Second virial coefficient for one dimensional system *

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This work is dedicated to the memory of S.P.Merkuriev.

1 Introduction

Exactly solvable models are very important in the modern statistical physics. Such models can give essential information about investigating physical objects. Unfortunately these models can not posses all properties of the real systems. But analytical exact solutions give us possibility to carry out calculations of very important quantities, which can not be done for the real ones, or can be done only numerically. One of the most popular models in statistical mechanics is the model of hard core spheres. This model have been used to investigate properties of the second ([8,9]) and third ([10]) virial coefficients. Even phase transitions can be observed in this model [7].

Another method which allows one to construct exactly solvable quantum mechanical problems is the method of zero range potentials [5] which is wide spread in mathematical, nuclear and atomic physics [1,4]. Meanwhile constructions in the framework of the method of zero range potentials are rather poor to give a realible description of many real physical processes. Moreover direct application of the zero range potentials method to some

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physical problems can lead to paradoxes ([4]). This method is based on the theory of selfadjoint extensions for symmetric operators [2]. Standard Fermi delta potential can be generalized considering selfadjoint extensions with some additional degrees of freedom. This method of zero range potentials with internal structure was developed first in [14,15]. Rigorous mathematical treatment of the two- and three-body scattering problems in one dimension can be found in [12,13]. The first three-body exactly solvable model with Fermi delta potentials was considered in [3].

Present paper is devoted to the second virial coefficient which is investigated for the case of one-dimensional particles. We chose this system as one of the simplest models in statistical physics which gives nontrivial results. We discuss the method of zero-range potentials applied to this problem. It is shown that the standard Fermi zero-range potentials leads to a "nonphysical" behaviour of the cluster integral. Considering of the additional space of interactions gives us possibility to prepare a realistic model of the problem. Exact calculation of the second cluster integral for the model operator is carried out. Important high and low temperature limits are investigated.

2 Two-body hamiltonian.

We shall consider in this section model scattering problem for two one-dimensional particles. Interaction between the particles will be introduced with the help of the extensions theory for selfadjoint operators. The spectrum and the eigenfunctions for this model operator can be calculated exactly and expressed in terms of the elementary functions.

We start from the orthogonal sum of the unperturbed kinetic operator for two one-dimensional particles $\mathcal{A} = -d^2/dx^2$ and some finite dimensional operator $\mathcal{A}_{in}$ acting in the othogonal sum of the Hilbert spaces $L_2(\mathbf{R}) \oplus H_{in}$. Restriction of the differential operator on the set of functions vanishing with the first derivative in a neighbourhood of the origin gives us symmetric operator $\mathcal{A}_0 \oplus \mathcal{A}_{in}, Dom(\mathcal{A}_0) = \{u \in W_2^2(\mathbf{R}), u(0) = 0, u'(0) = 0\}$ (after a closure). The adjoint operator is given by the formula $\mathcal{A}_0^* \oplus \mathcal{A}_{in}, Dom(\mathcal{A}_0^*) = \{u \in W_2^2(\mathbf{R} \setminus \{0\})\}$. Operator with the interaction will be defined as follows:

$$\mathcal{L}\begin{pmatrix} u \\ u_{in} \end{pmatrix} = \begin{pmatrix} \mathcal{A}_0 u \\ \mathcal{A}_{in} u_{in} + \left(a[\frac{du}{dx}]|_{x=0} + b\{u\}|_{x=0}\right) < u_{in}, \theta > \end{pmatrix},$$

where $\theta \in H_{in}, a$ and b are real numbers, $< *, * >$ denotes the scalar product in the internal space H_{in}. Vector θ and numbers a, b are parameters of the interaction. The bracket and the brace denote the jump and the average value of the function:

$$[f]|_x = \lim_{y \to x+0} f(y) - \lim_{y \to x-0} f(y),$$

$$2\{f\}|_x = \lim_{y \to x+0} f(y) + \lim_{y \to x-0} f(y).$$

The operator $\mathcal{L}$ is a selfadjoint operator on the domain of functions from $Dom(\mathcal{A}_0^*) \oplus H_{in}$ satisfying the boundary conditions

$$\left(c[\frac{du}{dx}] + d\{u\} \right) |_{x=0} =< u_{in}, \theta >,$$

$$[u]|_{x=0} = 0, \tag{1}$$

with real parameters c and d, such that

$$\det \left| \begin{array}{cc} a & b \\ c & d \end{array} \right| = -1. \tag{2}$$

Proof of this result can be carried out following the papers [12,13].

Constructed operator can be investigated in details. Equation for the eigenfunction $\Psi(\lambda) = (\psi(\lambda, x), \psi_{in}(\lambda))$ corresponding to the energy λ can be reduced to the Hemgholtz equation for the first component in $L_2(\mathbf{R})$

$$-\frac{d^2}{dx^2}\psi(\lambda, x) = \lambda \psi(\lambda, x) \tag{3}$$

with the energy dependent boundary conditions at the origin:

$$[\frac{d\psi}{dx}] \, |_{x=0} = -\mathcal{D}(\lambda)\{\psi\} \, |_{x=0} = 0$$

$$[\psi] \, |_{x=0} = 0. \tag{4}$$

The function $\mathcal{D}(\lambda)$ is defined by the internal operator and parameters θ, a, b, c, d:

$$\mathcal{D}(\lambda) = \frac{b\mathbf{R}(\lambda) + d}{a\mathbf{R}(\lambda) + c}, \quad \mathbf{R}(\lambda) =< (\mathcal{A}_{in} - \lambda)^{-1}\theta, \theta > . \tag{5}$$

It is a function with the positive imaginary part in the upper half plane of the spectral parameter λ. We note that the standard method of zero-range potentials [1,4] gives the same boundary conditions but with some real constant $\mathcal{D}$.

The two-body scattering matrix can be introduced using the following ansatz for the continuous spectrum eigenfunctions:

$$\psi(\lambda, x) = \frac{1}{\sqrt{2\pi k}} \begin{cases} e^{\imath kx} + R(k)e^{-\imath kx}, & x < 0; \\ T(k)e^{\imath kx}, & x > 0. \end{cases} . \tag{6}$$

The transition and reflection coefficients can be calculted from the boundary conditions

$$T(k) = \frac{2ik}{\mathcal{D}(k^2) + 2ik} \quad R(k) = \frac{-\mathcal{D}(k^2)}{\mathcal{D}(k^2) + 2ik}. \tag{7}$$

The dispersion equation for the eigenvalues $-\xi_s^2$

$$2\xi_s = \mathcal{D}(-\xi_s^2) \tag{8}$$

has finite number of negative solutions.

3 The second cluster integral

The second virial coefficient can be calculated using the second cluster integral B. Contributions of the discrete and continuous spectrums to the cluster integral can be separated:

$$B = B_d + B_c. \tag{9}$$

The discrete spectrum contribution B_d is given by the following expression

$$B_d = \sum_{\sigma_d} e^{\gamma \xi_s^2} \tag{10}$$

where the sum is taken over all bound states and $-\xi_s^2$ are the energies of the bound states; $\gamma = (k_B T)^{-1}$, k_B - Boltzman constant, T - the absolute temperature. This sum can be calculated using the dispersion relations (8) .

To calculate the contribution of the continuous spectrum the corresponding integral should be regularized because continuous spectrum eigenfunctions are not square integrable on the real axis:

$$B_c = \int_{\sigma_c} dE \int_{-\infty}^{+\infty} dx(\mid \psi(E,x) \mid^2 - \mid \psi_0(E,x) \mid^2) e^{-\gamma E} \tag{11}$$

Here the first integral is the integral over the continuous spectrum with the measure $dE = 2k\,dk$. The function $\psi_0(E,x)$ is the eigenfunction of the unperturbed operator. The eigenfunctions of the perturbed and original operators should be normalized by the standard condition:

$$\int_{-\infty}^{+\infty} \psi(\lambda,x)\overline{\psi}(\lambda',x)dx = \delta(\lambda-\lambda').$$

The probability density of the perturbed state characterized by the function $|\psi|^2$ is reduced by the probability density of the unperturbed (free) state (function $|\psi_0|^2$). The regularisation mentioned above leads to the exclusion of the free state probability. The integrals in (11) don't diverge contrary to the ordinary form of the second cluster integral [11]. In order to calculate B_c we shall use the orthogonal decomposition of $L_2(\mathbf{R})$ on the subspaces of the symmetric and antisymmetric functions:

$$\psi(\lambda,x) = \psi_s(\lambda,x) + \psi_a(\lambda,x),$$

where

$$\psi_s(\lambda,x) = \frac{1}{2}(\psi(\lambda,x) + \psi(\lambda,-x)),$$

$$\psi_a(\lambda,x) = \frac{1}{2}(\psi(\lambda,x) - \psi(\lambda,-x)).$$

According to (4) the antisymmetric wave ψ_a isn't perturbed by the boundary condition and consequently coincides with the free one. The continuous spectrum contribution can be calculated integrating the symmetric waves only

$$\psi_s(E,x) = \frac{1}{2\sqrt{2\pi k}}(e^{-ik|x|} + S(k)e^{ik|x|}) \tag{12}$$

where

$$S(k) = T(k) + R(k) = \frac{2ik - \mathcal{D}(k^2)}{2ik + \mathcal{D}(k^2)} \tag{13}$$

and

$$\psi_{0\ s}(E,x) = \frac{1}{2\sqrt{2\pi k}}(e^{-ik|x|} + e^{ik|x|}) \tag{14}$$

As the result B_c can be expressed by the following formula:

$$B_c = \frac{1}{2\pi}\int_0^{+\infty} dk \int_0^{+\infty} dx((S(k)-1)e^{2ikx} + (\overline{S(k)}-1)e^{-2ikx})e^{-\gamma k^2}. \tag{15}$$

This integral can be transformed to the integral over the real line with respect to the spectral parameter k. In this way a delta-functional singularity should be extracted:

$$B_c = \frac{S(0)-1}{4} + \frac{1}{2\pi}\int_{-\infty}^{+\infty} dk \int_0^{+\infty} dx (S(k)-S(0)) e^{2ikx} e^{-\gamma k^2} \tag{16}$$

and we have the following expression for the continuous spectrum contribution into the cluster integral

$$B_c = \frac{S(0)-1}{4} + \frac{\imath}{4\pi}\int_{-\infty}^{+\infty} dk \frac{S(k)-S(0)}{k} e^{-\gamma k^2}. \tag{17}$$

4 Low and high temperature limits.

In this section the limits of the cluster integral for the high and low values of the absolute temperature will be investigated. The limits of the bound states contribution B_d can be easily calculated and we restrict our consideration to the continuous spectrum part only.

The low temperature asymptotics of B_c can be calculated with the help of the steepest descent method

$$B_c \sim_{T\to 0} \frac{S(0)-1}{4} + \frac{i}{4\pi}\sqrt{\frac{\pi}{\gamma}}\frac{dS}{dk} \mid_{k=0} . \tag{18}$$

The derivative of the scattering matrix at the origin is pure imaginary $\frac{dS}{dk} \mid_{k=0} = \Im(\frac{dS}{dk} \mid_{k=0})$ and the asymptotic expansion for B_c is real. Then the asymptotics of B_c at low temperatures is given by the following expression:

$$B_c(T) \sim_{T\to 0} \frac{S(0)-1}{4} + \sqrt{T}\frac{\imath}{4}\sqrt{\frac{k_B}{\pi}}\frac{dS}{dk} \mid_{k=0} .$$

Zero order term vanishes if no zero energy resonance or bound state is present. In this case $S(0) = 1$ and B_c vanishes like $\sqrt{T}$. We want to underline that this condition coincides with the condition obtained for the usual Schroedinger equation with the potentials from the Faddeev class $\int_0^\infty |xV(x)|dx < \infty$ (see [6]). Standard zero-range potentials gives the scattering matrices $S(k)$ such that $S(0) = -1$ and $B_c \mid_{T=0}$ is not trivial in this case. Using zero range potentials with internal structure one can consider this condition as some

additional restriction on the model. It leads to the following restriction on the function $\mathcal{D}(\lambda)$

$$\mathcal{D}(0) = 0. \tag{19}$$

This condition can be easily satisfied for a special choice of the parameters.

For the large values of the absolute temperature $T \to \infty$ formula (17) can be simplified

$$B_c = \frac{\imath}{4\pi} \int_{-\infty}^{+\infty} dk \frac{S(k) - 1}{k}. \tag{20}$$

We notice that this integral exists iff

$$S(k) \to_{|k| \to \infty} S(0). \tag{21}$$

This condition is not satisfied for the standard zero-range potentials $\mathcal{D} = const$, and it gives another one restriction on our model. Combining conditions (19,21) we get the following restriction on the function $\mathcal{D}(\lambda)$

$$\mathcal{D}(\lambda) \to_{\lambda \to \infty} 0. \tag{22}$$

Conditions (19,21) define natural vanishing of the quantum corrections after the transition to the classical case $S(k) \to_{|k| \to \infty} 1$, which takes place at hight temperatures (large values of k). The function $S(k)$ in this case can be presented by finite Blaschke product as a ratio of two rational functions

$$S(k) = \prod_{j=1}^{n} \frac{k + k_j}{k - k_j}. \tag{23}$$

Then the continuous part of the cluster integral for large temperatures is given by the following expression

$$B_c \sim_{T \to \infty} - \sum_{\Im k_j > 0} \prod_{l \neq j} \frac{k_l + k_j}{k_l - k_j}. \tag{24}$$

Formula for the low temperature asymptotics can be simplified also. Using the representation (23) the function $dS/dk \mid_{k=0}$ can be calculated explicitely

$$\frac{dS}{dk} \mid_{k=0} = 2 \sum_{l=1}^{n} \frac{1}{k_l}.$$

Then the asymptotic expansion has the form

$$B_c \sim_{T\to 0} \sqrt{T}\frac{\imath}{2}\sqrt{\frac{k_B}{\pi}}\sum_{l=1}^{n}\frac{1}{k_l}.$$

Two restrictions on the model were introduced during the calculation of the limits for the continuous spectrum contribution into the cluster integral. These two conditions can be satisfied for the zero range potentials with internal structure only. Constructed model problem can be used for the calculation of the third cluster integral (see [13]).

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