Virial coefficients expressed by heat kernel coefficients

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Abstract

In this paper, we generally expressed the virial expansion of ideal quantum gases by the heat kernel coefficients for the corresponding Laplace type operator. As examples, we give the virial coefficients for quantum gases in \(d\)-dimensional confined space and spheres, respectively. Our results show that, the relative correction from the boundary to the second virial coefficient is independent of the dimension and it always enhances the quantum exchange interaction. In \(d\)-dimensional spheres, however, the influence of the curvature enhances the quantum exchange interaction in two dimensions, but weakens it in higher dimensions \((d > 3)\).

1 Introduction

Virial expansion is a powerful tool to study the effects of interaction on the thermodynamic properties of many-particle systems [1, 2, 3]. Virial expansion is first introduced to describe weakly interacting classical gases. It expresses the equation of state of the gas as a series of the number density, and the influence of interaction is embodied in the higher-order terms. After the establishment of quantum statistical mechanics, the virial expansion becomes even more important. On the one hand, a quantum gas is usually treated in the grand canonical ensemble in order to perform the sum over the states, but this treatment introduces a non-independent parameter, the fugacity \(z\), into the equation of state. However, this parameter is eliminated in the virial expansion, which leads to an equation of state without the extra parameter. On the other hand, the virial expansion for a quantum gas directly reflects the influence of quantum exchange interaction. Even for an ideal quantum gas in which there is no classical interaction among the particles, the virial expansion contains infinite number of terms, which reflect the influence of the exchange symmetry of identical particles on the thermodynamic properties of the gas. In other words, the virial expansion contains the contributions not only from the classical interaction, but also from the quantum exchange interaction.

The heat kernel, as a kind of spectral functions, has close connections with the spectrum asymptotics [4] and other spectral functions, such as the spectral zeta function.
and the counting functions \[7\] in mathematics. Since the first several heat kernel coefficients can be analytically expressed in terms of geometric invariants of the manifold \[8, 9, 10]\, the asymptotic expansion of heat kernel, i.e., the heat kernel expansion, becomes a very important tool \[8, 11, 12]\. The heat kernel expansion has been applied in many fields of physics, such as quantum field theory \[13, 14, 15]\, quantum gravity \[16, 17]\, and string theory \[18]\. In quantum statistical mechanics, the sum over the spectrum is a key component to calculate the grand partition function, so the heat kernel approach also plays an important role \[11, 19, 20]\.

In this paper, we will discuss the virial expansion of nonrelativistic ideal quantum gases by using the approach of the heat kernel expansion. We will first give the general expressions of the virial coefficients in terms of the heat kernel coefficients. By these results, as long as the heat kernel coefficients are known, the virial expansion of the equation of state of quantum gases can be obtained straightforward. Then as examples, we will calculate the virial expansions for quantum gases in \(d\)-dimensional confined space and in \(d\)-dimensional sphere \(S^d\), respectively. According to the virial coefficients, we will analyze the influence of the boundary and the curvature on the thermodynamic properties of quantum gases.

The paper is organized as follows. In section 2, we will give the general results of the virial coefficients for ideal quantum gases expressed by the global heat kernel and the heat kernel coefficients. In section 3, we will take \(d\)-dimensional confined space and spheres as examples, and analyze the influence of the boundary and the curvature on the virial expansion. The conclusion is summarized in section 4. In Appendix A, the concrete results of the virial coefficients for ideal Bose gases in \(S^d\) are given.

2 The relation between virial coefficients and heat kernel coefficients

In statistical mechanics, quantum gases are usually treated within the grand canonical ensemble. For a nonrelativistic ideal Bose gas with a fixed particle number, the equation of state can be expressed as

\[
\frac{PV}{k_B T} = \ln \Xi = - \sum_n \ln \left(1 - z e^{-\beta \varepsilon_n}\right),
\]

(1)

\[
N = \left(z \frac{\partial}{\partial z} \ln \Xi \right)_{V,T},
\]

(2)

where \(k_B\) is the Boltzmann constant, \(\Xi\) is the grand partition function, and \(\varepsilon_n\) denotes the single-particle eigenenergies. For clarity, in the following we will only consider Bose
gases; at the end of this paper, we will show how to obtain the Fermi results from the Bose ones. Since the number of particles $N$ is a constant, the fugacity $z$ is not an independent parameter and should be eliminated from the equation of state. However, the explicit expression of the fugacity $z$ is hard to find out. Only for some special cases, $z$ is solvable and the equation of state can be expressed in an explicit form without $z$. Among them, the most important approximate method is the virial expansion. When $z \ll 1$, eqs. (1) and (2) can be expanded as serieses of $z$ so that a series solution of $z$ can be obtained. Then the form of the equation of state becomes a series of the number density of particles, which is the virial expansion.

According to eqs. (1) and (2), to obtain the equation of state of a quantum gas, one needs to know the energy spectrum $\varepsilon_n$ of the particles and to perform the sum over the spectrum in principle, but this is usually very difficult. Fortunately, this difficulty can be overcome by the help of the heat kernel approach. In the following we will generally discuss how to achieve the virial expansion of the equation of state in terms of the global heat kernel and the heat kernel expansion.

The global heat kernel of a Laplace type operator $D$ on a $d$-dimensional manifold is defined as

$$ K(t) = \sum_n e^{-\lambda_n t}, $$

where $\{\lambda_n\}$ is the spectrum of the operator $D$. When $t \ll 1$, it can be expanded as a series, which is the heat kernel expansion,

$$ K(t) \approx (4\pi t)^{-d/2} \sum_{k=0, \frac{1}{2}, 1, \cdots} B_k t^k; \quad (t \to 0) \quad (4) $$

where $B_k$ ($k = 0, 1/2, 1, \cdots$) are the heat kernel coefficients.

To deal with the sum in eq. (1), we first expand the logarithm term to a series, then exchange the order of these two sums. Concretely, when $z \ll 1$, we have

$$ \ln \Xi = \sum_{k=1}^{\infty} \frac{z^k}{k} \sum_n e^{-k\beta \varepsilon_n}. \quad (5) $$

Since the eigenenergy $\varepsilon_n$ satisfies the equation

$$ \left[ -\nabla^2 + \frac{2m}{\hbar^2} U(x) \right] \psi_n(x) = \frac{2m}{\hbar^2} \varepsilon_n \psi_n(x), \quad (6) $$

the sum in eq. (5) can be represented by the global heat kernel for the $D = -\nabla^2 + \left(\frac{2m}{\hbar^2}\right)U(x)$ as

$$ \ln \Xi = \sum_{k=1}^{\infty} \frac{1}{k} K \left( \frac{\hbar^2 \beta}{2m} \right) z^k = \sum_{k=1}^{\infty} K \left( \frac{k \lambda^2}{4\pi} \right) \frac{z^k}{k}, \quad (7) $$

3
where \( \lambda = \hbar \sqrt{2\pi \beta/m} \) is the mean thermal wavelength. Therefore, the grand potential can be expressed as a series of the global heat kernels. Similarly, we can rewrite the particle number eq. (2) as

\[
N = \sum_{k=1}^{\infty} K \left( \frac{k \lambda^2}{4\pi} \right) z^k,
\]

or

\[
n\lambda^d = \frac{\lambda^d}{V} \sum_{k=1}^{\infty} K \left( \frac{k \lambda^2}{4\pi} \right) z^k,
\]

where \( V \) is the volume of the system in \( d \)-dimensional space, and \( n = N/V \) is the number density of particles. To solve the asymptotic solution of the fugacity \( z \) from eq. (9), assume that

\[
z = \sum_{k=1}^{\infty} c_k \left( n\lambda^d \right)^k, \quad \left( n\lambda^d \ll 1 \right)
\]

Substituting it into eq. (9) gives the coefficients \( c_k \). Then from eq. (7), we can obtain the virial expansion of the equation of state as

\[
\frac{PV}{Nk_BT} = b_1 + b_2 n\lambda^d + b_3 \left( n\lambda^d \right)^2 + b_4 \left( n\lambda^d \right)^3 + \cdots,
\]

where the virial coefficients are

\[
b_1 = 1,
\]

\[
b_2 = -\frac{K \left( \frac{2\lambda^2}{4\pi} \right) V}{2K^2 \left( \frac{\lambda^2}{4\pi} \right) \lambda^d},
\]

\[
b_3 = \left[ -\frac{2K \left( \frac{3\lambda^2}{4\pi} \right)}{3K^3 \left( \frac{\lambda^2}{4\pi} \right)} + \frac{K^2 \left( \frac{2\lambda^2}{4\pi} \right)}{K^4 \left( \frac{\lambda^2}{4\pi} \right)} \right] \left( \frac{V}{\lambda^d} \right)^2,
\]

\[
b_4 = \left[ -\frac{3K \left( \frac{4\lambda^2}{4\pi} \right)}{4K^4 \left( \frac{\lambda^2}{4\pi} \right)} + \frac{3K \left( \frac{5\lambda^2}{4\pi} \right) K \left( \frac{3\lambda^2}{4\pi} \right)}{2K^6 \left( \frac{\lambda^2}{4\pi} \right)} \right] \left( \frac{V}{\lambda^d} \right)^3,
\]

\[
\vdots
\]

Thus we have expressed the virial coefficients for ideal Bose gases by the global heat kernel for the corresponding operator.

On the other hand, the exact solutions of global heat kernels are not easy to achieve, but the heat kernel expansion is easier to obtain. Expressing the virial coefficients by heat kernel coefficients will provide a more powerful way to perform the virial expansion. By use of the heat kernel expansion (11), we can write

\[
K \left( \frac{\lambda^2}{4\pi} \right) \approx \sum_{k=0,\frac{1}{2},1,\cdots}^{\infty} \frac{B_k}{(4\pi)^k} \lambda^{2k-d}.
\]
Note that the heat kernel coefficient $B_k$ has a dimension $[L]^{d-2k}$, so the sum in eq. (13) can be regarded as a series of $\lambda/\bar{L}$, where $\bar{L}$ represents the characteristic length scale of the system. This result will be seen more clearly from the specific examples in the next section.

Applying eq. (13) to the equation of the grand potential eq. (7), we arrive

$$\ln \Xi \approx \sum_{k=0, \frac{1}{2}, 1, \cdots}^{\infty} \frac{B_k}{(4\pi)^k} \lambda^{2k-d} g_{d/2+1-k} (z),$$

where

$$g_{\sigma} (z) = \frac{1}{\Gamma (\sigma)} \int_{0}^{\infty} \frac{x^{\sigma-1}}{z^{-1} e^x - 1} dx = \sum_{k=1}^{\infty} \frac{z^k}{k^\sigma}$$

is the Bose-Einstein integral. Similarly, the equation for particle number can be rewritten as

$$n \lambda^d \approx \sum_{k=0, \frac{1}{2}, 1, \cdots}^{\infty} \frac{B_k}{(4\pi)^k V} \lambda^{2k} g_{d/2+1-k} (z).$$

Eqs. (14) and (16) show that the asymptotic behavior of an ideal Bose gas always takes the form of a series of the Bose-Einstein integrals. This form of the equation of state has been used to discuss the properties of quantum gases for decades [11, 19, 20]. Since the information of shape and topology of a system, as well as the external potential, is embodied in the heat kernel coefficients, this approach is widely applied to the quantum gases, especially the phenomenon of Bose-Einstein condensation, in cavities [20, 21, 22], in external potentials [22, 23] and on different manifolds [24, 25]. For electromagnetic fields, the heat kernel expansion is an effective tool to study the Casimir effect for various geometries [26, 27, 28]. The thermodynamical properties of relativistic quantum gases and the Bose-Einstein condensation are also discussed in flat and curved space [19, 29, 30]. However, there are few works to systematically discuss the virial expansion in terms of the heat kernel expansion.

Taking advantaging of the expansion of the Bose-Einstein integral eq. (15) and following the same procedure as above, we can obtain the final result of the virial coefficients expressed by the heat kernel coefficients. However, the complete expressions are too complicated to present here, so we will divide the problem into two parts according to whether the heat kernel expansion contains half-integer power terms or not.

When the heat kernel expansion eq. (14) contains half-integer power terms, the first
several virial coefficients take the forms as

\begin{align*}
b_1 &= 1, \\
b_2 &\approx -\frac{1}{2d/2+1} + \frac{\sqrt{2} - 1}{2(2d+3)/2} \frac{\lambda B_{1/2}}{\sqrt{\pi V}} - \frac{3 - 2\sqrt{2}}{2(2d+6)/2} \left(\frac{\lambda B_{1/2}}{\sqrt{\pi V}}\right)^2, \\
b_3 &\approx -\left(\frac{2}{3d/2+1} - \frac{1}{2d}\right) + \left(\frac{\sqrt{2} - 1}{2d-1/2} + \frac{\sqrt{3} - 1}{3(2d+1)/2}\right) \frac{\lambda B_{1/2}}{\sqrt{\pi V}} + \left(\frac{3 - 2\sqrt{2}}{2d - 2 - \sqrt{3}}\right) \left(\frac{\lambda B_{1/2}}{\sqrt{\pi V}}\right)^2, \\
b_4 &\approx -\left(\frac{3}{4d/2+1} - \frac{1}{2d^2} \cdot \frac{3d/2-1}{2d+2} \cdot \frac{5}{2d^2+1}\right) + \left(\frac{3}{2d^2} + \frac{15 \left(\frac{\sqrt{2} - 1}{2d^2-1} - \frac{5\sqrt{2} - \sqrt{6} - 2}{2d^2-1}\right)}{2(d+3)/2 \cdot 2d/2+1}\right) \frac{\lambda B_{1/2}}{\sqrt{\pi V}} \\
&\quad + \left[\frac{3}{2d+3} - \frac{45 \left(\frac{3 - 2\sqrt{2}}{2d+3} + \frac{3}{2d+3} - \frac{5\sqrt{6}}{2d+3}\right)}{2d+3-1}\right] \left(\frac{\lambda B_{1/2}}{\sqrt{\pi V}}\right)^2, \quad (17)
\end{align*}

where we have used the relation \( B_0 = V \). These expressions are accurate to the second order in \( \lambda \). From eq. (17), we can find that both the terms proportional to \( \lambda^1 \) and \( \lambda^2 \) are only related to the coefficient \( B_{1/2} \). Other higher-order heat kernel coefficients only contribute higher-power terms of \( \lambda \).

When the heat kernel expansion only contains integer power terms, the virial coefficients are

\begin{align*}
b_1 &= 1, \\
b_2 &\approx -\frac{1}{2d/2+1} + \frac{1}{2d/2+5} \frac{\lambda^4 \left( B_1^2 - 2VB_2 \right)}{\pi^2 V^2}, \\
b_3 &\approx -\left(\frac{2}{3d/2+1} - \frac{1}{4d/2}\right) + \left(\frac{1}{2d^2} - \frac{1}{2d+3}\right) \frac{\lambda^4 \left( B_1^2 - 2VB_2 \right)}{\pi^2 V^2}, \\
b_4 &\approx -\left(\frac{3}{4d/2+1} - \frac{1}{2d/2} \cdot \frac{3d/2-1}{2d+2} \cdot \frac{5}{2d/2+1}\right) + \left(\frac{9}{2d+5} - \frac{1}{2d^2+2d+2} + \frac{15}{2d/2+5}\right) \frac{\lambda^4 \left( B_1^2 - 2VB_2 \right)}{\pi^2 V^2}, \quad (18)
\end{align*}

where we have also taken \( B_0 = V \). In these expressions we only include the leading correction terms which are proportional to \( \lambda^4 \). Clearly, the leading correction to the virial coefficients is related to both the heat kernel coefficients \( B_1 \) and \( B_2 \). Furthermore, the leading correction to each virial coefficient (except \( b_1 \)) has a similar form. They are all proportional to the same factor \( \lambda^4 \left( B_1^2 - 2VB_2 \right) / V^2 \), only with different numeric constants.

In the following, we will consider two specific cases as the examples of the above results.
3 Examples

3.1 \textit{d}-dimensional confined space

A thermodynamic system is usually assumed to be extensive, which implies that the effect of boundary is neglected. For a macro system, this is a good approximation, but for a small-scale system, the influence of boundary becomes large and may not be ignored. For example, when considering quantum dots or quantum wires with dimensions in the nanometer range, the effects of boundary must be included. In recent years, much research on the influence of boundary on the thermodynamic properties has been carried out \cite{21, 31, 32, 33, 34}.

Now we will consider the influence of boundary on the virial expansion of an ideal Bose gas by use of the approach given in the above section. On a manifold with boundary, the heat kernel expansion of the Laplace operator has half-integer power terms. For the Dirichlet boundary conditions, only taking the first two terms, the heat kernel expansion has the general form \cite{8}

\begin{equation}
K(t) \approx \frac{1}{(4\pi t)^{d/2}} \left(V - \frac{\sqrt{\pi}}{2} S t^{1/2}\right),
\end{equation}

where \(V\) and \(S\) represent the volume and surface area of the \(d\)-dimensional manifold, respectively. In other words, the second heat kernel coefficient has the general form \(B_{1/2} = - (\sqrt{\pi}/2) S\) in arbitrary dimensions. Substituting it into eq. \((17)\) immediately gives the virial coefficients of an ideal Bose gas in \(d\)-dimensional confined space.

Clearly, the most important correction to the thermodynamic properties of the quantum gas is described by the second virial coefficient \(b_2\). In confined space, the main contribution of the boundary is embodied in the correction to \(b_2\). To describe the correction, we introduce the relative correction parameter \(\eta\) as the ratio of the correction to \(b_2\) and its zero-order term. From eq. \((17)\), we find

\begin{equation}
\eta = \frac{2 - \sqrt{2} S \lambda}{4} V + \frac{3 - 2 \sqrt{2}}{16} \left(\frac{S \lambda}{V}\right)^2.
\end{equation}

Therefore, the relative correction is only related to the factor \(S \lambda/V\) but is independent of the dimension. It indicates that regardless of the dimension of the system, the influence of the boundary on the thermodynamic properties of quantum gases is almost the same.

In a roughly isotropic system, since \(V/S\) represents the length scale of the system \(\bar{L}\), the relative correction \(\eta\) given in eq. \((20)\) only related to the ratio of the mean wavelength and the scale of the system \(\lambda/\bar{L}\). This is consistent with the general analysis about the expansion parameter of the heat kernel expansion in last section. It indicates that eq. \((20)\) holds for small values of \(\lambda/\bar{L}\). As a result, the influence of the boundary
will become manifest for a small-scale system under a relatively low temperature, in which the mean thermal wavelength of particles is not much smaller than the scale of the system and $\lambda/L$ is not negligible. For example, in a cube with side length $L$, when the temperature satisfies $\lambda/L = 0.1$, the influence of boundary to the second virial coefficient $b_2$ is $\eta = 9.2\%$ according to eq. (20). On the other hand, in an highly anisotropic system, e.g., a long and narrow one, the ratio $S/V$ is larger, so the influence of boundary is more important in such cases.

### 3.2 $d$-dimensional sphere

In this section, we will consider the virial expansion of Bose gases when the corresponding heat kernel expansion only contains integer terms. A typical example is the heat kernel of the Laplace operator on a smooth curved manifold. For simplification, in the following we will consider the case of $d$-dimensional sphere $S^d$, which is a typical representative of constant curvature spaces.

We denote the sectional curvature of the space as $\kappa$. The heat kernel in $S^d$ can be generally expressed as

$$K_{2k+1}(\rho, t) = \frac{(-1)^k}{2^{k-1} \kappa^k \sqrt{4\pi t}} \left( \frac{\sqrt{\kappa}}{\sin(\sqrt{\kappa} \rho)} \frac{\partial}{\partial \rho} \right)^k e^{\kappa t \rho^2 - \frac{\rho^2}{4}};$$

$$K_{2k+2}(\rho, t) = \frac{(-1)^k}{2^{k+1} \sqrt{\pi k+3/2} 3^{3/2}} e^{(2k+1)^2/4 \kappa t} \left( \frac{\sqrt{\kappa}}{\sin(\sqrt{\kappa} \rho)} \frac{\partial}{\partial \rho} \right)^k \int_{\rho}^{\delta/\sqrt{|\kappa|}} \frac{\sqrt{\kappa} e^{-s^2/4}}{\sqrt{\cos(\sqrt{\kappa} \rho) - \cos(\sqrt{\kappa} s)}} ds,$$

where $\rho$ is the geodesic distance and $0 < \delta < \pi/2$. Taking trace of the heat kernel and after some calculations, we can obtain the following expressions for the global heat kernel for different dimensions.

$$K_2(t) = V \frac{e^{\kappa t}}{4\pi t} \left[ 1 + \sum_{l=1}^{\infty} \left( 2^{1-2l} - 1 \right) B_{2l} \frac{(-\kappa t)^l}{l!} \right],$$

$$K_3(t) = V \frac{e^{\kappa t}}{(4\pi t)^{3/2}},$$

$$K_4(t) = V \frac{e^{\kappa t}}{(4\pi t)^2} \left\{ 1 - \frac{\kappa t}{4} + \sum_{l=2}^{\infty} \frac{(-\kappa t)^l}{l!} \left[ (l-1) \left( 2^{1-2l} - 1 \right) B_{2l} + \frac{l}{4} \left( 2^{3-2l} - 1 \right) B_{2(l-1)} \right] \right\},$$

$$K_5(t) = V \frac{e^{\kappa t}}{(4\pi t)^{5/2}} \left( 1 - \frac{2}{3} \kappa t \right).$$

These results show a difference between odd and even dimensions. The expression for the odd dimension only contains finite number of terms but that for the even dimension
contains infinite terms, which is a natural result led by the heat kernel for different dimensions, eq. (21).

In the expressions (22), the 3-d case is special since the global heat kernel $K_3(t)$ differs to that in flat 3-d space only by an exponential factor $e^{\kappa t}$. One can generally prove that when the only difference between two heat kernels is an exponential factor, i.e., $K^{(2)}(t) = K^{(1)}(t) e^{\xi t}$, the virial coefficients related to them are the same. This result can be directly verified from eq. (12). Therefore, the virial expansion of ideal quantum gases in a 3-d sphere $S^3$ is exactly the same as that in 3-d flat space. Notice that a trivial case is that the spectra of two systems only differ by a translation, which corresponds a different choice of the zero-point energy, and this certainly does not affect the statistical or thermodynamic properties of the system. Nevertheless, the above example is different. The spectrum of the Laplace operator in a 3-d sphere has a different structure from that in 3-d flat space. The equivalence of these systems is not trivial.

Further expanding the exponential factor in eq. (22) will give the heat kernel expansion. Then the virial coefficients in the corresponding space can be obtained directly. We list the virial coefficients in different dimensions in Appendix A.

As discussed before, the influence of the curvature on the quantum gas is mainly reflected by the relative correction $\eta$, which is the proportion of the correction to $b_2$. From the results given in Appendix A, we can find that, different from the case of confined space, the relative correction in $S^d$ is tightly related the dimension. The value of $\eta$ in different dimensions are listed in Table 1, in which we only consider the leading contribution.

As shown in Table 1, the leading correction to the virial coefficient $\eta \sim (\lambda/R)^4$, where $R$ is the radius of the $d$-sphere and it also represents the length scale of the system, which is consistent with the analysis of the heat kernel expansion in last section. From Table 1, we can find the two-dimensional case is different from others. The relative correction $\eta$ in two dimensions is positive, which means that the influence of the curved space has the same sign as the quantum exchange interaction, or, the curved space enhances the quantum exchange interaction. However, in the space with $d > 3$, the sign of $\eta$ becomes negative, which means that the influence of the curvature will weaken the quantum exchange interaction, and this influence becomes larger with the increase of

| dimension | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|-----------|---|---|---|---|---|---|---|---|----|
| $\eta \left( \frac{\lambda^2}{\pi^2} \right)$ | $\frac{1}{120}$ | 0 | $-\frac{1}{120}$ | $-\frac{1}{36}$ | $-\frac{1}{16}$ | $-\frac{7}{60}$ | $-\frac{7}{36}$ | $-\frac{3}{10}$ | $-\frac{7}{16}$ |

Table 1: The leading relative correction $\eta$ in $d$-dimensional sphere.
the dimension. The three-dimensional space is the critical case, in which the correction vanishes, just as the above analysis.

4 Discussion and Conclusion

In the above sections we only consider the Bose gases for clarity. As for Fermi gases, the treatment is exactly the same, and the results only have some minor differences: Besides the grand potential changes to \( \ln \Xi = \sum_n \ln (1 + z e^{-\beta \epsilon_n}) \) and the Bose-Einstein integrals in eqs. and change to the Fermi-Dirac integrals, the main difference is that all of the even-order virial coefficients \( b_2, b_4, \cdots \) will have an extra negative sign while the odd-order ones \( b_1, b_3, \cdots \) are the same as the Bose case. Therefore, the virial expansion for Fermi gases can be obtained from the above Bose results directly.

In this paper we focus on the virial expansion, which is in principle applicable to the high temperature and low density region. The applicability range is often represented as \( n \lambda^3 \ll 1 \). However, we know that the virial expansion usually can be applied to a wider range of the parameter. Taking the 3-d flat space case as an example, in which the virial expansion for an ideal Bose gas is

\[
\frac{PV}{Nk_B T} \approx 1 - 0.1768 n \lambda^3 - 0.0033 \left( n \lambda^3 \right)^2 - 0.00011 \left( n \lambda^3 \right)^3 + \cdots .
\] (23)

Due to the rapid decrease of the virial coefficients, the approximation is usually quite good. For example, even for \( n \lambda^3 \sim 1 \), only taking into account the first two terms gives an error about 0.3%; if taking first three terms, the error is about 0.01%. As a comparison, the Bose-Einstein condensation for a free ideal gas occurs at \( n \lambda^3 \approx 2.612 \), which implies that the virial expansion is a good approximation as long as the temperature is not very closed to the critical temperature. In Ref. [36], the authors detailed analyze the applicability range of the virial expansion for relativistic pion gases and reach a similar conclusion.

Our results can be verified by experiments in small-scale systems. Since a real system exists in no more than three dimensions, in our results, those can be directly compared with experiments mainly includes two- or three-dimensional systems with boundaries and two-dimensional spheres with the length scales in the nanometer range. In experiments, the effect of boundary can be found for non-interacting real particles or quasiparticles, e.g., electrons or excitons, in some nanoparticles and nanofilms at an appropriate temperature. Our results show that the influence of boundary becomes stronger in highly anisotropic systems. The influence of curvature is expected to be observed in some systems with cage shapes, e.g., electrons in a fullerene, or quasiparticles on the surface of a spherical system, e.g., surface excitons on the surface of xenon clusters [37].
In summary, in this paper, we discuss the relation between the virial coefficients of an ideal quantum gas and the heat kernel coefficients for the corresponding Laplace type operator, and give the expressions of the virial coefficients expressed by the heat kernel coefficients. As examples, we discuss the quantum gases in confined space and in spheres in any dimensions, and give the explicit results for the virial expansions. Our results show that, in confined space, the influence of boundary is almost independent of the dimension of space, and its effect enhances the quantum exchange interaction of the gas. On the other hand, the influence of curvature on quantum gases is tightly related to the dimension of space. It can enhance \((d = 2)\) or weaken \((d > 3)\) the effect of the quantum exchange interaction.

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**Appendix A**

The first four virial coefficients for ideal Bose gases in \(d\)-dimensional spheres \(S^d\) are

1. **2-d:**
   
   \[
   \begin{align*}
   b_1 & = 1, \\
   b_2 & \approx -\frac{1}{4} - \frac{\kappa^2 \lambda^4}{2880 \pi^2} - \frac{\kappa^3 \lambda^6}{15120 \pi^3} - \frac{\kappa^4 \lambda^8}{69120 \pi^4}, \\
   b_3 & \approx \frac{1}{36} - \frac{\kappa^2 \lambda^4}{4320 \pi^2} - \frac{\kappa^3 \lambda^6}{9720 \pi^3} - \frac{\kappa^4 \lambda^8}{4354560 \pi^4}, \\
   b_4 & \approx -\frac{\kappa^2 \lambda^4}{11520 \pi^2} - \frac{\kappa^3 \lambda^6}{12096 \pi^3} - \frac{29 \kappa^4 \lambda^8}{483840 \pi^4}.
   \end{align*}
   \]

2. **3-d:**
   
   \[
   \begin{align*}
   b_1 & = 1, \\
   b_2 & = -\frac{1}{4\sqrt{2}}, \\
   b_3 & = -\left(\frac{2}{9\sqrt{3}} - \frac{1}{5}\right), \\
   b_4 & = -\left(\frac{5}{32\sqrt{2}} - \frac{1}{2\sqrt{6}} + \frac{3}{32}\right),
   \end{align*}
   \]

which are the same as those in flat space.
(3) 4-d:

\[ b_1 = 1, \]
\[ b_2 \approx -1 + \frac{\kappa^2 \lambda^4}{960 \pi^2} + \frac{\kappa^3 \lambda^6}{3360 \pi^3} + \frac{7 \kappa^4 \lambda^8}{92160 \pi^4} + \frac{61 \kappa^5 \lambda^{10}}{2956800 \pi^5}, \]
\[ b_3 \approx -\frac{5}{432} + \frac{7 \kappa^2 \lambda^4}{8640 \pi^2} + \frac{37 \kappa^3 \lambda^6}{90720 \pi^3} + \frac{989 \kappa^4 \lambda^8}{5806080 \pi^4}, \]
\[ b_4 \approx -\frac{1}{384} + \frac{5 \kappa^2 \lambda^4}{9216 \pi^2} + \frac{13 \kappa^3 \lambda^6}{32256 \pi^3}. \]

(4) 5-d:

\[ b_1 = 1, \]
\[ b_2 \approx -\frac{1}{8 \sqrt{2}} + \frac{\kappa^2 \lambda^4}{288 \sqrt{2 \pi^2}} + \frac{864 \sqrt{2 \pi^3}}{\sqrt{2 \pi^2}} + \frac{3456 \sqrt{2 \pi^4}}{\sqrt{2 \pi^3}} + \frac{15552 \sqrt{2 \pi^5}}{\sqrt{2 \pi^4}}, \]
\[ b_3 \approx \frac{1}{32} - \frac{2}{27 \sqrt{3}} + \left( \frac{1}{162 \sqrt{3}} - \frac{1}{576} \right) \frac{\kappa^2 \lambda^4}{\pi^2} - \left( \frac{1}{1728} - \frac{2}{729 \sqrt{3}} \right) \frac{\kappa^3 \lambda^6}{\pi^3} + \left( \frac{5}{5832 \sqrt{3}} - \frac{5}{41472} \right) \frac{\kappa^4 \lambda^8}{\pi^4}, \]
\[ b_4 \approx -\left( \frac{3}{128} + \frac{5}{256 \sqrt{2}} - \frac{1}{12 \sqrt{6}} \right) + \left( \frac{1}{108 \sqrt{6}} + \frac{5}{3072 \sqrt{2}} + \frac{1}{256} \right) \frac{\kappa^2 \lambda^4}{\pi^2}. \]

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