Energy spectrum of interacting gas: cluster expansion method

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Abstract: In this paper, we calculate the energy spectrum of interacting gases by converting the cluster expansion method in statistical mechanics into a method of solving energy eigenvalues. We obtain an explicit expression of the energy eigenvalue, by which we can calculate the eigenvalue of an interacting gas from the interparticle potential directly. As an example, we calculate the energy spectrum for an interacting gas with soft-sphere potentials.

Keywords: Interacting gas, Energy spectrum, Cluster expansion, Soft-sphere gas.

1. Introduction

The energy spectrum of an interacting many-body system, in principle, can be obtained by solving the eigenequation of the Hamiltonian $H$:

$$H\psi = E\psi,$$

where $E$ is the energy eigenvalue and $\psi$ is the eigenfunction. However, it is very difficult to solve the eigenequation (1.1) for interacting many-body systems. In this paper, instead of solving eigenequations, we solve the energy spectrum based on the cluster expansion in statistical mechanics. This approach comes from an observation of the partition function. The partition function is defined as

$$Z(\beta) = \sum_s e^{-\beta E_s},$$

where $\beta = \frac{1}{kT}$ and the sum runs over all states. If the energy eigenvalue $E_s$ is known, the partition function $Z(\beta)$ can be obtained by performing the sum in Eq. (1.2). However, if what we know is the partition function rather than the energy eigenvalue, then Eq. (1.2) is a sum (or, equivalently, an integral) equation of eigenvalues. This inspires us that when the partition function is known, we can seek the energy eigenvalue by solving the sum (an integral) equation (1.2). In statistical mechanics, many methods have been developed for calculating partition functions, which do not need to know the energy eigenvalues in advance. Therefore, we can first work out the partition function in statistical mechanics, and then solve the energy eigenvalue by solving the sum (integral) equation (1.2).

In statistical mechanics, mechanical quantities are replaced by their average values. Taking average, of course, loses information. Let us see what information is lost and what information is retained after averaging. The definition of the partition function (1.2) contains only eigenvalues, but no eigenfunctions. That is, after the statistical average, the eigenfunction information is lost, but the eigenvalue information is retained. It is worth noting that all the eigenvalue information is retained in the partition function. This is because although the partition function is an average value, it is the average value of all temperatures, i.e., the average value is a function of temperature. In other words, the partition function is not...
a single average value, but an infinite number of average values, as informative as all the eigenvalues. All thermodynamic quantities can be calculated from the partition function, so the thermodynamic quantity also contains eigenvalue information. In this paper, we take the partition function as an example to illustrate the method. The method is also applicable to various thermodynamic quantities.

The method directly solves the eigenvalue from the partition function, without solving the eigenfunction at the same time. Seeking a method for solving eigenvalues without solving the eigenfunctions is important in quantum mechanics. Recall that in quantum mechanics, in most cases, even if we do not need the eigenfunction, we still usually have to solve the eigenfunction at the same time when solving the eigenvalue. For example, in perturbation theory, in order to solve the $n$-th order perturbation of eigenvalues, we must first solve the $(n-1)$-th order perturbation of eigenfunctions. The partition function contains the information of eigenvalues, but the information of the eigenfunction has been averaged out. Therefore, only the eigenvalue can be extracted from the partition function. In fact, this is just the advantage of this method: solving eigenvalues without solving eigenfunctions at the same time. In statistical mechanics, many methods for calculating partition functions have been developed, which calculate the partition function without knowing the eigenvalues in advance, such as the cluster expansion method. Our method converts a method for calculating partition functions and thermodynamic quantities in statistical mechanics into a method of calculating the energy eigenvalue of interacting gas systems.

In this paper, using the method, we find an explicit expression for the energy eigenvalue of interacting gases. By this result, we can calculate the energy eigenvalue from the interparticle potential directly.

The method is based on the canonical partition function. As long as the canonical partition function is known, the energy eigenvalue spectrum can be calculated using the method. Many methods for calculating the canonical partition function are developed [1–7], such as the cluster expansion [8–12]. Canonical partition functions are also calculated through the virial expansion [13–15]. The eigenvalue spectrum of interacting many-body systems is an important problem and many methods are developed [16–19], such as classical limit of the quantum-mechanical canonical partition function [20], the effect of particle-wall interactions on gases [21], and the configuration-interaction method [22]. Quantum gases are important topics in statistical mechanics [23–26]. The energy spectrum of gas systems are studied, such as interacting as Bose gases [27].

In section 3, we calculate the cluster expansion for the canonical partition function. In section 4, we calculate the cluster expansion for the spectral counting function. In section 5, we construct an equation for energy eigenvalues. In section 6, we calculate the energy spectrum of an interacting gas with soft-sphere potentials. Conclusions are given in section 7.

2. Cluster expansion of energy spectrum for interacting many-body system: scheme

The main aim of this paper is to convert the cluster expansion method in statistical mechanics into a method for solving the energy eigenvalue of interacting gases. By this method, the perturbation series of the energy eigenvalue of an interacting gas can be expressed in terms of the cluster expansion coefficient, as long as the interparticle potential is given.

2.1. Equation of energy spectrum of interacting many-body system

Calculating the energy spectrum from the canonical partition function follows two steps. *Calculating spectral counting function from canonical partition function.* Both the partition function and the counting function are spectral functions, i.e., functions defined by
eigenvalues. For the Hamiltonian whose eigenvalue spectrum is \( \{E_n\} \), the canonical partition function is defined as

\[
Z(\beta) = \sum_n e^{-\beta E_n},
\]  

(2.1)

the spectral counting function \( \Omega(E) \) is defined as the number of eigenvalues less than \( E \):

\[
\Omega(E) = \sum_n \theta(E - E_n).
\]  

(2.2)

In Refs. [28–30], we prove a relation between the spectral counting function and the canonical partition function:

\[
\Omega(E) = \mathcal{L}^{-1} \left[ \frac{Z(\beta)}{\beta} \right] + c,
\]

(2.3)

where \( \mathcal{L}^{-1} \) denotes the inverse Laplace transform. By this relation, we can calculate the spectral counting function from the canonical partition function.

*Calculating energy spectrum from spectral counting function.* The \( n \)-th eigenvalue \( E_n \) can be solved from the equation [28,31]:

\[
\Omega(E_n) = n.
\]  

(2.4)

As long as the spectral counting function is known, the energy spectrum can be solved.

2.2. Cluster expansion of canonical partition function

The cluster expansion method works in grand canonical ensembles. In order to use the method of calculating the eigenvalue described in section 2.1, we need canonical partition functions rather than grand canonical partition functions. This requires us to construct cluster expansions for canonical partition functions. Based on the mathematical result of the integer partition function and the symmetric function [32–35], we suggest a method which allows us to calculate the cluster expansion of canonical partition functions from the cluster expansion of grand canonical partition functions [36].

In Ref. [36], we give an expression of canonical partition functions expressed by quantum and classical cluster expansion coefficients for \( N \)-particle interacting gases:

\[
Z(\beta,N) = \frac{1}{N!} B_N(\Gamma_1,\ldots,\Gamma_N).
\]  

(2.5)

Here \( B_N(\Gamma_1,\ldots,\Gamma_N) \) is the Bell polynomial [36], where \( \Gamma_i = \frac{\mu V}{\lambda} b_i \) with \( b_i \) the cluster-expansion coefficient [37], \( \lambda = \hbar \sqrt{\frac{\mu}{2m}} \) the thermal wavelength, and \( V \) the volume. It should be noted that for classical gases, \( Z(\beta,N) = B_N(\Gamma_1,\ldots,\Gamma_N) \), while for identical-particle gases, \( Z(\beta,N) = \frac{1}{N!} B_N(\Gamma_1,\ldots,\Gamma_N) \).

3. Cluster expansion of canonical partition function

In this section, we calculate the cluster expansion of canonical partition functions.
The Bell polynomial in the canonical partition function (2.5) can be expressed as [36]

\[
B_N(\Gamma_1, \ldots, \Gamma_N) = \det \begin{bmatrix}
\Gamma_1 & C^1_{N-1} \Gamma_2 & C^2_{N-2} \Gamma_3 & \cdots & \cdots & \Gamma_N \\
-1 & \Gamma_1 & C^1_{N-2} \Gamma_2 & \cdots & \cdots & \Gamma_{N-1} \\
0 & -1 & \Gamma_1 & \cdots & \cdots & \Gamma_{N-2} \\
0 & 0 & -1 & \cdots & \cdots & \Gamma_{N-3} \\
\vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & -1 & \Gamma_1 
\end{bmatrix},
\]

(3.1)

where \( C^q_p = \frac{p!}{q!(p-q)!} \). Writing the canonical partition function (2.5) as

\[
Z(\beta, N) = \frac{1}{N! \left( \frac{V}{\lambda^3} \right)^N} \det(1 - A)
\]

with

\[
A = \begin{bmatrix}
0 & -2b_2 & -3b_3 & \cdots & \cdots & -Nb_N \\
(N-1)\frac{\lambda^3}{V} & 0 & -2b_2 & \cdots & \cdots & -(N-1)b_{N-1} \\
0 & (N-2)\frac{\lambda^3}{V} & 0 & \cdots & \cdots & -(N-2)b_{N-2} \\
0 & 0 & (N-3)\frac{\lambda^3}{V} & \cdots & \cdots & -(N-3)b_{N-3} \\
\vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & 1\frac{\lambda^3}{V} & 0
\end{bmatrix}
\]

(3.3)

Note that here \( b_1 = 1 \).

We rewrite the determinant in Eq. (3.2) as

\[
det(1 - A) = \exp(\ln[det(1 - A)])
\]

\[
= \exp(\text{tr}[\ln(1 - A)])
\]

(3.4)

and for weak interparticle interactions we expand the determinant:

\[
det(1 - A) = \exp \left( -\sum_{n=1}^{\infty} \frac{\text{tr}A^n}{n} \right)
\]

\[
= 1 - \text{tr}A - \frac{1}{2} \text{tr}A^2 - \frac{1}{3} \text{tr}A^3 + \cdots.
\]

(3.5)

It should be noted that since according to Eq. (3.3) \( \text{tr}A = 0 \), there are no cross terms in the first three orders of the expansion, and the cross term will appear in higher-order terms. In this paper, we only consider the first three-order contributions.

From Eq. (3.3) we obtain

\[
\text{tr}A = 0,
\]

\[
\text{tr}A^2 = -2N(N-1)\frac{\lambda^3}{V} b_2,
\]

\[
\text{tr}A^3 = -3N(N-1)(N-2)\left( \frac{\lambda^3}{V} \right)^2 b_3,
\]

\[
\cdots.
\]

(3.6)

The canonical partition function then reads

\[
Z(\beta, N) = \frac{1}{N! \left( \frac{V}{\lambda^3} \right)^N} + \frac{1}{(N-2)! \left( \frac{V}{\lambda^3} \right)^{N-1}} b_2 + \frac{1}{(N-3)! \left( \frac{V}{\lambda^3} \right)^{N-2}} b_3 + \cdots.
\]

(3.7)
This is the canonical partition function of an \( N \) particle interacting gas expressed by the cluster expansion coefficient \( b_l \).

The cluster expansion coefficient \( b_l \) here is obtained in the grand canonical ensemble, which can be expressed by the two-particle function

\[
f_{ij} \equiv e^{-\beta u_{ij}} - 1
\]

with \( u_{ij} \) the two-particle interaction [37]:

\[
b_2 = \frac{1}{2!A^3V} \int f_{12}d^3r_1d^3r_2,
\]

\[
b_3 = \frac{1}{3!A^3V} \int (f_{12}f_{13} + f_{12}f_{23} + f_{13}f_{23} + f_{12}f_{13}f_{23})d^3r_1d^3r_2d^3r_3, ...
\]

Substituting Eq. (3.9) into Eq. (3.7) gives

\[
Z(\beta,N) = \frac{V^N}{N!} \left( \frac{2\pi m}{\hbar^3 N} \right)^{\frac{3N}{2}} + \frac{V^{N-2}}{2!(N-2)!} \left( \frac{2\pi m}{\hbar^3 N} \right)^{\frac{3N}{2}} \int f_{12}d^3r_1d^3r_2
\]

\[
+ \frac{V^{N-3}}{3!(N-3)!} \left( \frac{2\pi m}{\hbar^3 N} \right)^{\frac{3N}{2}} \int (f_{12}f_{13} + f_{12}f_{23} + f_{13}f_{23} + f_{12}f_{13}f_{23})d^3r_1d^3r_2d^3r_3 + ... .
\]

\[
(3.10)
\]

4. Cluster expansion of spectral counting function

According to the scheme illustrated in section 2, we calculate the spectral counting function \( \Omega(E) \) using the relation (2.3). Substituting the canonical partition function (3.10) into Eq. (2.3), we have

\[
\Omega(E) = \frac{V^N}{N!} \left( \frac{2\pi m}{\hbar^3 N} \right)^{\frac{3N}{2}} \mathcal{L}^{-1} \left[ \beta^{-\frac{3N}{2}-1} \right]
\]

\[
+ \frac{V^{N-2}}{2!(N-2)!} \left( \frac{2\pi m}{\hbar^3 N} \right)^{\frac{3N}{2}} \mathcal{L}^{-1} \left[ \beta^{-\frac{3N}{2}-1} \int d^3r_1d^3r_2f_{12} \right]
\]

\[
+ \frac{V^{N-3}}{3!(N-3)!} \left( \frac{2\pi m}{\hbar^3 N} \right)^{\frac{3N}{2}} \mathcal{L}^{-1} \left[ \beta^{-\frac{3N}{2}-1} \int d^3r_1d^3r_2d^3r_3(f_{12}f_{13} + f_{12}f_{23} + f_{13}f_{23} + f_{12}f_{13}f_{23}) \right]
\]

\[
+ ... .
\]

\[
(4.1)
\]

Next, we calculate the inverse Laplace transform in Eq. (4.1) in virtue of the convolution theorem [38],

\[
\mathcal{L}^{-1}[f(s)g(s)] = F(t) * G(t) = \int_0^t F(t-\tau)G(\tau)d\tau,
\]

where \( F(t) = \mathcal{L}^{-1}[f(s)] \) and \( G(t) = \mathcal{L}^{-1}[g(s)] \).

The inverse Laplace transforms in Eq. (4.1) are

\[
\mathcal{L}^{-1}\left[ \beta^{-\frac{3N}{2}-1} \right] = \frac{E^{\frac{3N}{2}}}{\Gamma\left(\frac{3N}{2} + 1\right)} \theta(E),
\]

\[
(4.3)
\]
\[ \mathcal{L}^{-1}\left[ \beta^{-\frac{3}{2}N-1} \int d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 f_{12} \right] = \mathcal{L}^{-1}\left[ \beta^{-\frac{3}{2}N-1} \right] \ast \mathcal{L}^{-1}\left[ \int d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 f_{12} \right] \]

\[ = \int d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 \left[ \frac{E_N^{\frac{3N}{2}}}{\Gamma\left(\frac{3N}{2} + 1\right)} \theta(E) \right] \ast \tilde{f}_{12}, \quad (4.4) \]

\[ \mathcal{L}^{-1}\left[ \beta^{-\frac{3}{2}N-1} \int d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 d^3 \mathbf{r}_3 (f_{12} f_{13} + f_{12} f_{23} + f_{13} f_{23} + f_{13} f_{13} f_{23}) \right] \]

\[ = \int d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 d^3 \mathbf{r}_3 \left[ \frac{E_N^{\frac{3N}{2}}}{\Gamma\left(\frac{3N}{2} + 1\right)} \theta(E) \right] \ast (\tilde{f}_{12} \ast \tilde{f}_{13} \ast \tilde{f}_{23} \ast \tilde{f}_{13} \ast \tilde{f}_{23} \ast \tilde{f}_{13} \ast \tilde{f}_{23}), \quad (4.5) \]

where \( \tilde{f}_{ij} \) is the inverse Laplace transform of \( f_{ij} \),

\[ \tilde{f}_{ij} = \mathcal{L}^{-1}[f_{ij}] \quad (4.6) \]

and \( \theta(E) \) is the Heaviside theta function.

The spectral counting function \( (4.1) \) then reads

\[ \Omega(E) = \frac{V^N}{N!} \frac{(2\pi m)^{\frac{3N}{2}}}{\hbar^{3N}} \frac{E_N^{\frac{3N}{2}}}{\Gamma\left(\frac{3N}{2} + 1\right)} \theta(E) \]

\[ + \frac{V^{N-2}}{2!(N-2)!} \frac{(2\pi m)^{\frac{3N}{2}}}{\hbar^{3N}} \int d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 \left\{ \left[ \frac{E_N^{\frac{3N}{2}}}{\Gamma\left(\frac{3N}{2} + 1\right)} \theta(E) \right] \ast \tilde{f}_{12} \right\} \]

\[ + \frac{V^{N-3}}{3!(N-3)!} \frac{(2\pi m)^{\frac{3N}{2}}}{\hbar^{3N}} \int d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 d^3 \mathbf{r}_3 \left\{ \left[ \frac{E_N^{\frac{3N}{2}}}{\Gamma\left(\frac{3N}{2} + 1\right)} \theta(E) \right] \ast (\tilde{f}_{12} \ast \tilde{f}_{13} \ast \tilde{f}_{23} \ast \tilde{f}_{13} \ast \tilde{f}_{23} \ast \tilde{f}_{13} \ast \tilde{f}_{23}) \right\} \]

\[ + \cdots. \quad (4.7) \]

For the calculation of the second term in Eq. \( (4.7) \), we consider the inverse Laplace transform of Eq. \( (3.8) \) as

\[ \tilde{f}_{ij} = \mathcal{L}^{-1}[e^{-\beta u_{ij}} - 1] = \delta(E - u_{ij}) - \delta(E) \quad (4.8) \]

and the convolution in Eq. \( (4.7) \) can be calculated by Eq. \( (4.2) \):

\[ \left[ \frac{E_N^{\frac{3N}{2}}}{\Gamma\left(\frac{3N}{2} + 1\right)} \theta(E) \right] \ast \tilde{f}_{12} = \frac{E_N^{\frac{3N}{2}}}{\Gamma\left(\frac{3N}{2} + 1\right)} \ast [\delta(E - u_{12}) - \delta(E)] \]

\[ = \int_{\delta = 0}^{E} \frac{(E - \epsilon)^{\frac{3N}{2}}}{\Gamma\left(\frac{3N}{2} + 1\right)} \delta(\epsilon - u_{12}) d\epsilon - \int_{\delta = 0}^{E} \frac{(E - \epsilon)^{\frac{3N}{2}}}{\Gamma\left(\frac{3N}{2} + 1\right)} \delta(\epsilon) d\epsilon \]

\[ = \frac{E_N^{\frac{3N}{2}}}{\Gamma\left(\frac{3N}{2} + 1\right)} \left(1 - \frac{u_{12}}{E}\right)^{\frac{3N}{2}} \theta(E - u_{12}) - \theta(E) \right]. \quad (4.9) \]
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Then

Therefore

are used.

For the calculation of the third term in Eq. (4.7), we consider the inverse Laplace transform of \( \hat{f}_{ij} \) and \( \hat{f}_{hl} \) and \( \hat{f}_{hl} \). A direct calculation gives

Then

Therefore

Then the spectral counting function (4.7) becomes

\[
\begin{align*}
\Omega(E) &= \frac{V^N (2\pi m)^{\frac{3N}{2}}}{N! h^{3N}} \frac{E^{\frac{3N}{2}}}{\Gamma(\frac{3N}{2} + 1)} \theta(E) + \frac{V^N (2\pi m)^{\frac{3N}{2}}}{3!(N - 2)! h^{3N}} \frac{E^{\frac{3N}{2}}}{\Gamma(\frac{3N}{2} + 1)} \times \left[ \frac{1}{V^2} \int d^3 r_1 d^3 r_2 \left( 1 - \frac{u_{12}}{E} \right)^{\frac{3N}{2}} \theta(E - u_{12}) - \theta(E) \right] + \frac{V^N (2\pi m)^{\frac{3N}{2}}}{h^{3N}} \frac{E^{\frac{3N}{2}}}{\Gamma(\frac{3N}{2} + 1)} \times \left[ \frac{1}{V^2} \int d^3 r_1 d^3 r_2 \left( 1 - \frac{u_{12} + u_{13} + u_{23}}{E} \right)^{\frac{3N}{2}} \theta(E - (u_{12} + u_{13} + u_{23})) \right] \\
&\quad - \frac{1}{V^2} \int d^3 r_1 d^3 r_2 \left( 1 - \frac{u_{12}}{E} \right)^{\frac{3N}{2}} \theta(E - u_{12}) - \frac{1}{V^2} \int d^3 r_1 d^3 r_3 \left( 1 - \frac{u_{13}}{E} \right)^{\frac{3N}{2}} \theta(E - u_{13}) \\
&\quad - \frac{1}{V^2} \int d^3 r_1 d^3 r_3 \left( 1 - \frac{u_{13}}{E} \right)^{\frac{3N}{2}} \theta(E - u_{23}) + 2\theta(E) \nu^5. \tag{4.14}
\end{align*}
\]
Expanding (4.14) by use of \((1 - \frac{a}{E})^{2N} \approx 1 - \frac{3N}{2} \frac{a}{E} + \frac{3N(3N-2)}{8} \frac{a^2}{E^2} + \cdots\) gives

\[
\Omega(E) = \sum_{k=0}^{2N} (-1)^k \frac{c_k}{\Gamma(1 + \frac{3N}{2} - k)} E^{\frac{3N}{2} - k}
\]

\[
= \frac{c_0}{\Gamma\left(\frac{3N}{2} + 1\right)} E^{\frac{3N}{2}} - \frac{c_1}{\Gamma\left(\frac{3N}{2}\right)} E^{\frac{3N}{2} - 1} + \frac{c_2}{\Gamma\left(\frac{3N}{2} - 1\right)} E^{\frac{3N}{2} - 2} - \frac{c_3}{\Gamma\left(\frac{3N}{2} - 2\right)} E^{\frac{3N}{2} - 3} + \cdots, \quad (4.15)
\]

where

\[
c_0 = \frac{V^N}{N!} \frac{(2\pi m)^{\frac{3N}{2}}}{\hbar^{3N}} \left\{ \frac{(N-2)(N-3)(2N+1)}{6} \theta(E) - \frac{N(N+1)(N-5)}{3! V^2} \int d^3r_1 d^3r_2 \theta(E - u_{12}) - \frac{N(N-1)(N-2)}{3! V^2} \int d^3r_1 d^3r_2 \theta(E - u_{13}) - \frac{N(N-1)(N-2)}{3! V^2} \int d^3r_1 d^3r_2 d^3r_3 \theta(E - u_{12} + u_{13} + u_{23}) \right\}, \quad (4.16)
\]

\[
c_1 = \frac{1}{2!(N-2)!} \frac{V^N}{2!(N-2)!} \frac{(2\pi m)^{\frac{3N}{2}}}{\hbar^{3N}} \left\{ \frac{N-2}{3V^3} \int d^3r_1 d^3r_2 d^3r_3 (u_{12} + u_{13} + u_{23}) \right. \times \left. \theta(E - (u_{12} + u_{13} + u_{23})) \right\} - \frac{N-5}{3V^2} \int d^3r_1 d^3r_2 \theta(E - u_{12}) - \frac{N-2}{3V^2} \int d^3r_1 d^3r_2 d^3r_3 \theta(E - u_{12} + u_{13} + u_{23}) \right\}, \quad (4.17)
\]

\[
c_2 = \frac{1}{2!(N-2)!} \frac{V^N}{2!(N-2)!} \frac{(2\pi m)^{\frac{3N}{2}}}{\hbar^{3N}} \left\{ \frac{N-2}{3V^3} \int d^3r_1 d^3r_2 d^3r_3 (u_{12} + u_{13} + u_{23}) \right. \times \left. \theta(E - (u_{12} + u_{13} + u_{23})) \right\} - \frac{N-5}{3V^2} \int d^3r_1 d^3r_2 u_{12}^2 \theta(E - u_{12}) - \frac{N-2}{3V^2} \int d^3r_1 d^3r_2 d^3r_3 u_{12}^2 \theta(E - u_{23}) \right\}, \quad (4.18)
\]

5. Energy eigenvalue

Now we solve the energy eigenvalue. By Eqs. (2.4) and (4.15), we arrive at an equation of the energy eigenvalue \(E_n\):

\[
\sum_{k=0}^{2N} (-1)^k \frac{c_k}{\Gamma(1 + \frac{3N}{2} - k)} E^{\frac{3N}{2} - k} = n.
\]

We first consider the leading order contribution:

\[
\frac{c_0}{\Gamma\left(\frac{3N}{2} + 1\right)} E^{\frac{3N}{2}} = n
\]
which gives

\[ E_n = \Gamma \left( \frac{3N}{2} + 1 \right) \cdot n^{\frac{2}{3N}}. \]  \hfill (5.3)

To solve the equation, we expand \( E_n \) as [28]

\[ E_n = \frac{\Gamma \left( \frac{3N}{2} + 1 \right)}{c_0} n^{\frac{2}{3N}} + \sum_{m=0}^{\infty} \alpha_{m+1} n^{-\frac{2m}{3N}}. \]  \hfill (5.4)

Then Eq. (5.1) becomes

\[
\frac{c_0}{\Gamma \left( \frac{3N}{2} + 1 \right)} \left[ \frac{\Gamma \left( \frac{3N}{2} + 1 \right)}{c_0} n^{\frac{2}{3N}} + \alpha_1 n^0 \right]^{\frac{3N}{2}} - \frac{c_1}{\Gamma \left( \frac{3N}{2} \right)} \left[ \frac{\Gamma \left( \frac{3N}{2} + 1 \right)}{c_0} n^{\frac{2}{3N}} + \alpha_1 n^0 \right]^{\frac{3N}{2}-1} + \cdots = n. \]  \hfill (5.5)

By the Newton binomial theorem [39]

\[ (x + y)^a = \sum_{k=0}^{\infty} \binom{a}{k} x^{a-k} y^k, \]  \hfill (5.6)

where \( a \) is a real number and \( \binom{a}{k} = \frac{\Gamma(a+1)}{\Gamma(a-k+1)} \Gamma(k+1) \), we have

\[
\left[ \frac{\Gamma \left( \frac{3N}{2} + 1 \right)}{c_0} n^{\frac{2}{3N}} + \alpha_1 n^0 \right]^{\frac{3N}{2}-r} \sum_{j=0}^{r} \binom{\frac{3N}{2} - r}{j} \left[ \frac{\Gamma \left( \frac{3N}{2} + 1 \right)}{c_0} n^{\frac{2}{3N}} + \alpha_1 n^0 \right]^{\frac{3N}{2} - j} \alpha_1^j, \quad 0 \leq r \leq \frac{3N}{2}. \]  \hfill (5.7)

Then Eq. (5.5) becomes

\[
\frac{c_0}{\Gamma \left( \frac{3N}{2} + 1 \right)} \left\{ \frac{\Gamma \left( \frac{3N}{2} + 1 \right)}{c_0} n^{\frac{2}{3N}} + \alpha_1 n^0 \right\}^{\frac{3N}{2} - j} - \frac{c_1}{\Gamma \left( \frac{3N}{2} \right)} \left\{ \frac{\Gamma \left( \frac{3N}{2} + 1 \right)}{c_0} n^{\frac{2}{3N}} + \alpha_1 n^0 \right\}^{\frac{3N}{2} - j - 1} + \cdots = n. \]  \hfill (5.8)

Keeping the first- and second-order contributions, we have

\[
\frac{c_0}{\Gamma \left( \frac{3N}{2} + 1 \right)} \left\{ \frac{\Gamma \left( \frac{3N}{2} + 1 \right)}{c_0} n^{\frac{2}{3N}} + \alpha_1 n^0 \right\}^{\frac{3N}{2} - 1} \alpha_1 \}
\[
- \frac{c_1}{\Gamma \left( \frac{3N}{2} \right)} \left[ \frac{\Gamma \left( \frac{3N}{2} + 1 \right)}{c_0} n^{\frac{2}{3N}} \right]^{\frac{3N}{2} - 1} = n. \]  \hfill (5.9)

Equating the coefficients at each power of \( n \), we have

\[ \alpha_1 = 2 \frac{c_1}{\Gamma \left( \frac{3N}{2} \right)} \frac{c_0}{\Gamma \left( \frac{3N}{2} + 1 \right)} \]  \hfill (5.10)
Substituting \( \alpha_1 \) into \( E_n \), we obtain the energy eigenvalue,

\[
E_n = \frac{\Gamma(\frac{3N}{2} + 1)}{c_0^{3/2}} n^{3/2} + \frac{2}{3N} \frac{\Gamma(\frac{3N}{2} + 1)}{\Gamma(\frac{3N}{2})} c_1 n^0 + \ldots. \tag{5.11}
\]

For higher orders, we use the multinomial theorem [39]

\[
(x_1 + x_2 + \cdots + x_l)^p = \sum_{p_1+p_2+\cdots+p_l=p} \binom{p}{p_1,p_2,\ldots,p_l} \prod_{i=1}^{l} x_i^{p_i}, \tag{5.12}
\]

where \( \binom{p}{p_1,p_2,\ldots,p_l} = \frac{\Gamma(p+1)}{\Gamma(p_1+1)\Gamma(p_2+1)\cdots\Gamma(p_l+1)} \). Similar calculation gives

\[
a_2 = \frac{3N-2}{6N} c_1^2 \frac{\Gamma(\frac{3N}{2} + 1)}{\Gamma(\frac{3N}{2})} - \frac{\Gamma(\frac{3N}{2} - 1)}{\Gamma(\frac{3N}{2})} \frac{c_2}{c_0} \tag{5.13}
\]

Then the energy eigenvalue reads

\[
E_n = \frac{\Gamma(\frac{3N}{2} + 1)}{c_0^{3/2}} n^{3/2} + \frac{2}{3N} \frac{\Gamma(\frac{3N}{2} + 1)}{\Gamma(\frac{3N}{2})} c_1 n^0 + \\
\left[ \frac{3N-2}{6N} c_1^2 \frac{\Gamma(\frac{3N}{2} + 1)}{\Gamma(\frac{3N}{2})} - \frac{\Gamma(\frac{3N}{2} - 1)}{\Gamma(\frac{3N}{2})} \frac{c_2}{c_0} \right] n^{-3/2} + \ldots. \tag{5.14}
\]

In an interacting gas, there are three typical length scales: the range of the interparticle interaction, the mean particle distance, and the thermal wavelength. The range of the interparticle interaction is determined by the interparticle potential (e.g., the radius of the gaseous molecule of a soft-sphere gas), the mean particle distance is determined by the density of the gas, and the thermal wavelength is determined by the temperature. The comparison between these three typical length scales determines the properties of the gas; for example, if the thermal wavelength is greater than the mean particle distance, it is a quantum gas, and so on.

The density that determines the distance between gaseous molecules will influence the energy spectrum of a gas. This requires us to discuss the energy spectrum case by case with different gas densities.

The temperature determines the thermal wavelength. For a given density, the longer the thermal wavelength is, the larger the overlapping region of the particle wave function and the stronger the quantum exchange interaction, and vice versa.

For the cluster expansion method, the effect of the interparticle interaction is reflected in the factor \( f_{ij} = e^{-u_{ij}/(kT)} - 1 \) defined by Eq. (3.8). It can be seen from \( f_{ij} \) that the effect of the interparticle interaction decreases at high temperatures and increases at low temperatures. Although the expression of the eigenvalue (5.14) does not include the temperature, the temperature will influence the eigenvalue. The energy spectrum of gas is different at different temperatures.

Concretely, the effect of temperature on the partition function leads to the effect of temperature on the counting function and then leads to the effect of temperature on the expansion coefficient \( c_k \) in the energy spectrum. The coefficient \( c_k \) (\( k \neq 0 \)) decreases with increasing temperature. The greater \( k \), the faster \( c_k \) decreases with increasing temperature.
In other words, although the temperature does not appear in \( c_k \), the effect of temperature influences \( c_k \) through its effect on \( f_{ij} \). The higher-order contribution in the eigenvalue decreases with the temperature increase. Higher-order contributions will become important in low-temperature systems.

6. Soft-sphere gas

The soft-sphere potential is

\[
u(r) = \begin{cases} 
0, & r > D \\
v_0, & r \leq D 
\end{cases}
\] (6.1)

where \( v_0 > 0 \).

As discussed in section 5, the density influences the eigenvalue of the gas. The eigenvalue of gases with different densities is different. In the following, we discuss the energy spectrum in four density conditions, from high densities to low densities: high-density, medium-high-density, medium-low-density, and low-density cases.

High-density case: In the high-density case, \(|\mathbf{r}_1 - \mathbf{r}_2| < D\), \(|\mathbf{r}_1 - \mathbf{r}_3| < D\), and \(|\mathbf{r}_2 - \mathbf{r}_3| < D\), i.e., \( E > 3v_0 \times \frac{N(N-1)(N-2)}{3!} \), we have

\[
\int d^3r_1 d^3r_2 \phi(E - u_{ij}) = V^2,
\]

\[
\int d^3r_1 d^3r_2 \phi(u_{ij}) = V^4 \frac{4\pi D^3}{3} v_0,
\]

\[
\int d^3r_1 d^3r_2 d^3r_3 \phi(E - (u_{12} + u_{13} + u_{23})) = V \frac{5\pi^2 D^6}{6},
\]

\[
\int d^3r_1 d^3r_2 d^3r_3 (u_{12} + u_{13} + u_{23}) \phi(E - (u_{12} + u_{13} + u_{23})) = V \frac{5\pi^2 D^6}{6} 3v_0.
\] (6.2)

Then by Eqs. (4.16) and (4.17), we have

\[
c_0 = \frac{V N (2\pi m)^{3N}}{N! h^{3N}} \left( \frac{N}{3} \right) \frac{5\pi^2 D^6}{6V^2} \left( \frac{N^2 + 2(N-3)}{6} \right),
\] (6.3)

\[
c_1 = \frac{V N}{2(N-2)!} \frac{(2\pi m)^{3N}}{h^{3N}} v_0 \left( (N-2) \frac{5\pi^2 D^6}{6V^2} - (N-3) \frac{4\pi D^3}{3V} \right).
\] (6.4)

The energy eigenvalue of a soft-sphere gas, by Eq. (5.11), reads

\[
E_n = E_n^{\text{free}} \left( \frac{N!}{3} \right)^2 \frac{\left( \frac{N}{3} \right) \frac{5\pi^2 D^6}{6V^2} - \left( \frac{N^2 + 2(N-3)}{6} \right)}{h^{3N}}
\]

\[
+ \frac{N(N-1)}{2} v_0 \left( \frac{N-2}{3} \frac{5\pi^2 D^6}{6V^2} - \left( \frac{N^2 + 2(N-3)}{6} \right) \right) n^0 + \ldots,
\] (6.5)

where \( E_n^{\text{free}} \) is the energy of ideal gases:

\[
E_n^{\text{free}} = \frac{\hbar^2}{2\pi m V} \Gamma \left( \frac{3}{2} N + 1 \right) n^{3N/2}.
\] (6.6)
Medium-high-density case: In the Medium-high-density case, $|\mathbf{r}_1 - \mathbf{r}_2| < D$, $|\mathbf{r}_2 - \mathbf{r}_3| < D$, $|\mathbf{r}_1 - \mathbf{r}_3| < D$, $|\mathbf{r}_1 - \mathbf{r}_2| > D$ or $|\mathbf{r}_1 - \mathbf{r}_2| < D$, $|\mathbf{r}_1 - \mathbf{r}_3| > D$, and $|\mathbf{r}_2 - \mathbf{r}_3| < D$, i.e., $2v_0 \times \frac{N(N-1)(N-2)}{3} < E < 3v_0 \times \frac{N(N-1)(N-2)}{3}$, we have

\[
\int d^3 r_i d^3 r_j \theta(E - u_{ij}) = V^2,
\]
\[
\int d^3 r_i d^3 r_j u_{ij} \theta(E - u_{ij}) = V \frac{4\pi D^3}{3} v_0,
\]
\[
\int d^3 r_1 d^3 r_2 d^3 r_3 \theta(E - (u_{12} + u_{13} + u_{23})) = \frac{17V}{32} \left( \frac{4\pi D^3}{3} \right)^2,
\]
\[
\int d^3 r_1 d^3 r_2 d^3 r_3 (u_{12} + u_{13} + u_{23}) \theta(E - (u_{12} + u_{13} + u_{23})) = 2v_0 \frac{17V}{32} \left( \frac{4\pi D^3}{3} \right)^2.
\] (6.7)

Then by Eqs. (4.16) and (4.17), we have

\[
c_0 = \frac{V^N}{N!} \frac{(2\pi m)^\frac{3N}{2}}{\hbar^{3N}} \left[ \frac{17}{32} \left( \frac{4\pi D^3}{3} \right)^2 - \frac{(N^2 + 2)(N - 3)}{6} \right],
\] (6.8)
\[
c_1 = \frac{V^N}{2(N - 2)!} \frac{(2\pi m)^\frac{3N}{2}}{\hbar^{3N}} \frac{4\pi D^3}{3} v_0 \left[ \frac{17(N - 2)}{48} \frac{4\pi D^3}{3} - \frac{(N - 3)}{3} \right].
\] (6.9)

The energy eigenvalue of a soft-sphere gas, by Eq. (5.11), reads

\[
E_n = E_n^\text{free} \left( \frac{(N!)^\frac{2N}{2}}{N!} \right) \left[ \frac{17}{32} \left( \frac{4\pi D^3}{3} \right)^2 - \frac{(N^2 + 2)(N - 3)}{6} \right] v_0^2
\]
\[+ \frac{N(N - 1)}{2} \frac{4\pi D^3}{3} \frac{17(N - 2)}{48} \frac{4\pi D^3}{3} - \frac{(N - 3)}{3} \cdot \frac{17}{32} \left( \frac{4\pi D^3}{3} \right)^2 - \frac{(N^2 + 2)(N - 3)}{6} n^0 + \cdots.
\] (6.10)

Medium-low-density case: In the Medium-low-density case, $|\mathbf{r}_1 - \mathbf{r}_2| < D$, $|\mathbf{r}_1 - \mathbf{r}_3| > D$, $|\mathbf{r}_2 - \mathbf{r}_3| > D$, i.e., $v_0 \times \frac{N(N-1)(N-2)}{3} < E < 2v_0 \times \frac{N(N-1)(N-2)}{3}$, we have

\[
\int d^3 r_i d^3 r_j \theta(E - u_{ij}) = V^2,
\]
\[
\int d^3 r_i d^3 r_j u_{ij} \theta(E - u_{ij}) = V \frac{4\pi D^3}{3} v_0,
\]
\[
\int d^3 r_1 d^3 r_2 d^3 r_3 \theta(E - (u_{12} + u_{13} + u_{23})) = V^2 \frac{4\pi D^3}{3} \left( 1 - \frac{49\pi D^3}{24V} \right),
\]
\[
\int d^3 r_1 d^3 r_2 d^3 r_3 (u_{12} + u_{13} + u_{23}) \theta(E - (u_{12} + u_{13} + u_{23})) = V^2 \frac{4\pi D^3}{3} v_0 \left( 1 - \frac{49\pi D^3}{24V} \right).
\] (6.11)

Then by Eqs. (4.16) and (4.17), we have

\[
c_0 = \frac{V^N}{N!} \frac{(2\pi m)^\frac{3N}{2}}{\hbar^{3N}} \left[ \frac{N}{3} \frac{4\pi D^3}{3V} \left( 1 - \frac{49\pi D^3}{24V} \right) - \frac{(N^2 + 2)(N - 3)}{6} \right],
\] (6.12)
\[
c_1 = - \frac{V^N}{2(N - 2)!} \frac{(2\pi m)^\frac{3N}{2}}{\hbar^{3N}} \frac{4\pi D^3}{3V} \frac{v_0}{3} \left( 2N - 7 \right) + (N - 2) \frac{49\pi D^3}{24V}.
\] (6.13)
The energy eigenvalue of a soft-sphere gas, by Eq. (5.11), reads

\[ E_n = E_n^{\text{free}} \left( \frac{(N)! \frac{4\pi D^3}{3V}}{\left[ \frac{N}{3} \right] \frac{4\pi D^3}{3V} \left( 1 - \frac{4\pi D^3}{24V} \right) - \frac{(N^2+2)(N-3)}{6} } \right) ^{\frac{1}{3V}} - \frac{N(N-1)}{6} v_0 \frac{4\pi D^3}{3V} \left( \frac{(N) \frac{4\pi D^3}{3V} \left( 1 - \frac{4\pi D^3}{24V} \right) - \frac{(N^2+2)(N-3)}{6} } { \pi^3 } \right) ^{\frac{1}{3V}} n^0 + \cdots, v_0 < E < 2v_0. \] (6.14)

**Low-density case:** In the low-density case, \(|\mathbf{r}_1 - \mathbf{r}_2| > D, |\mathbf{r}_1 - \mathbf{r}_3| > D, |\mathbf{r}_2 - \mathbf{r}_3| > D\), i.e., \(0 < E < v_0 \times \frac{N(N-1)(N-2)}{3!}\), we have

\[ \int d^3r_i d^3r_j \theta(E - u_{ij}) = V \left( V - \frac{4\pi D^3}{3} \right), \]
\[ \int d^3r_i d^3r_j u_{ij} \theta(E - u_{ij}) = 0, \]
\[ \int d^3r_1 d^3r_2 d^3r_3 \theta(E - (u_{12} + u_{13} + u_{23})) = V^3 \left( 1 - \frac{4\pi D^3}{3V} \right), \]
\[ \int d^3r_1 d^3r_2 d^3r_3 (u_{12} + u_{13} + u_{23}) \theta(E - (u_{12} + u_{13} + u_{23})) = 0. \] (6.15)

Then by Eqs. (4.16) and (4.17), we have

\[ c_0 = \frac{V^N (2\pi m)^{\frac{3\lambda}{2}}}{N! \hbar^{3N}} \left[ 1 + \left( \frac{N}{2} \right) \frac{2N - 7 \cdot 4\pi D^3}{3V} \right], \] (6.16)
\[ c_1 = 0. \] (6.17)

The energy eigenvalue of a soft-sphere gas, by Eq. (5.11), reads

\[ E_n = E_n^{\text{free}} \left( \frac{(N)! \frac{4\pi D^3}{3V}}{\left[ \frac{N}{3} \right] \frac{4\pi D^3}{3V} \left( 1 - \frac{4\pi D^3}{24V} \right) - \frac{(N^2+2)(N-3)}{6} } \right) ^{\frac{1}{3V}}, \] (6.18)

### 7. Conclusions and outlook

In this paper, we provide a formula for the energy eigenvalue of interacting gases, by converting the cluster method in statistical mechanics into a method for calculating energy eigenvalues.

The steps to solve the energy eigenvalue spectrum are as follows. (1) Calculate the cluster expansion of canonical partition functions from the cluster expansion of grand partition functions. (2) Calculate the cluster expansion of the spectral counting function from the cluster expansion of the canonical partition function. (3) Calculate energy eigenvalues from spectral counting functions.

Using the method, we calculate the energy eigenvalue of an interacting gas with soft-sphere potentials.

The method used in this paper is to convert various statistical mechanical methods into methods of finding the energy spectrum of many-body systems. In principle, all kinds of statistical mechanics methods for solving partition functions, grand partition functions, and thermodynamic quantities can be converted into methods for solving energy spectra.

In this paper, we convert the cluster expansion method in statistical mechanics into a method to calculate the energy spectrum of interacting gases. The cluster expansion method applies to the weak degenerate gases, so the resulting energy spectrum is also for weak degenerate cases. Although the most direct way to obtain the strong degenerate result is to
convert some kind of statistical mechanical method for dealing with strong degenerate gases into a method for solving energy spectra, there is still a possibility of extending the cluster expansion method which originally applies only to weak degenerate gases into a method for dealing with strong degenerate gases. This method is based on the Padé approximant. In Ref. [40], we suggest a method that converts the virtual expansion method for high-temperature and low-density gases into a method applying to low-temperature and high-density gases. After the Padé approximant treatment, the virtual expansion method can be used to consider the BEC phase transition and calculate the low-temperature properties of Fermi gases. Similarly, the Padé approximation method suggested in Ref. [40] can also be used to extend the cluster expansion method to strong degenerate cases. Similar to the virial expansion, the cluster expansion also gives a truncated power series approximation, which is essentially a polynomial approximation. From the power series given by the cluster expansion, we can construct a rational function approximation by the Padé approximant. As can be seen from the experience in Ref. [40], this treatment will extend the method for weak degenerate to a method for strong degenerate.

The counting function, Green function, heat kernel [41], and even scattering phase shift [42,43] of a given operator $H$ are all spectral functions, defined by the eigenvalues of the operator. This work is based on the relation between counting functions and partition functions. The partition function is the trace of the local heat kernel which is the Green function of the initial-value problem of the heat-type equation defined by the operator $H$ [41]. There is also a trace formula for the operator $H$, which corresponds to its Green function [44–46]. In future works, we will consider calculating eigenvalues by trace formula from the Green function.

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