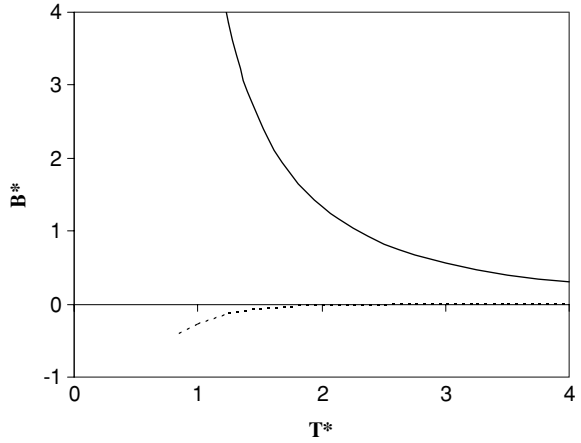

Figure 4. Reduced second virial coefficient as a function of reduced temperature: (—) $\tilde{a}_1 = 1.3$, $\tilde{v}_1 = 6.0$, $\tilde{v}_2 = 0.0$; $(\ldots)$ $\tilde{a}_1 = 1.3$, $\tilde{v}_1 = 0.0$, $\tilde{v}_2 = -6.0$.

cross section defined as

$$\sigma_l = \frac{4\pi}{\tilde{q}^2}(2l+1)\sin^2\delta_l \tag{6.4}$$

is shown in figure 3, where l is the angular momentum quantum number, which is zero for s-wave scattering. The resonance and associated partial cross-section peak is positioned at about 2.1, 0.6 and 2.2 for the first, second and third cases of figure 2, respectively.

Finally, the second virial coefficient of our potential model has been calculated analytically in terms of the potential parameters. Figures 4 and 5 show the reduced second virial coefficient $B^*(T^*)$ as a function of the reduced temperature T^*. At low temperatures the attractive part of the potential dominates the integrand and $B(T)$ is negative, whereas at high temperatures

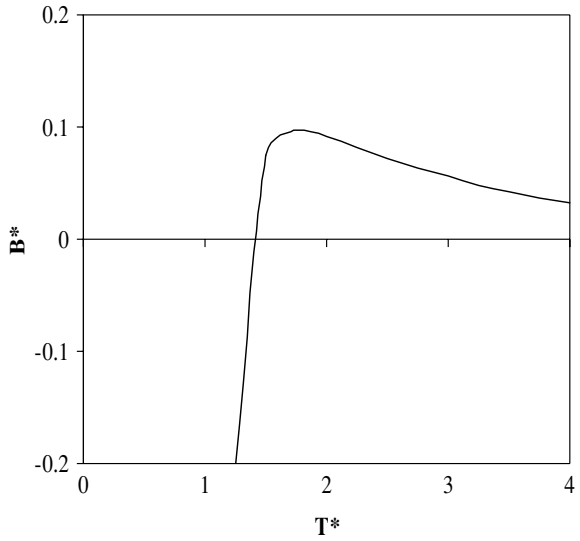

Figure 5. Reduced second virial coefficient as a function of reduced temperature for a system with $\tilde{a}_1 = 1.3$, $\tilde{v}_1 = 6.0$ and $\tilde{v}_2 = -23$.

$B(T)$is positive due to the repulsive effects of the potential. The temperature at which $B(T)$passes zero is called the Boyle temperature.

Acknowledgments

Financial support received from the University of Tehran Research Council is greatly appreciated. The authors wish to thank Professor M N Sarbolouki and Professor Alavi Moghaddam for helpful suggestions.

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