Virial expansion with Feynman diagrams

X. Leyronas

Laboratoire de Physique Statistique, Ecole Normale Supérieure, UPMC Univ Paris 06, Université Paris Diderot, CNRS, 24 rue Lhomond, 75005 Paris, France.

We present a field theoretic method for the calculation of the second and third virial coefficients $b_2$ and $b_3$ of 2-species fermions interacting via a contact interaction. The method is mostly analytic. We find a closed expression for $b_3$ in terms of the 2 and 3-body $T$-matrices. We recover numerically, at unitarity, and also in the whole BEC-BCS crossover, previous numerical results for the third virial coefficient $b_3$.

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I. INTRODUCTION

The topic of interacting ultracold fermions has witnessed some spectacular experimental developments since the first formation of a molecular Bose Einstein Condensate [1]. The Bose Einstein Condensate (BEC)-Bardeen Cooper Schrieffer (BCS) crossover has been the subject of numerous experimental and theoretical works [2]. Recently, the authors of Ref.[3] have found an accurate and elegant way of measuring the equation of state of an ultracold gas. In particular, they were able to measure the equation of state of a mixture of $^6$Li atoms in two internal states $\uparrow$ and $\downarrow$. In this experiment, the pressure was measured as a function of the chemical potential $\mu$ and the temperature $T$. The so called unitary limit (see below), where the interactions are known to be strong, was studied, starting from high temperature down to low temperature (close to the superfluid transition). In the high temperature regime, the data was compared to a virial expansion [4] 

$$P(\mu, T) = 2 T (\Lambda_T)^{-3} \left\{ z + b_2 z^2 + b_3 z^3 + \cdots + b_n z^n + \cdots \right\}$$

where $\Lambda_T = \sqrt{\frac{2 \mu}{m T}}$ is the thermal wavelength (we take $\hbar = 1$ and the Boltzmann constant $k_B = 1$). $z = e^{\beta \mu}$ is the fugacity and $\beta = \frac{1}{T}$ is the temperature. In this way, the authors of Ref.[3] were able to extract the numerical values of $b_3$ and $b_4$.

The theoretical calculation of virial coefficients started in the late 30’s with the work of Beth and Uhlenbeck [5] on the calculation of $b_2$ (see also [4] and [6]). The problem of computing $b_3$ was considered later in Ref. [7]. In the context of ultracold atoms, $b_3$ for ultracold bosons was studied in Ref. [8] and later for ultracold fermions in Refs.[9][12]. It is the goal of this paper to present a diagrammatic method to calculate $b_3$. Our results are in full agreement with Refs. [10][12] and therefore disagree with Ref.[11]. The idea of the method is that one needs to include the 3-body problem in the many-body problem if one wants to calculate $b_3$. In some sense, this is similar to the zero temperature low density expansion of Refs. [13][14]. In this work too, we will need to use the $T$-matrix of the 3-problem. Since the 3-body problem is basically solved [15][17], we can calculate $b_3$.

The paper is organized as follows. In section II the general formalism is introduced. The technical key point is to work in (imaginary) time, rather than with frequencies. In section III we apply the method to the determination of $b_2$ and recover in a rather efficient way the Beth-Uhlenbeck result [5]. Section IV is the main part of the paper, and it explains how to determine diagrammatically $b_3$. Several technical details are given in the Appendices. The main analytical results are given in Eqs.(37),(39),(33) and (45). Numerical results are shown in Fig.7 and Eq.(44). Finally, we conclude in section V.

II. GENERAL FORMALISM

We describe now the method we develop to get an expansion in power of the fugacity. We first consider the Green’s function for free fermions in imaginary time (for a general reference on diagrammatic techniques, see Ref.[18]). We have

$$G^0(p, \tau) = e^{-(\epsilon_p - \mu)\tau} \left\{ -\Theta(\tau) + n_F(\epsilon_p - \mu) \right\}$$

with $n_F(x) = (e^{\beta x} + 1)^{-1}$ and $\epsilon_p = p^2/(2m)$ is the kinetic energy of a fermion of mass $m$. $\Theta(x)$ is the Heaviside function. In the high temperature limit we consider, the fugacity $z = e^{\beta \mu}$ is smaller than one, and we can expand the Fermi-Dirac distribution according to

$$n_F(\epsilon_p - \mu) = \frac{z e^{-\beta \epsilon(p)}}{1 + z e^{-\beta \epsilon(p)}} = \sum_{n \geq 1} z^n (-1)^{n-1} e^{-n \beta \epsilon(p)}$$

From Eq.(2) and (3) we find an expansion in powers of the fugacity for the free fermions Green’s function

$$G^0(p, \tau) = e^{\beta \tau} \left[ \sum_{n \geq 0} G^{(0,n)}(p, \tau) z^n \right]$$

We have defined

$$G^{(0,0)}(p, \tau) = -\Theta(\tau) e^{-\epsilon_p \tau}$$

$$G^{(0,n)}(p, \tau) = (-1)^{n-1} e^{-\epsilon_p \tau} e^{-n \beta \epsilon(p), n \geq 1}$$
Therefore \( G^{(0,0)} \) is \textit{retarded}, while \( G^{(0,n)} \), for \( n \geq 1 \), is \textit{not retarded}. Notice that \( G^{(0,n)} \) does not depend on the chemical potential \( \mu \). Diagrammatically, since \( G^{(0,0)} \) is a retarded function, we represent it as a line with an arrow going \textit{from left to right} if increasing time goes to the right (this is the Green’s function of a particle in vacuum). On the other hand, \( G^{(0,n)} \), for \( n \geq 1 \), is not retarded, and we represent it as a \( n \)-times slashed line, which can be oriented from left to right or \textit{vice versa}. In order to calculate the virial coefficients, we expand the density \( n(\mu, T) \) (per spin species for spin 1/2 fermions) in power of the fugacity \( z = e^{\beta \mu} \).

\[
n(\mu, T) = (\Lambda_T)^{-3} \left\{ z + 2b_2z^2 + 3b_3z^3 + \cdots + nb_nz^n + \cdots \right\}
\]  

(7)

which comes from Eq. (1) and the Gibbs-Duhem identity \( n = (\partial P/\partial \mu)_T/2 \). The density per spin is related to the full Green’s function \( G(k, \tau) \) via the equation

\[
n(\mu, T) = \sum_k G(k, \tau = 0_-)
\]  

(8)

where we denote \( \sum_k = \int \frac{d^3k}{(2\pi)^3} \) in 3 dimensions.

It is convenient to define the densities \( \delta n^{(p)} \) such that

\[
n(\mu, T) = \delta n^{(1)} z + \delta n^{(2)} z^2 + \delta n^{(3)} z^3 + \cdots
\]  

(9)

The principle of the method is the following: in order to calculate \( \delta n^{(p)} \), we need to find all the diagrams for \( G_I(k, 0_-) \) of order \( z^p \). Those are the diagrams with one \( G^{(0,p)} \), or one \( G^{(0,p-1)} \) and one \( G^{(0,1)} \), or one \( G^{(0,p-2)} \) and one \( G^{(0,2)} \), or one \( G^{(0,p-2)} \) and two \( G^{(0,1)} \)'s etc. Of course, the higher the value of \( p \), the more cases we have to consider, and the calculation becomes more and more difficult. Nevertheless, we have been able to use this method for the second and third viriel coefficients \( b_2 \) and \( b_3 \). We notice immediately that in order to calculate \( n(\mu, T) \), hence \( G_I(p, 0_-) \), all the \( e^{\beta \tau} \) terms in prefactors of the \( G^{(p)} \)'s (cf. Eq. 2) cancel in the expressions. Therefore we do not consider them in the following. The chemical potential \( \mu \) therefore appears only in the fugacity.

At lowest order, we have simply \( G \approx G^{(0,0)} + z G^{(0,1)} \). \( G^{(0,0)} \) is retarded and therefore does not contribute to \( G(k, 0_-) \). Hence we find

\[
\delta n^{(1)} = \sum_k G^{(0,1)}(k, \tau = 0_-)
\]  

(10)

which is shown in the diagram of Fig. 1. The calculation is easily done using Eq. 8, and we find

\[
\delta n^{(1)} = (\Lambda_T)^{-3}
\]  

(11)

This is the ideal classical gas result.

In the following, we focus on the problem of distinguishable fermions of 2 species \( \uparrow \) (respectively \( \downarrow \)) of mass \( m_\uparrow \) (respectively \( m_\downarrow \)) typical of the BEC-BCS crossover (for a review, see [2]). Specifically, we consider equal masses \( (m_\uparrow = m_\downarrow = m) \) and equal densities (unpolarized case) or equal chemical potential \( \mu_\uparrow = \mu_\downarrow \).

III. \textbf{CALCULATION OF} \( b_2 \)

In order to calculate \( b_2 \) [19], we must consider all the diagrams with one \( G^{(0,2)} \) (Fig. 2(a)) or 2 \( G^{(0,1)} \)'s (Fig. 2(b)).

The two diagrams contributing to the viriel coefficient \( b_2 \). (a) is the diagrammatic expansion of the Fermi-Dirac distribution. (b) gives the Beth-Uhlenbeck contribution.

\[
\delta n^{(2,a)} = \sum_k G^{(0,2)}(k, \tau = 0_-)
\]  

(12)

One easily finds using Eqs. 8

\[
\delta n^{(2,a)} = -(\Lambda_T)^{-3} 2^{-3/2}
\]  

(13)

This is of course just the free fermions contribution.

We consider now the contribution of the diagram of Fig. 2(b). It contains explicitly the effect of interactions, through the 2-body \( T \) matrix. We show now that it gives the Beth-Uhlenbeck contribution [3]. The imaginary time integration is in the time domain \( \{ 0 < \tau_1 < \tau_2 < \beta \} \), corresponding to the domain for time differences \( \{ t_1 >\)
0, t_2 > 0, \beta - (t_1 + t_2) > 0 \}$. We therefore find

\[
\delta n^{(2,b)} = \sum_{k,P} \int dt_1 \, dt_2 \Theta(t_1) \Theta(t_2) \Theta(\beta - (t_1 + t_2)) \left( T_2(P, t_2) e^{-(\beta - t_2)}(\varepsilon_{\uparrow,k} + \varepsilon_{\downarrow,P-k}) \right)
\]

where $\varepsilon_{\uparrow,k} = k^2/(2m_{\uparrow,k})$. The integration on $t_1$ is easily performed and gives a factor $(\beta - t_2) \Theta(\beta - t_2)$. The remaining integral on $t_2$ (for given $P$ and $k$) is of the form

\[
I = \int dt_2 \, f_1(\beta - t_2) f_2(t_2)
\]

with $f_1$ and $f_2$ two retarded functions (i.e. which are equal to zero for a non positive argument). The convolution theorem for Laplace transforms gives

\[
I = \int \frac{ds}{2\pi i} e^{-\beta s} F_1(s) F_2(s)
\]

where $C_\gamma$ is the Bromwich contour of the problem. It is a straight line in the $s$ complex plane parallel to the imaginary axis with a given real part $\gamma$. $\gamma$ is such that the integrand is analytic to the left of the contour. We have also defined $F_1(s) = \int_0^{\infty} dx e^{sx} F_1(\tau)$ (and similarly for $F_2(s)$) for a complex variable $s$. The usual Laplace transform is defined with a minus sign in the exponential, but the usual expressions for propagators are recovered with this definition.

In our problem, we have $f_1(\tau) = T_2(P, \tau)$ and $f_2(\tau) = \tau e^{-\tau(\varepsilon_{\uparrow,k} + \varepsilon_{\downarrow,P-k})}$, and $F_1(s) = t_2(s - P^2/(2M))$, with

\[
M = m_\uparrow + m_\downarrow = 2m
\]

the total mass of the 2-body problem, and (in 3D)

\[
t_2(s) = \frac{2\pi}{m_r} \frac{1}{(a^2 - 1) - \sqrt{-2m_r s}}
\]

This expression for $t_2(s)$ is easily found by writing down the integral (ladder) equation in time and taking the Laplace transform. This is just the usual result for a dimer propagator in vacuum, with energy $s$. $a$ is the scattering length and

\[
m_r = \frac{m_\uparrow m_\downarrow}{m_\uparrow + m_\downarrow} = \frac{m}{2}
\]

the 2-body reduced mass. Next we go to the center of mass frame and make the change of variable $k = k' + (m_\uparrow/M)P$. By the change of variable $s' = s - P^2/(2M)$, the center of mass momentum $P$ decouples. The integration on $P$ gives a prefactor $(M/m_\uparrow)^{3/2}(\Lambda_T)^{-3}$. Here $\Lambda_T$ is the thermal wavelength for $\uparrow$ particles. The integration on $k'$ is also easily performed using (in 3D)

\[
\sum_{k'} \left( s' - \frac{k'^2}{2m_r} \right)^2 = \frac{(m_r)^2}{2\pi} \frac{1}{\sqrt{-2m_r s'}}
\]

Finally, we get the result

\[
\delta n^{(2,b)}(\Lambda_T)^3 = \left( \frac{M}{m_\uparrow} \right)^{3/2} \int_{C_\gamma} ds' e^{-\beta s'} \frac{t_2(s')}{\sqrt{-2m_r s'}} \frac{m_r^2}{2\pi}
\]

We show now that we recover the Beth-Uhlenbeck result [3] from Eq.[22]. The integral on the variable $s'$ is transformed by deforming the integration contour along the real axis. There comes two kinds of contributions. The first contribution comes from the molecular pole of $t_2(s)$ (if there is one) at the molecular energy $-|E_0| = -1/(2m_r a^2)$. The second contribution comes from the branch cut along the positive part of the real axis (physically the continuum of scattering states). We finally get for the contribution to the density

\[
\delta n^{(2,b)}(\Lambda_T)^3 = \left( \frac{M}{m_\uparrow} \right)^{3/2} \{ \bar{n}_{mol} + \bar{n}_{scatt} \}
\]

with

\[
\bar{n}_{mol} = e^{\beta |E_0|}, \text{if } a > 0
\]

\[
= 0, \text{if } a \leq 0
\]

\[
\bar{n}_{scatt} = \frac{1}{\pi} \int_0^{\infty} dx e^{-\beta x} \frac{m_r}{\sqrt{2m_r x}} \frac{a^{-1}}{(a^2 + 2m_r x)}
\]

We can recover the Beth-Uhlenbeck [3] result by making the change of variable $x = p^2/(2m_r)$

\[
\bar{n}_{scatt} = \frac{1}{\pi} \int_0^{\infty} dp e^{-\beta p^2} \frac{a}{(1 + p^2 a^2)}
\]

For equal masses, $(m_\uparrow = m_\downarrow)$ we have for the second order virial coefficient $b_2$

\[
b_2 = 2^{-5/2} = \sqrt{2} (\bar{n}_{mol} + \bar{n}_{scatt})
\]

where $\bar{n}_{mol}$ is given by Eqs.[24],[25] and $\bar{n}_{scatt}$ by Eq.[27]. In the unitary limit, if $a \rightarrow +\infty$ we find from Eqs.[25],[27] $\bar{n}_{mol} = 1$ and $\bar{n}_{scatt} = -1/2$ thus (for equal masses $m_\uparrow = m_\downarrow$) $\delta n^{(2,b)}(\Lambda_T)^3 = \sqrt{2}$ (corresponding to $b_2 = 2/\sqrt{2}$ [20]). If $a \rightarrow -\infty$, $\bar{n}_{mol} = 0$ and $\bar{n}_{scatt} = 1/2$ and we find the same result.

IV. CALCULATION OF $b_3$

We now come to the calculation of the third virial coefficient $b_3$, which is the main result of this work. We focus on the 3D situation but the method works in any dimension. We proceed following the general method presented in section [1] and developed in section [II]. We want to gather all the diagrams of order $z^3$. There are three sorts of diagrams (the partition number of 3) : 1) with one $G^{(0,3)}$, 2) with one $G^{(0,2)}$ and one $G^{(0,1)}$, 3) with three $G^{(0,1)}$’s. We will denote the corresponding corrections
to the density $\delta n^{(3,1)}$, $\delta n^{(3,2)}$,... and $\delta n^{(3,3)}$ (there are several contributions in the last two cases).

The diagram 1 is nothing but the free fermion result and it amounts to expand the Fermi-Dirac distribution in power of $z$. This is a standard result, and we find for the density the correction for free fermions (in $d = 3$ dimensions)

$$\delta n^{(3,1)} \Lambda_T^3 = 3^{-3/2} \tag{29}$$

\textbf{A.} $\delta n^{(3,2)}$

The diagrams with one $G^{(0,2)}$ and one $G^{(0,1)}$ are shown in Fig.\ 3. The diagrams of Fig. 3(a) and 3(b) are very similar to the diagram of Fig.2(b). Indeed, by noticing that $G^{(0,2)}(k, -(t_1 + t_2)) = (-e^{-\beta s})G^{(0,1)}(k, -(t_1 + t_2))$ we just have to multiply the time integral in Eq. (14) by $-e^{-\beta s}$ in order to get the contribution of diagram of Fig. 3(a). We can therefore skip directly to Eq. (16) in order to evaluate the time integrals. Then we make the following change of variables (the Jacobian is unity).

$$s' = s - \frac{P^2}{4m} \tag{30}$$

$$k' = k - \frac{1}{2}P \tag{31}$$

$$P' = \frac{2}{3} (k + P) \tag{32}$$

The integral on $P'$ decouples and can be done analytically. The angular integration on $k'$ can also be performed, and we get

$$\delta n^{(3,2,a)} \Lambda_T^3 = \frac{8}{3\sqrt{3}} \int_0^{+\infty} \frac{dk'}{2\pi} e^{-\beta s} \int_0^{\infty} \frac{ds'}{2\pi} e^{-\beta s'} \frac{t_2(s')}{(s' - \frac{k'^2}{2mr})^2} \tag{33}$$

The diagram of Fig. 3(b) can be calculated along the same line. We just have to exchange the role of $\uparrow$ and $\downarrow$ particles. As a result we find

$$\delta n^{(3,2,b)} = \delta n^{(3,2,a)} \tag{34}$$

At unitarity ($a^{-1} = 0$), the integrals can be done analytically.

$$\delta n^{(3,2,a)} \Lambda_T^3 = \delta n^{(3,2,b)} \Lambda_T^3 = -\left(\frac{8}{3\sqrt{3}} - \frac{2}{3\pi}\right) \approx -0.300994 \tag{35}$$

\textbf{B.} $\delta n^{(3,3)}$

We want to find all the diagrams with three $G^{(0,1)}$ propagators. A given diagram always contains an incoming $k\uparrow$ line to the imaginary time $\tau = 0$. The initial time of this fermionic line must be in the interval $[0, \beta]$. Therefore, this line can not correspond to a retarded propagator $G^{(0,0)}$, and it must be a $G^{(0,1)}$ (slashed) line. A given diagram also always contains an outgoing $k\uparrow$ line from the imaginary time $\tau = 0$. This can be a $G^{(0,1)}$ (slashed) line (first case) or a retarded $G^{(0,0)}$ line (second case).

\begin{itemize}
  \item \textbf{1.} $\delta n^{(3,3,1)}$
  
  In the first case, the only possible diagram is shown in Fig. 4 and is similar to diagrams of Figs. 2(b) and Fig. 3. If we follow the same line of reasoning than for the calculation of these diagrams, we easily find
  
  $$\delta n^{(3,3,1)} = \delta n^{(3,2,a)} \tag{36}$$

  \item \textbf{2.} $\delta n^{(3,3,2)}$
  
  The second case is the most interesting. A general diagram is drawn in Fig. 5. It contains two $G^{(0,1)}$'s and
FIG. 4: The diagram contributing to $\delta n^{(3,3,1)}$

FIG. 5: The general structure of a diagram contributing to $\delta n^{(3,3,2)}$

\[
\delta n^{(3,3,2,a)} \Lambda_T^3 = -3^{3/2} m_2^2 \frac{\pi}{2} \int_C ds' e^{-\beta s'} \int_0^{+\infty} \frac{dp}{2 \pi} \frac{[t_2(s' - \frac{p^2}{2 m_{A^\uparrow,D}})]^2}{\sqrt{-2 m_r(s' - \frac{p^2}{2 m_{A^\uparrow,D}})}} \left( \sum_{l \geq 0} t_{3,l}^\uparrow(p, p'; s') \right) \tag{37}
\]

$C$ is a Bromwich contour such that the integrand is analytical to the right of $C$.

\[
m_{A^\uparrow,D} = \frac{m_2 (m_2 + m_1)}{2 (m_2 + m_2)} = \frac{2}{3} m
\tag{38}
\]

\[
\delta n^{(3,3,2,b)} \Lambda_T^3 = 3^{3/2} \sum_{l \geq 0} \int_C ds' e^{-\beta s'} \int_0^{+\infty} \frac{dp}{2 \pi} \frac{[t_2(s' - \frac{p^2}{2 m_{A^\uparrow,D}})]^2}{\sqrt{-2 m_r(s' - \frac{p^2}{2 m_{A^\uparrow,D}})}} \int_0^{+\infty} \frac{dp'}{2 \pi} \frac{t_2(s' - \frac{p'^2}{2 m_{A^\uparrow,D}})}{t_2(s' - \frac{p'^2}{2 m_{A^\uparrow,D}})} \times \left( \frac{m}{p p'} \right)^2 \bar{Q}_1 \left( \frac{m}{p p'} \left( s' - \frac{p^2 + p'^2}{2 m_r} \right) \right) t_{3,l}^\uparrow(p, p'; s') \tag{39}
\]

with $\bar{Q}_1(z) = -\frac{dQ_1(z)}{dz} = \frac{1}{2} \int_{-1}^{1} du \frac{F_1(u)}{(z-u)^2}$ ($Q_1$ is the Legendre function of the second kind).
The calculation of diagrams of Fig.6(c) and 6(d) is done in the same way and we find that

$$\delta n^{(3,3,2,d)} = \delta n^{(3,3,2,a)}$$  \hspace{1cm} (40)
$$\delta n^{(3,3,2,c)} = \delta n^{(3,3,2,b)}$$  \hspace{1cm} (41)

Moreover, it is also easy to verify that $\delta n^{(3,3,2,c)}$ (respectively $\delta n^{(3,3,2,f)}$) is obtained from the expression for $\delta n^{(3,3,2,a)}$ (respectively $\delta n^{(3,3,2,b)}$) by exchanging the role of $\uparrow$ and $\downarrow$ particles (this amounts to exchange $m_\uparrow$ and $m_\downarrow$ in the analytical expressions).

C. Calculation of $b_3$ in the case $m_\uparrow = m_\downarrow$

In general, $b_3$ is obtained from $\delta n^{(3)}$ by summing all the contributions $\delta n^{(3,1)}, \delta n^{(3,2,a \text{ and } b)}, \delta n^{(3,3,1)}$, and the six $\delta n^{(3,3,2)}$'s. However, in the case of equal masses, we have $\delta n^{(3,3,1)} = \delta n^{(3,2,a)} = \delta n^{(3,2,b)}, \delta n^{(3,3,2,a)} = \delta n^{(3,3,2,d)}$. In this way we get

$$\delta n^{(3)} \Lambda_T^3 = 3^{-5/2} + 3 \left( \delta n^{(3,2,a)} + \delta n^{(3,3,2,a)} + \delta n^{(3,3,2,b)} \right) \Lambda_T^3$$

And therefore for $b_3 = \delta n^{(3)} \Lambda_T^3 / 3$

$$b_3 = 3^{-5/2} + \left( \delta n^{(3,2,a)} + \delta n^{(3,3,2,a)} + \delta n^{(3,3,2,b)} \right) \Lambda_T^3$$  \hspace{1cm} (43)

The numerical result is shown in Fig.7. In order to reveal the effect of interactions, we have plotted the difference $b_3 - 3^{-5/2}$ as a function of $\Lambda_T/a$. In practice, in order to integrate safely on $s'$, we deform the contour $C$ into two semi straight lines, symmetric with respect to the real axis, and making an angle $\alpha \in [0, \pi/2]$ with it. In this way, the exponential goes to zero at the extremities of the contour. We checked for different values of $\alpha$, that the result is independent of $\alpha$. We discretized the values of $s', p$ and $p'$ on a grid in order to determine $t_{3,l}^{\uparrow \downarrow}$ numerically from the linear integral equation (B7), which transforms into the problem of solving linear algebraic equations. Finally, for a given value of $l$, we sum on $s', p$ and $p'$ in order to get $\delta n^{(3,3,2,a)}$ and $\delta n^{(3,3,2,b)}$. The curve of

FIG. 7: The third virial coefficient $b_3 - 3^{-5/2}$ as a function of the dimensionless parameter $\Lambda_T/a$.

Fig. 7 is in excellent agreement with the results of Ref.[10]. At unitarity, we find for the $b_3$ coefficient (we sum the harmonics in Eqs.(37), (39) up to $l = 7$ for the four digits we show)

$$b_3 - 3^{-5/2} \approx -0.3551$$  \hspace{1cm} (44)

in excellent agreement with the results of Refs.[10, 12]. This is therefore an independent check for the value of $b_3$, since our method is very different from the method of [10, 12].

V. CONCLUSION

We have calculated the third order virial coefficient $b_3$ in the problem of 2-species fermions interacting via a short range interaction. We have developed a diagrammatic method which leads to explicit analytic expressions. This approach might be extended to the calculation of the 4th order virial coefficient $b_4$, which was recently calculated [12].

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Appendix A: Calculation of $\delta t_{i(3,3,2,a)}$

In order to calculate the diagram of Fig. 6(a) we first look at the "Born" approximation of $T_3^I$. The diagram is shown in Fig. 8. In this figure, we have indicated the 4 relevant time differences $t_1, t_2, t_3, t_4$ as well as a convenient way to choose the momentum variables. Physically $P$ is the total momentum of the 3-body problem $(2 \uparrow, 1 \downarrow)$. $p$ is the momentum of the incoming $\uparrow$, in the centre of mass reference frame, scattering with a dimer of opposite momentum in the centre of mass reference frame. We have defined

$$\alpha = \frac{m_\uparrow}{(2m_\uparrow + m_\downarrow)} = \frac{1}{3} \quad (A1)$$

We give expressions valid for any masses $m_\downarrow$ and $m_\uparrow$.

FIG. 8: Diagram of Fig. 6(a) with $T_3^I$ taken in the Born approximation.

\[
I = - \int \Pi_{i=2}^{4} dt_i \left( T_2 (\mathbf{p} + (1 - \alpha)\mathbf{P}, t_2) e^{-\varepsilon_i ((\mathbf{p} + \alpha \mathbf{P}) t_2 \Theta(t_2))} (e^{-(2\varepsilon_i ((\mathbf{p} + \alpha \mathbf{P}) + \varepsilon_i (-(2p + (1-2\alpha)\mathbf{P})) t_3 \Theta(t_3))} \right. \\
\left. \times \left( T_2 (-\mathbf{p} + (1 - \alpha)\mathbf{P}, t_3) e^{-\varepsilon_i ((\mathbf{p} + \alpha \mathbf{P}) t_4 \Theta(t_4))} \right. \\
\left. \times \left( (\beta - (t_2 + t_3 + t_4)) \Theta (\beta - (t_2 + t_3 + t_4)) e^{-(\beta - (t_2 + t_3 + t_4)) (\varepsilon_i ((\mathbf{p} + \alpha \mathbf{P}) + \varepsilon_i (\mathbf{p} + \alpha \mathbf{P} + \varepsilon_i (-\mathbf{p} + (1 - 2\alpha)\mathbf{P}))) \right) \right) \right) \\
(A2)
\]

This apparently complicated expression is actually a convolution integral of the type studied in Appendix C.

We then easily find

\[
I = \int \frac{ds}{2\pi i} e^{-\beta s} \left[ t_2 \left( s - \frac{P^2}{2(2m_\uparrow + m_\downarrow)} - \frac{p^2}{2m_{\uparrow, D}} \right) \right]^2 \\
\times \left( \frac{1}{(s - \frac{P^2}{2(2m_\uparrow + m_\downarrow)}) - \frac{p^2}{2m_\uparrow} + \frac{p^2}{2m_\downarrow}} \right) \\
(A3)
\]
If we look at the next order Feynman diagrams for $T_3^t$, we see by inspection that we still find a convolution integral, and we just have to replace the last line of the above equation by $l_3^t(p; p, (s - \frac{p^2}{2(2m_\uparrow + m_\downarrow)}))$. In this way, the multidimensional time integrals are replaced by a single integral on the variable $s$.

We now come to the summation on wave vectors. For the summation on the total momentum $P$, we see that, similarly to what was found in the calculation of $b_2$, $P$ enters only through the combination $s - \frac{p^2}{2(2m_\uparrow + m_\downarrow)}$. This enables to decouple the summation on $P$ (by the change of variable $s' = s - \frac{p^2}{2(2m_\uparrow + m_\downarrow)}$). After summation on $P$, we get a factor $(\Lambda_T s)^{-3} \left( \frac{2m_\uparrow + m_\downarrow}{m_\downarrow} \right)^{3/2}$.

Finally, for $\delta\eta(3,3,2,a)$, it is also possible to integrate on $p'$, since $p'$ enters only the expression through $1/(s - \frac{p^2}{2m_\uparrow} - (\frac{p^2}{2m_\downarrow} + \frac{p^2}{2m_\uparrow + m_\downarrow}))$. The integration is done via the change of variable $p'' = p' + (m_\uparrow)/(m_\uparrow + m_\downarrow)p$, and the use of Eq. (21). In this way we get a factor $(m_r)^2/(2\pi)/\sqrt{-2m_r(s' - p'^2/(2m_\uparrow + m_\downarrow))}$.

The last step is to express $l_3^t(p, p, s')$ in terms of the Legendre Polynomials components $l_3^t$’s. This is done thanks to

$$l_3^t(p, p; s') = \sum_{l \geq 0} l_3^t(p, p; s')$$

which physically represents the forward scattering of an atom on a dimer (we used $P_l(1) = 1$). In this way, we recover Eq. (37).

**Appendix B: Integral equation for the 3-body problem in the center of mass frame of reference.**

We first recall the integral equation for $T_3^t(p_1, p_2; P)$ (for complex frequencies) following the approach of [17]

$$T_3^t(p_1, p_2; P) = -G_1(P - p_1 - p_2) - \sum_q G_1(q)G_\downarrow(P - p_1 - q)T_2(P - q)T_3^t(q, p_2; P)$$

In order to be as general as possible, we also give here formulas valid for any masses $m_\downarrow$ and $m_\uparrow$. In Eq. (B1), it is possible to perform the integration on the variable $s_q$ by deforming the integration contour in the half plane $Re(s_q) > \gamma$. The only singularity in this domain is the pole $s_q = \varepsilon(q)$, and we end up, as usual, with an integral equation where $T_3^t$ in the integral term is evaluated "on the shell". The next step is to make a change of variables and function according to

$$p_1 = p_1 + \frac{m_\uparrow}{2m_\uparrow + m_\downarrow}P$$
$$p_2 = p_2 + \frac{m_\downarrow}{2m_\uparrow + m_\downarrow}P$$
$$s_p = s_p - \frac{P^2}{2(2m_\uparrow + m_\downarrow)}$$

$$l_3^t(p_1, p_2; s_p) = T_3^t([p_1, \varepsilon(q)(p_1)], [p_2, \varepsilon(q)(p_2)]; [P, s_p])$$

This amounts to go to the center of mass reference frame and to evaluate $T_3^t$ “on the shell”. $p'_1$ is the momentum of a $\uparrow$ incoming atom in the center of mass reference frame (total impulsion $P$ in “laboratory” frame). $s'_p$, can be seen as the total "energy” minus the center of mass kinetic energy, i.e. the energy in the center of mass reference frame. In this way, we get

$$l_3^t(p_1, p_2; s'_p) = \int \frac{d^3q'}{(2\pi)^3} \left[ \frac{t_2(s_p - \frac{(q')^2}{2m_\uparrow + m_\downarrow})}{(\frac{(p_1')^2 + (p_2')^2}{2m_\uparrow} + \frac{(p_1')^2 + (q')^2}{2m_\uparrow + m_\downarrow} - s'_p)} \right] t_3^t(q', p_2; s'_p)$$

We do not suppose here that the two species have equal masses. $m_r = \frac{m_\uparrow + m_\downarrow}{(m_\uparrow + m_\downarrow)}$ is the 2-body reduced mass, and $m_A1,D = \frac{m_\uparrow (m_\uparrow + m_\downarrow)}{(2m_\uparrow + m_\downarrow)}$ is the atom$\uparrow$-dimer reduced mass.
\[ I(\beta) = \int_{t_1, t_2} \beta (t - (t_2 + t_3 + t_4)) g_2(t_2) f_3(t_3) f_4(t_4) \]  
(C1)

We first integrate with respect to \( t_2 \), and use the convolution theorem for Laplace transforms

\[ \int_0^t dt_2 g(t - t_2) f_2(t_2) = \mathcal{L}^{-1} \left( G(s) F_2(s) \right) \]  
(C2)

where \( G(s) = \int_0^{\infty} dt e^{-s t} g(t) \) and \( F_2(s) = \int_0^{\infty} dt e^{-s t} f_2(t) \). We use a notation such that the Laplace transforms of a given function is denoted by the corresponding capital letter. The symbol \( \mathcal{L} \) denotes the Laplace transform, and \( \mathcal{L}^{-1} \) the inverse Laplace transform. The integration with respect to \( t_2 \) therefore gives the contribution

\[ g_2(\beta - (t_2 + t_3 + t_4)) = \mathcal{L}^{-1} \left( G(s) F_2(s) \right)_{t=\beta - (t_2 + t_3 + t_4)} \]  
(C3)

The integration on \( t_3 \) can be done similarly, and we get

\[ g_3(\beta - t_4) = \mathcal{L}^{-1} \left( G(s) F_3(s) \right)_{t=\beta - t_4} = \mathcal{L}^{-1} \left( G(s) F_2(s) F_3(s) \right)_{t=\beta - t_4} \]  
(C4)

The last integration on \( t_4 \) gives the full integral

\[ I(\beta) = \mathcal{L}^{-1} \left( G(s) F_2(s) F_3(s) F_4(s) \right)_{t=\beta} \]  
(C5)

In this way, we have transformed the 4-dimensional integral Eq.(C7) in the 1-dimensional following integral

\[ I(\beta) = \int_{\gamma} ds \frac{e^{-s \beta}}{2 \pi i} G(s) F_2(s) F_3(s) F_4(s) \]  
(C6)

with \( \gamma \), a contour parallel to the imaginary axis with \( \text{Re}(s) = \gamma \), such that \( G, F_2, F_3 \) and \( F_4 \) are analytical for \( \text{Re}(s) < \gamma \).

This can be generalized easily to any \( n \)-dimensional integral of the form

\[ I_n(\beta) = \int_{t_1, \ldots, t_n} \beta ((t_2 + \cdots + t_n)) g(\beta - (t_2 + \cdots + t_n)) f_2(t_2) \cdots f_n(t_n) \]  
(C7)

Following the same method as before, we get

\[ I_n(\beta) = \int_{\gamma} ds \frac{e^{-s \beta}}{2 \pi i} G(s) F_2(s) \cdots F_n(s) \]  
(C8)
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