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Partial-wave Scattering and Statistical Mechanics via the l-wave Non-local Separable Potential of Rank-two

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Abstract The equilibrium statistical mechanics relations are shown to be related to T-matrix, which describes the scattering processes taking place in the thermodynamic system consisting of free particles and independent correlated pairs, interacting via the separable non-local potential of rank two in the ℓth partial wave. Thermodynamic properties are related to the correlated states, when making a pole expansion of the analytically continued momentum matrix element of $R_\ell(z)$, the difference between the resolvents of the interacting and free Hamiltonians. It is shown that local potentials equivalent to the nonlocal ones have an attractive part which is responsible for a bound state and negative values of some thermodynamic properties.

Keywords Boltzmann statistics · Partial-wave scattering · Local equivalent of nonlocal potential

1 Introduction

The scattering properties by a s-wave three dimensional separable potential of rank-two and their explicit expressions for a number of scattering properties, such as phase shifts, cross-sections and T and S-matrices were calculated in our previous work [1]. Moreover, we have presented a formulation for statistical mechanics of a thermodynamic system consisting of free particles and independent correlated pairs, interacting via s-wave separable potential, in terms of the scattering properties [2]. This paper deals with the generalization of our previous formulation, to ℓ-wave non-local separable interaction of rank-two.

In thermal equilibrium the ℓ-wave correlations between two particles is given by the partial Ursell operator [3]

$$\hat{U}_\ell(T) = (e^{-\beta \hat{H}_\ell} - e^{-\beta \hat{H}_0}) \tag{1}$$

The author died when the manuscript was under editorial process. So his friend, Mahtab Gharibi (*email: gharibi@tmu.ac.ir*) pursued the publication.

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Here $\hat{H}_\ell = \hat{H}_0 + \hat{V}_\ell$ is defined as the partial interacting Hamiltonian, in which $\hat{H}_0$ and $\hat{V}_\ell$ are the free Hamiltonian and ℓ-wave potential for relative motion, respectively. It can be shown that the partial Ursell operator is related to the interacting and free resolvent operators by the Laplace transform

$$\hat{U}_\ell(T) = \frac{1}{2\pi i}\int_C e^{-\beta z}\hat{R}_\ell(z)dz \tag{2}$$

where $z = q^2/2\mu$ is the complex energy parameter and $R_\ell(z)$ is the difference between the resolvents of interacting and free motion Hamiltonians

$$\hat{R}_\ell(z) \equiv \left(\frac{1}{z-\hat{H}_\ell} - \frac{1}{z-\hat{H}_0}\right) \tag{3}$$

The contour integral in (2) either over the complex energy parameter $z \equiv E + i\varepsilon$ or its equivalent complex momentum parameter q. The contour must lie to the left of the eigenvalues of both $\hat{H}_\ell$ and $\hat{H}_0$ for the z integral and equivalently, above the eigenvalues for the q integral with the small positive number ε constraining q to have a positive imaginary component. The spectrum for $\hat{H}_0$ is simply identified as the positive real axis, but $\hat{H}_\ell$ may have bound states that lies on negative real axis with their equivalent momenta positive imaginary, so the contours must be chosen appropriately.

Furthermore, there is an explicit relation between the partial transition operator $\hat{T}_\ell(z)$ and resolvent operator $\hat{R}_\ell(z)$ as

$$\begin{aligned}\hat{R}_\ell(z) &\equiv \frac{1}{z-\hat{H}_\ell} - \frac{1}{z-\hat{H}_0}\\ &= \frac{1}{z-\hat{H}_0}\hat{T}_\ell(z)\frac{1}{z-\hat{H}_0}\end{aligned} \tag{4}$$

The connection between thermophysical and scattering properties for the system can be created by (4), since some of the resolvent matrix poles are the same as the transition matrix (or scattering matrix) poles. In fact, there are two types of poles; one set determined by $\langle \boldsymbol{p}|\hat{T}_\ell(z)|\boldsymbol{p}\rangle$, will be referred to as "correlated-state" poles. The two other second order poles at $p = \pm q$ will be referred to as "structural" poles. Except for the poles associated with possible bound states, the correlated- state poles are all in the lower half q plane.

The arrangement of the paper is as follows. Section 2 is devoted to the two-particle partial-wave scattering problem by the ℓ-wave nonlocal separable potential of rank-two. In Sect. 3 we construct local potentials equivalent to the nonlocal ones. Some thermodynamic properties of the described system such as second virial coefficient, virial pressure and quantum correction of kinetic energy are given in terms of the Ursell operator in Sect. 4. A brief discussion is given in Sect. 5. The explicit expressions required for s-, p- and d-wave calculations are presented in the Appendices.

2 Nonlocal Separable Potential and Its Scattering Properties

The separable potentials are widely used in electronic structure calculations on atoms, molecules, and solids [4–7] and in the areas of nuclear and condensed matter [8–11]. A general form of central non-local separable potential of rank-two, which produces scattering in only the ℓth partial wave, can be written as [12]

$$\hat{V}_\ell = 4\pi \sum_{i=1}^{2} \sum_{m} |\chi_{\ell,i};\ell,m\rangle \lambda_{\ell,i} \langle \chi_{\ell,i};\ell,m| \tag{5}$$

where $\lambda_{\ell,i}$ is the potential energy strength, which is a real number and $|\chi_{\ell,i};\ell,m\rangle$ is state of the system, which its momentum representation is given by

$$\langle \boldsymbol{p}|\chi_{\ell,i};\ell,m\rangle = f_{\ell,i}(p) Y_{\ell,m}(\hat{\boldsymbol{p}}), \tag{6}$$

where $f_{\ell,i}(p)$ and $Y_{\ell,m}(\hat{\boldsymbol{p}})$ are the form factor for the ℓth partial wave and the spherical harmonics of angular variables $\hat{\boldsymbol{p}}$ respectively. In the present work we have been used the following normalized form factor

$$f_{\ell,i}(p) = N_{\ell,i} \frac{p^\ell}{(p^2 + a_{\ell,i}^2)^{\ell+1}} \tag{7}$$

where $a_{\ell,i}$ is the range parameter and $N_{\ell,i}$ the normalization constant is given by

$$N_{\ell,i} = \left(\frac{2^{2\ell}\ell!}{\Gamma(\ell+\frac{1}{2})} \frac{a_{l,i}^{2\ell+1}}{\pi^{3/2}} \right)^{1/2} \tag{8}$$

in which $\Gamma(n)$ is the Gamma function.

Ghirardi and Rimini [13] have examined general properties of separable potential. 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. The potential allows all quantities of interest, such as resonance energy, lifetime, phase shift, etc., to be expressed in a completely analytical form. It is well known that separable ones of a certain rank [14] can accurately approximate almost all short-range potential models.

Moreover, a rank-two separable potential with Yamaguchi form factor leads to algebraic expressions for most quantities of interest. Such potentials have been studied as models for a variety of physical problems [15–19].

The momentum representation of the separable potential of rank-two, can be shown as

$$\begin{aligned} \langle \boldsymbol{p}|\hat{V}_\ell|\boldsymbol{p}'\rangle &= 4\pi \sum_{i=1}^{2} \lambda_{\ell,i} f_{\ell,i}(p) f_{\ell,i}(p') \sum_{m} Y_{\ell,m}(\hat{\boldsymbol{p}}) Y_{\ell,m}^*(\hat{\boldsymbol{p}}') \\ &= (2\ell+1) \sum_{i=1}^{2} \lambda_{\ell,i} f_{\ell,i}(p) f_{\ell,i}(p') P_\ell(\hat{\boldsymbol{p}}.\hat{\boldsymbol{p}}') \end{aligned} \tag{9}$$

where $P_\ell(\hat{\boldsymbol{p}}.\hat{\boldsymbol{p}}')$ is Legendre polynomials for ℓth partial wave.

A striking feature of the non-local separable potential (5) is that it gives rise to scattering only for the ℓth partial wave.

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

$$\hat{T}_\ell = \hat{V}_\ell \hat{\Omega}_\ell \tag{10}$$

where the partial Møller wave operator $\hat{\Omega}_\ell$ is an operator by which a free state changes into the ℓth partial wave of scattering one [20]. The resolvent form of the Møller operator is represented as

$$\hat{\Omega}_\ell(z) = 1 + (z - \hat{H}_\ell)^{-1}\hat{V}_\ell = 1 + (z - \hat{H}_0)^{-1}\hat{V}_\ell\hat{\Omega}_\ell(z) \tag{11}$$

where $\hat{H}_\ell = \hat{H}_0 + \hat{V}_\ell$ is the partial interacting Hamiltonian, in which $\hat{H}_0$ is the free Hamiltonian. Defining the partial interacting resolvent $\hat{Q}_\ell \equiv (z - \hat{H}_\ell)^{-1}$ and free motion resolvent $\hat{Q}^0 \equiv (z - \hat{H}_0)^{-1}$, it can be easily shown that the Møller operator can be rewritten as

$$\hat{\Omega}_\ell(z) = \hat{1} + (\hat{1} - \hat{Q}^0\hat{V}_\ell)^{-1}\hat{Q}^0\hat{V}_\ell \tag{12}$$

Therefore, the partial transition matrix $\hat{T}_\ell$, may be written as

$$\begin{aligned}\hat{T}_\ell &= \hat{V}_\ell[\hat{1} + (\hat{1} - \hat{Q}^0\hat{V}_\ell)^{-1}\hat{Q}^0\hat{V}_\ell] \\ &= \hat{V}_\ell(\hat{1} - \hat{Q}^0\hat{V}_\ell)^{-1}\end{aligned} \tag{13}$$

It can be shown that when using the separable potential of rank-two (5), partial transition matrix operator $\hat{T}_\ell$, also becomes separable. By inserting (5), (6) and (7) into (13) and after some manipulations, it is found that

$$\hat{T}_\ell = \frac{4\pi}{d_\ell(q)} \sum_{i,j=1}^{2} \sum_m |\chi_{\ell,i}; \ell, m\rangle \tau_{\ell,ij} \langle \chi_{\ell,j}; \ell, m| \tag{14}$$

where $\tau_{\ell,ij}$ is the matrix element of τ_ℓ, which is given by

$$\tau_\ell \equiv \begin{pmatrix} \lambda_{\ell,1}(1 - Q^0_{\ell,22}\lambda_{\ell,2}) & Q^0_{\ell,12}\lambda_{\ell,1}\lambda_{\ell,2} \\ Q^0_{\ell,21}\lambda_{\ell,1}\lambda_{\ell,2} & \lambda_{\ell,2}(1 - Q^0_{\ell,11}\lambda_{\ell,1}) \end{pmatrix} \tag{15}$$

and

$$d_\ell(q) = (1 - Q^0_{\ell,11}\lambda_{\ell,1})(1 - Q^0_{\ell,22}\lambda_{\ell,2}) - \lambda_{\ell,1}\lambda_{\ell,2}Q^{0^2}_{\ell,12} \tag{16}$$

in which $Q^0_{\ell,ij}$, the matrix elements of the free motion resolvent $\hat{Q}^0 = (z - \hat{H}_0)^{-1}$, are given by

$$Q^0_{\ell,ij}(q) = (4\pi)(2\mu)\int_c \frac{f_{\ell,i}(p) f_{\ell,j}(p)}{q^2 - p^2} p^2 dp \tag{17}$$

where $q \equiv \sqrt{2\mu z}$, and the contour C goes from $-\infty$ to $+\infty$ passing above all the singularities. Substituting (7) in (17) it is found that

$$Q^0_{\ell,ij}(q) = (4\pi)(2\mu)N_{\ell,i}N_{\ell,j}I^{(1)}_{\ell,ij}(q) \tag{18}$$

where $I^{(1)}_{\ell,ij}(q)$ is defined as

$$I^{(1)}_{\ell,ij}(q) \equiv \int_c \frac{p^{2l+2}}{(p^2 + a^2_{l,i})^{l+1}(p^2 + a^2_{l,j})^{l+1}(q^2 - p^2)} dp \tag{19}$$

It is obvious from (19) that the matrix elements $Q^0_{\ell,ij}$ can be calculated analytically for any particular value of ℓ. Some explicit expressions will be given in the Appendix A.

Using (14), the momentum representation of $\hat{T}_\ell$ is given by the following expression

$$\langle \boldsymbol{p}|\hat{T}_\ell|\boldsymbol{p}'\rangle = \frac{(2\ell+1)}{d_\ell(q)} \sum_{i,j=1}^{2} f_{\ell,i}(p)\tau_{\ell,ij}(q) f_{\ell,j}(p')P_\ell(\hat{\boldsymbol{p}}.\hat{\boldsymbol{p}}') \tag{20}$$

For elastic scattering $\boldsymbol{p}'^2 = \boldsymbol{p}^2 = 2\mu E = q^2$, the partial transition operator $\hat{T}_\ell$ can be written as

$$\begin{aligned} T_\ell(q) &= \frac{1}{4\pi^2\mu q}\left(\frac{Y_\ell(q)}{X_\ell(q)+iY_\ell(q)}\right) \\ &= \frac{1}{4\pi^2\mu q}\left(\frac{Y_\ell(q)}{J_\ell(-q)}\right) \end{aligned} \tag{21}$$

in which, $X_\ell(q)$, $Y_\ell(q)$ and the Jost function $(J_\ell(q) = X_\ell(q) - iY_\ell(q))$ can be determined for particular values of l and n.

It is well known that the scattering problem is determined if the transition matrix is known. The poles of the $\hat{T}$-matrix, that is equivalent to the poles of the scattering wave function (correlated states), naturally include energies corresponding to resonance, virtual (defined analogously to the antibound state) and bound states. The poles of the $\hat{T}$-matrix can be obtained by solving the following equation

$$d_\ell(q_j) = 0 \tag{22}$$

The zeroes of $d_\ell(q)$ (16) with positive imaginary $q_{b,\ell} = i\kappa_{b,\ell}$, negative imaginary $q_{v,\ell} = -i\kappa_{v,\ell}$, and complex momenta $q_{r,\ell} = \pm k_{r,\ell} - i\kappa_\ell$, show the bound, virtual and resonance states, respectively.

3 Nonlocal Separable Potential and Its Local Equivalent

The purpose of this section is to introduce an equivalent local potential which corresponds to the nonlocal separable potential (5) (see also [21, 22]). This is done in the following way. The Schrödinger equation in r-space is

$$-\left(\frac{\hbar^2}{2\mu}\right)\nabla^2\Psi(\boldsymbol{r}) + \int V(\boldsymbol{r},\boldsymbol{r}')\Psi(\boldsymbol{r}')d\boldsymbol{r}' = E\Psi(\boldsymbol{r}) \tag{23}$$

The equivalent local potential in the present work is defined as the local potential $V_{EL}(\boldsymbol{r})$ which is equivalent to the nonlocal potential $V(\boldsymbol{r},\boldsymbol{r}')$ and thus can be written as

$$V_{EL}(\boldsymbol{r}) \equiv [\Psi(\boldsymbol{r})]^{-1} \int V(\boldsymbol{r},\boldsymbol{r}')\Psi(\boldsymbol{r}')d\boldsymbol{r}' \tag{24}$$

It is clear from the definition (24) that $V_{EL}(\boldsymbol{r})$ is energy-dependent, since the two body wave function $\Psi(\boldsymbol{r})$ is energy-dependent. The r-space nonlocal potential $V_\ell(\boldsymbol{r},\boldsymbol{r}')$ in (24) is the Fourier transform of the p-space $V_\ell(\boldsymbol{p},\boldsymbol{p}')$ (9) and can be obtained by employing the Rayleigh expansion of a plane wave, given by

$$\exp(i\boldsymbol{k}.\boldsymbol{r}) = \sum_{\ell,m} 4\pi i^\ell j_\ell(kr)Y^*_{\ell,m}(\hat{\boldsymbol{k}})Y_{\ell,m}(\hat{\boldsymbol{r}}) \tag{25}$$

in which $j_\ell(x)$ is the Bessel function.

The result can be shown as

$$V_\ell(\boldsymbol{r},\boldsymbol{r}') = 4\pi \sum_{i=1}^{2} \sum_{m} \lambda_{\ell,i} g_{\ell,i}(r) g^*_{\ell,i}(r') Y_{\ell,m}(\hat{\boldsymbol{r}}) Y^*_{\ell,m}(\hat{\boldsymbol{r}}') \tag{26}$$

where $g_{\ell,i}(r)$ is given by

$$g_{\ell,i}(r) = (i)^\ell \sqrt{\frac{2}{\pi}} N_{\ell,i} \int_0^\infty p^2 j_\ell(pr) f_{\ell,i}(p) dp \tag{27}$$

In order to constructing the local potential equivalent to the nonlocal interaction possessing a bound state, the bound state wave function must be calculated. It can be shown that the bound state wave function with the energy $E_b = -\frac{\kappa_b^2}{2\mu}$ in the momentum representation is given by

$$\psi_{b,\ell}(\boldsymbol{p}) = N_{b,\ell} \frac{2\mu}{(p^2+\kappa_b^2)} \sum_{i=1}^{2} c_{\ell,i} f_{\ell,i}(p) \sum_{m} Y_{\ell,m}(\hat{\boldsymbol{p}}) \tag{28}$$

in which

$$c_{\ell,1} = \frac{1-\lambda_{\ell,2} Q^0_{\ell,22}(i\kappa_b)}{Q^0_{\ell,12}(i\kappa_b)} \tag{29}$$

$$c_{\ell,2} = \lambda_{\ell,1} \tag{30}$$

where its validity may be confirmed by substituting in the Schrödinger equation for the bound state. The corresponding coordinate representation of the partial-wave bound state wave function $\psi_{b,\ell}(\boldsymbol{r})$ can be calculated from the Fourier transform of (28) as

$$\psi_{b,\ell}(\boldsymbol{r}) = i^\ell (2\mu N_{b,\ell}) \sum_{i=1}^{2} c_{\ell,i} R_{\ell,i}(r,\kappa_b) \sum_{m} Y_{\ell,m}(\hat{\boldsymbol{r}}) \tag{31}$$

where

$$R_{\ell,i}(r,\kappa_b) = \sqrt{\frac{2}{\pi}} \int_0^\infty \frac{j_\ell(pr) f_{\ell,i}(p)}{(p^2+\kappa_b^2)} p^2 dp \tag{32}$$

The equivalent local potential to the nonlocal interaction which supports a bound state with the energy $E_b = -\frac{\kappa_b^2}{2\mu}$, can be obtained by inserting (26) and (31) into (24) as

$$V_{EL,\ell}(r,\kappa_b) = 4\pi \frac{\sum_{i=1}^{2} c_{\ell,i} \lambda_{\ell,i} b_{l,i}(\kappa_b) g_{\ell,i}(r)}{\sum_{i=1}^{2} c_{\ell,i} R_{\ell,i}(r,\kappa_b)} \tag{33}$$

where $b_{l,i}(\kappa_b)$ is defined by the following integral

$$b_{l,i}(\kappa_b) = \int_0^\infty r^2 g^*_{\ell,i}(r) R_{\ell,i}(r,\kappa_b) dr \tag{34}$$

The integrals of (27) and (32), which are necessary for the computation of (33), can be calculated analytically by the straightforward method of contour integration in the complex

Fig. 1 Local potentials equivalent to the nonlocal interactions of Table 1

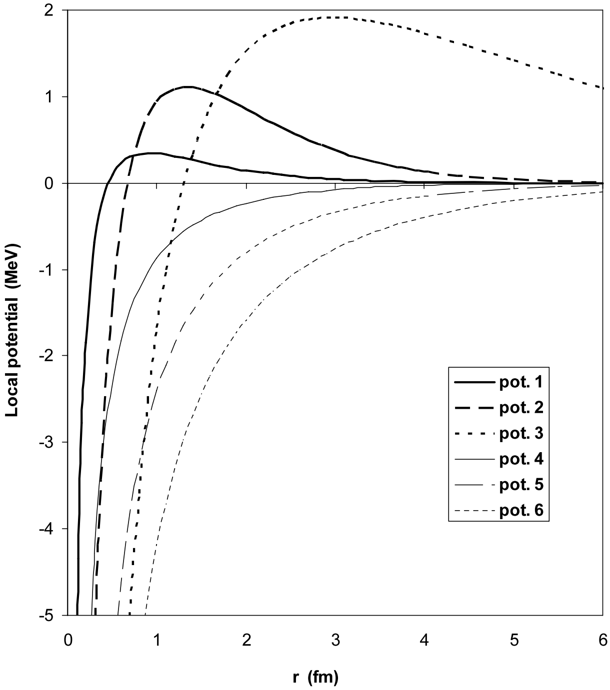


Table 1 The parameters for the nonlocal potentials of rank-two and rank-one which support a bound state with the energy $E_b = -1.00$ MeV

Pot.	$a_{\ell,1}$ (fm $^{-1}$)	$a_{\ell,2}$ (fm $^{-1}$)	$\lambda_{\ell,1}$ (MeV)	$\lambda_{\ell,2}$ (MeV)
1 ($\ell = 0$)	2.5	3.0	20.00	−33.23
2 ($\ell = 1$)	2.5	3.0	20.00	−29.50
3 ($\ell = 2$)	2.5	3.0	20.00	−27.30
4 ($\ell = 0$)	2.0	0.0	−4.50	0.00
5 ($\ell = 1$)	2.0	0.0	−3.12	0.00
6 ($\ell = 2$)	2.0	0.0	−2.86	0.00

p-plane. The explicit expressions for the s-, p- and d-wave interactions have been presented in Appendix B. Moreover, some graphical results for a specific bound state are given in Fig. 1.

4 Nonlocal Potential and Its Statistical Properties

For low density and moderate temperature, the effect of exchange symmetry plays a minor role and the system obeys the Boltzmann statistics. In this work, we assume that only binary correlations are taken into account in formulating thermodynamic properties. The N-particle the partition function for our system which includes free particles and independent correlated pairs, can be written as [23]

$$Z_{N,\ell} = \frac{1}{N!} \sum_{N_c}^{[N/2]} \frac{N!}{(N-2N_c)!N_c!2^{N_c}} Z_1^{N-2N_c} (2Z_2^{U_\ell})^{N_c} \tag{35}$$

where

$$Z_2^{U_\ell} \equiv \frac{1}{2}\,\mathrm{Tr}\,\hat{U}_\ell(T) \tag{36}$$

is the correlated pairs partition function which includes trace of binary Ursell operator and $Z_1 = W/\Lambda^3$, is free particle partition function, in which $\Lambda \equiv h/\sqrt{2\pi\mu k_B T}$ is the thermal de Broglie wavelength for relative motion, and W will be used for the volume.

In (35) N_c is the possible numbers of correlated pairs. Therefore using (35), the N-particle the partition function for the system can be approximated as

$$Z_{N,\ell} = \frac{Z_1^N}{N!}\left(1 + \frac{Z_2^{U_\ell}}{Z_1^2}\right)^{\frac{N}{2}} \tag{37}$$

The relation between N-particle partition function, $Z_{N,\ell}$ and the partial Helmholtz function can be shown as

$$A_\ell(N, W, T) = -NkT\ln\left(\frac{eW}{N\Lambda^3}\right) - NkT\ln\left(1 + \frac{Z_2^{U_\ell}}{Z_1^2}\right)^{\frac{1}{2}} \tag{38}$$

The various thermodynamic properties of the system such as partial energy, pressure and entropy, can be derived from (38) that includes evaluation of the correlated pairs partition function $Z_2^{U_\ell}$. It is obvious from (2) that, evaluation of $Z_2^{U_\ell}$ requires calculation of the trace (Tr) of the resolvent operator $\hat{R}_\ell(z)$. Considering only the ℓ-wave correlation, and using (18), the trace of operator $\hat{R}_\ell(z)$ for the rank-two interaction can be written as

$$\begin{aligned}\mathrm{Tr}[\hat{R}_\ell(z)] &= \int \langle \boldsymbol{p}|\hat{R}_\ell(z)|\boldsymbol{p}\rangle d\boldsymbol{p} = (2\mu)^2 \int \frac{1}{(p^2-q^2)^2}\langle \boldsymbol{p}|\hat{T}_\ell(z)|\boldsymbol{p}\rangle d\boldsymbol{p}\\ &= (4\pi)(2\mu)^2\frac{(2l+1)}{d_\ell(q)}\sum_{i,j=1}^{2} N_{\ell,i}N_{\ell,j}\tau_{\ell,ij}(q)I_{\ell,ij}^{(2)}(q)\end{aligned} \tag{39}$$

where $I_{\ell,ij}^{(2)}(q)$ is defined as

$$I_{\ell,ij}^{(2)}(q) \equiv \int_0^\infty \frac{p^{2\ell+2}}{(p^2+a_{\ell,i}^2)^{\ell+1}(p^2+a_{\ell,j}^2)^{\ell+1}(q^2-p^2)^2}dp \tag{40}$$

Therefore, using the equations of (2) and (39), the correlated pairs partition function for the ℓth partial wave, $Z_2^{U_\ell} \equiv \frac{1}{2}\,\mathrm{Tr}\,U_\ell$ can be obtained as

$$Z_2^{U_\ell} = \frac{1}{2\pi i}\sum_{i,j=1}^{n} N_{\ell,i}N_{\ell,j}\left(\int_C \frac{(4\pi)(2\mu)(2\ell+1)}{d_\ell(q)}\tau_{\ell,ij}(q)I_{\ell,ij}^{(2)}(q)e^{-\frac{\beta q^2}{2\mu}}q\,dq\right) \tag{41}$$

The integrand of the obtained equation can be expanded in terms of its poles, which includes correlated-state and structural poles. Therefore, $Z_2^{U_\ell}$ can be evaluated analytically. Moreover, the partial second virial coefficient $B_\ell(T)$ is related to the correlated pairs partition function as

$$B_\ell(T) = -\frac{\Lambda^3}{2}Z_2^{U_\ell} \tag{42}$$

The equation (38) for the partial Helmhotz function can be written approximately as

$$A_\ell(N,W,T) \approx -NkT \ln\left(\frac{eW}{\Lambda^3}\right) - NkT\frac{\Lambda^3 Z_2^{U_\ell}}{W} \tag{43}$$

The partial energy per particle ε_l would then be

$$\varepsilon_\ell(T) = \frac{1}{N}\left(A_\ell - T\left(\frac{\partial A_\ell}{\partial T}\right)_{N,W}\right) = \frac{3}{2}kT + kT^2\frac{d(\Lambda^3 Z_2^{U_\ell})}{dT} \tag{44}$$

In terms of molecular quantities, the last term of (44) can be explicitly expressed in a number of different ways

$$\begin{aligned} kT^2\frac{d(\Lambda^3 Z_2^{U_\ell})}{dT} &= -\frac{3}{2}kT\left(\frac{\Lambda^3}{2}\operatorname{Tr}\hat{U}_\ell\right) + \frac{\Lambda^3}{2}\operatorname{Tr}(\hat{H}_\ell e^{-\beta\hat{H}_\ell} - \hat{H}_0 e^{-\beta\hat{H}_0}) \\ &= \frac{\Lambda^3}{2}\operatorname{Tr}\left[\left(\hat{H}_\ell - \frac{3}{2}kT\right)e^{-\beta\hat{H}_\ell} - \left(\hat{H}_0 - \frac{3}{2}kT\right)e^{-\beta\hat{H}_0}\right] \\ &= \frac{\Lambda^3}{2}\operatorname{Tr}\left[\left(\hat{H}_0 - \frac{3}{2}kT\right)\hat{U}_\ell + (\hat{V}_\ell e^{-\beta\hat{H}_\ell})\right] \end{aligned} \tag{45}$$

while the first term is what arises by direct differentiation of $\hat{U}_\ell(T)$, the second form demonstrates how each of total and free particle energies deviates from $\frac{3}{2}kT$. The third form splits the energy into kinetic

$$\varepsilon^K \equiv \frac{3}{2}kT + \frac{\Lambda^3}{2}\operatorname{Tr}\left[\left(\hat{H}_0 - \frac{3}{2}kT\right)\hat{U}_\ell\right] \tag{46}$$

and potential

$$\varepsilon^V = \frac{\Lambda^3}{2}\operatorname{Tr}(\hat{V}_\ell e^{-\beta\hat{H}_\ell}) \tag{47}$$

energy part. The kinetic energy consists of the usual classical value of $\frac{3}{2}kT$ plus a quantum correction $\varepsilon^K_{q,\ell}$ from the noncommutation of position and momentum in the Ursell operator.

Using (46), quantum correction of the kinetic energy for particular value of ℓ, $\varepsilon^K_{q,\ell}$ can be written as

$$\varepsilon^K_{q,\ell} = \frac{\Lambda^3}{2}(\operatorname{Tr}(\hat{H}_0\hat{U}_\ell) - 3kTZ_2^{U_\ell}) \tag{48}$$

Using (2), (4) and (14), the first trace is given by

$$\operatorname{Tr}(\hat{H}_0\hat{U}_l) = \frac{1}{2\pi i}\sum_{i,j=1}^{n} N_{\ell,i}N_{\ell,j}\left(\int_C \frac{(4\pi)(2\ell+1)}{d_\ell(q)}\tau_{\ell,ij}(q)I^{(3)}_{\ell,ij}(q)e^{-\frac{\beta q^2}{2\mu}}q\,dq\right) \tag{49}$$

where $I^{(3)}_{\ell,ij}(q)$ is defined as

$$I^{(3)}_{\ell,ij}(q) \equiv \int_0^\infty \frac{p^{2\ell+4}}{(p^2+a^2_{\ell,i})^{\ell+1}(p^2+a^2_{\ell,j})^{\ell+1}(q^2-p^2)^2}dp \tag{50}$$

Substituting (50) in (39) leads to an explicit expression for $\varepsilon^{K}_{q,l}$.

Furthermore, the pressure can be separated into kinetic and the virial pressure P_{virial} contributions. The virial form for the pressure that is due to collisions can be shown as [24]

$$\begin{aligned} P_{virial,\ell} &= -\frac{\Lambda^3}{2}\operatorname{Tr}\left(\frac{2}{3}\hat{H}_0\hat{U}_\ell\right) \\ &= -\frac{\Lambda^3}{6}\operatorname{Tr}(\hat{r}\cdot\hat{\nabla}\hat{V}_\ell e^{-\beta\hat{H}_\ell}) \end{aligned} \tag{51}$$

Inserting (49) in first form of (51) leads to the following expression for the partial $P_{virial,\ell}$ as

$$P_{virial,\ell} = -\frac{2}{3}\frac{\Lambda^3}{2\pi i}\int_c \frac{(2\ell+1)(4\pi)}{d_\ell(q)}\sum_{i,j=1}^{2}\tau_{\ell,ij}(q)I^{(3)}_{\ell,ij}(q)e^{-\frac{\beta q^2}{2\mu}}q\,dq \tag{52}$$

It can be shown that the pole expansion of the integrands of (41), (49) and (52), leads to the analytic expressions for the related integrals, in term of the complementary error function [25]

$$\zeta(z) = \frac{1}{i\pi}\int_{-\infty}^{\infty}\frac{e^{-t^2}}{t-z}dt = e^{-z^2}\operatorname{erfc}(-iz) \quad (\operatorname{Im} z > 0) \tag{53}$$

The details of the method can be found in our previous work, [2].

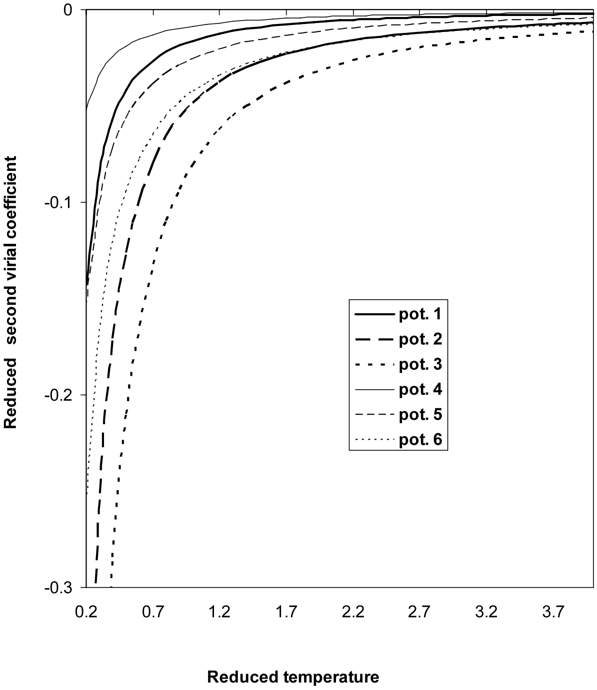
5 Results and Discussion

We have shown how the equilibrium statistical mechanics relations to be related to the partial transition matrix which includes all information of the scattering processes taking place in the thermodynamic system consisting of free particles and independent correlated pairs, interacting via the separable non-local potential of rank two in the ℓth partial wave. In fact the presented work describes a dilute gas in which binary correlations are important. Using a rank-two separable potential with Yamaguchi type form factor leads to solvability of the model and algebraic expressions for most quantities of interest.

The resonance poles of the partial transition matrix, which located on the complex q-plane, are obtained by calculating the zeros of (16) $d_\ell(q_j) = 0$. The qualitative features of every pole position depend on the values of potential parameters for particular values of ℓ. In the other hand, all the required integrals for calculation of the partition function and the other thermodynamic properties which appear in (41), (49) and (52) have the same poles as the transition matrix and pole expansion of these equations leads to the direct and analytic relation between thermodynamic properties and the resonance poles of the partial transition matrix (the correlated states).

Moreover, it is shown that the obtained equivalent local potentials of the nonlocal interactions by (33), can explain the behaviour of the calculated thermodynamic properties well. The equivalent local potentials of the nonlocal interactions of Table 1 are shown in Fig. 1 where all of these potentials support one bound state with the same value of $E_b = -1$ MeV. We can divide these potentials in two classes; the cases 1–3 are rank-two and it is seen that they are similar in shape, and have an attractive strength at short distances. Another aspect of these potentials should be noted, namely, the existence of a hump, which suggests a repulsion in the interaction region. We can see that for the rank-two interactions, the ranges

Fig. 2 Reduced second virial coeficient for the nonlocal interactions of Table 1



of attraction and repulsion increase with increasing the value of ℓ. The second class of the nonlocal potentials, the cases 4–6, are rank-one interactions. It is shown in Fig. 1 that the studied rank-one potentials loose repulsion humps and create attraction at wider range in comparison with the cases 1–3. The above-mentioned properties of the potentials play the axial role in determination of thermodynamic properties of the studied system.

In Figs. 2–5, we plot, the second virial coefficient, interaction part of the total energy, quantum correction for the kinetic energy, and the reduced virial pressure as a function of reduced temperature respectively. As can be seen from the figures, all of the studied properties grow monotonically towards the zero value at infinite temperature. The attractive strength of the equivalent local potentials of all cases become deeper (more negative value) with increasing the value of ℓ where leads to more negative values for the properties like the second virial coefficient (Fig. 2) and interaction part of the total energy (Fig. 3) at wide rang of the temperature. The existence of repulsion humps in the cases 1–3 are responsible to the more positive values of quantum correction for the kinetic energy in comparison with the cases 4–6, see Fig. 4. We can use the second expression of (51) for virial pressure, to explain Fig. 5. We can see from the second expression of (51) that virial pressure is appropriate to $-\frac{\partial V_\ell(r)}{\partial r}$ in the r-space where can be used to understanding Fig. 5 where $V_\ell(r)$ is substituted by the equivalent local potentials of the nolocal interactions.

In this paper, the thermodynamic properties have been calculated using the Boltzmann statistics. The application of the presented formulation for a system that obeys the quantum statistics will be reported in the future publications.

Fig. 3 Interaction part of reduced total energy for the nonlocal interactions of Table 1

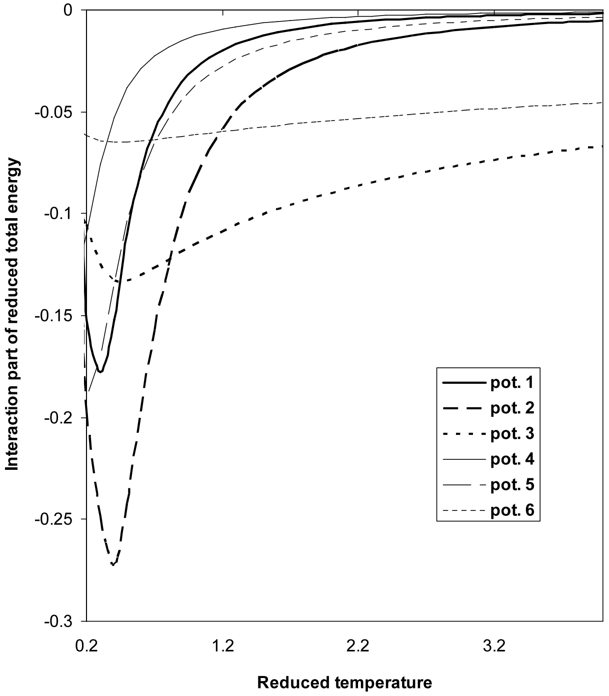
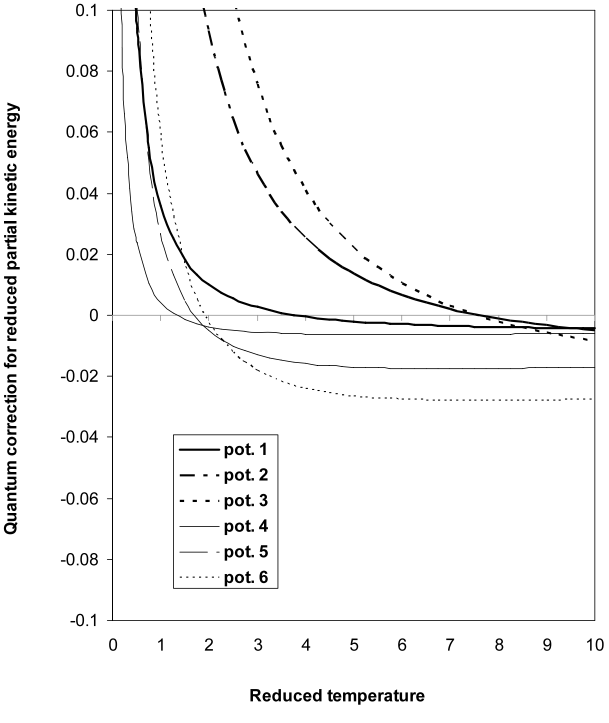


Fig. 4 Quantum correction for reduced kinetic energy for the nonlocal interactions of Table 1



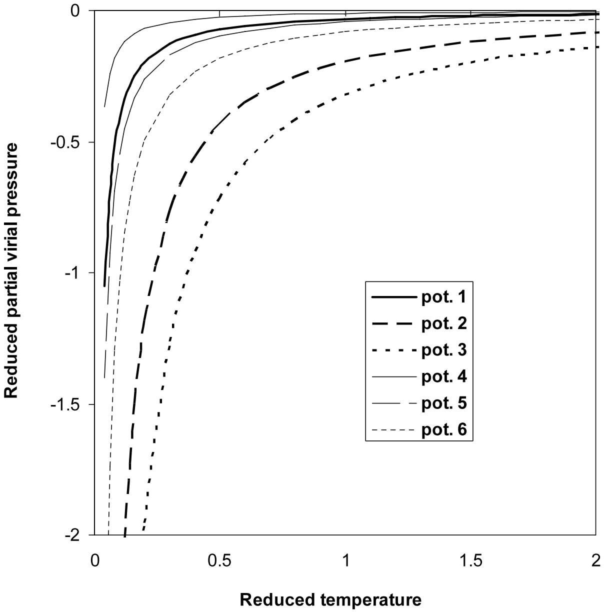


Fig. 5 Reduced virial pressure for the nonlocal interactions of Table 1

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Appendix A

The expressions required for evaluation of scattering and thermodynamic properties of (s-, p- and d-wave) separable potentials are as follows:

$$I^{(1)}_{\ell=0,ij}(q) = \frac{(a_{1,i}a_{1,j})^{1/2}}{2\pi(q+ia_{0,i})(q+ia_{0,j})(a_{0,i}+a_{0,j})} \tag{A.1}$$

$$I^{(2)}_{\ell=0,ij}(q) = \frac{i(a_{1,i}a_{1,j})^{1/2}(-2iq+a_{0,i}+a_{0,j})}{4\pi q(q+ia_{0,i})^2(q+ia_{0,j})^2(a_{0,i}+a_{0,j})} \tag{A.2}$$

$$I^{(3)}_{\ell=0,ij}(q) = -\frac{i(a_{1,i}a_{1,j})^{1/2}(a_{0,i}(q+2ia_{0,j})+qa_{0,j})}{4\pi(q+ia_{0,i})^2(q+ia_{0,j})^2(a_{0,i}+a_{0,j})} \tag{A.3}$$

$$I^{(1)}_{\ell=1,ij}(q) = \frac{2(a_{1,i}a_{1,j})^{3/2}(a_{1,i}(2iq-a_{1,j})+q(q+2ia_{1,j}))}{\pi(q+ia_{1,i})^2(q+ia_{1,j})^2(a_{1,i}+a_{1,j})^3} \tag{A.4}$$

$$I^{(2)}_{\ell=1,ij}(q) = \frac{2(a_{1,i}a_{1,j})^{3/2}(q^2+3ia_{1,i}(q+2ia_{1,j})+3ia_{1,j}q-(a^2_{1,i}+a^2_{1,j}))}{\pi(q+ia_{1,i})^3(q+ia_{1,j})^3(a_{1,i}+a_{1,j})^3} \tag{A.5}$$

$$I^{(3)}_{\ell=1,ij}(q) = \frac{2(a_{1,i}a_{1,j})^{3/2}(3qa_{1,i}a_{1,j}(q+ia_{1,j})+q^2a^2_{1,j}+a^2_{1,i}(q^2+3ia_{1,j}-a^2_{1,j}))}{\pi(q+ia_{1,i})^3(q+ia_{1,j})^3(a_{1,i}+a_{1,j})^3} \tag{A.6}$$

$$\begin{aligned} I^{(1)}_{\ell=2,ij}(q) = {} & 8(a_{2,i}a_{2,j})^{5/2}(3q^4 + q^2 a_{2,j}(9iq - 8a_{2,j}) + iqa_{2,i}(9q^2 + 22iqa_{2,j} - 9a^2_{2,j}) \\ & + a^2_{2,1}(-8q^2 + 3a_{2,j}(-3iq + a_{2,j}))) \\ & /(3\pi(q + ia_{2,i})^3(q + ia_{2,j})^3(a_{2,i} + a_{2,j})^5) \end{aligned} \tag{A.7}$$

$$\begin{aligned} I^{(2)}_{\ell=2,ij}(q) = {} & 8(a_{2,i}a_{2,j})^{5/2}(3q^4 + 4iqa_{2,j}(q + ia_{2,j})(3q + ia_{2,j}) + a^3_{2,i}(-4iq + a_{2,j}) \\ & + a^2_{2,i}(-16q^2 - 24iqa_{2,j} + 5a^2_{2,j}) + a_{2,i}(12iq^3 - 38q^2 a_{2,j} - 24iqa^2_{2,j} + a^3_{2,j}) \\ & /(3\pi(q + ia_{2,i})^4(q + ia_{2,j})^4(a_{2,i} + a_{2,j})^5) \end{aligned} \tag{A.8}$$

$$\begin{aligned} I^{(3)}_{\ell=2,ij}(q) = {} & 8(a_{2,i}a_{2,j})^{5/2}(q^2 a_{2,i}a_{2,j}(q + 4ia_{2,j})(5q + 4ia_{2,j}) \\ & + qa^2_{2,i}(q^3 + 24iq^2 a_{2,j} - 38qa^2_{2,j} - 12ia^3_{2,j}) \\ & + q^3 a^2_{2,j}(q + 4ia_{2,j}) + a^3_{2,j}(4iq^3 + a_{2,j}(-16q^2 + 3a_{2,j}(a_{2,j} - 4iq))) \\ & /(3\pi(q + ia_{2,i})^4(q + ia_{2,j})^4(a_{2,i} + a_{2,j})^5) \end{aligned} \tag{A.9}$$

Appendix B

The expressions required for derivation of local potentials equivalent to the (s-, p- and d-wave) nonlocal separable potentials are as follows:

$$g_{0,i}(r) = \frac{a^{1/2}_{0,i}}{\sqrt{2\pi}} \frac{\exp(-a_{0,i}r)}{r} \tag{B.1}$$

$$g_{1,i}(r) = \frac{a^{3/2}_{1,i}}{\sqrt{\pi}} \exp(-a_{1,i}r) \tag{B.2}$$

$$g_{2,i}(r) = \frac{a^{5/2}_{2,i}}{\sqrt{3\pi}} r \exp(-a_{2,i}r) \tag{B.3}$$

$$R_{0,i}(r,\kappa_b) = \frac{a^{1/2}_{0,i}}{\sqrt{2\pi}} \frac{\exp(-a_{0,i}r) - \exp(-\kappa_b r)}{r(\kappa_b^2 - a^2_{0,i})} \tag{B.4}$$

$$\begin{aligned} R_{1,i}(r,\kappa_b) = {} & \frac{a^{3/2}_{1,i}}{\sqrt{\pi}} \frac{\exp(-a_{1,i}r)}{r^2(\kappa_b^2 - a^2_{1,i})^2} \\ & \times [2\exp((a_{1,i} - \kappa_b)r)(1 + r\kappa_b) + r^2(\kappa_b^2 - a^2_{1,i}) - 2ra_{1,i} - 2] \end{aligned} \tag{B.5}$$

$$\begin{aligned} R_{2,i}(r,\kappa_b) = {} & \frac{1}{\sqrt{3\pi}} \frac{a^{5/2}_{2,i}}{r^3(\kappa_b^2 - a^2_{2,i})^3} \times [8\exp(-\kappa_b r)(r^2\kappa_b^2 + 3\kappa_b r - 3) \\ & + \exp(-a_{2,i}r)((24 - 4r^2\kappa_b^2 + r^4\kappa_b^4 + 4r^3 a^3_{2,i} + r^4 a^4_{2,i}) \\ & - 2ra_{2,i}(r^2\kappa_b^2 - 6)(2 + ra_{2,i}))] \end{aligned} \tag{B.6}$$

$$b_{0,i}(\kappa_b) = \frac{1}{4\pi(\kappa_b + a_{0,i})^2} \tag{B.7}$$

$$b_{1,i}(\kappa_b) = \frac{(\kappa_b^2 + 4\kappa_b a_{1,i} + a_{1,i}^2)}{4\pi(\kappa_b + a_{1,i})^4} \tag{B.8}$$

$$b_{2,i}(\kappa_b) = \frac{(3\kappa_b^4 + 18\kappa_b^3 a_{2,i} + 38\kappa_b^2 a_{2,i}^2 + 18\kappa_b a_{2,i}^3 + 3a_{2,i}^4)}{12\pi(\kappa_b + a_{2,i})^6} \tag{B.9}$$

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