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Second order virial expansion for an atomic gas in a harmonic waveguide

Tom Kristensen^{1,2,3}, Xavier Leyronas^{1,2,4} and Ludovic Pricoupenko^{1,2}

1- Sorbonne Universités, UPMC Univ Paris 06, UMR 7600,

Laboratoire de Physique Théorique de la Matière Condensée, F-75005, Paris, France

2- CNRS, UMR 7600, Laboratoire de Physique Théorique de la Matière Condensée, F-75005, Paris, France

3-Institut de Physique de Rennes, UMR 6251 du CNRS and Université de Rennes 1, 35042 Rennes Cedex, France

4- Laboratoire de Physique Statistique, École Normale Supérieure,

PSL Research University; Université Paris Diderot Sorbonne Paris-Cité; Sorbonne

Universités UPMC Univ Paris 06; CNRS; 24 rue Lhomond, 75005 Paris, France.

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The virial expansion for cold two-component Fermi and Bose atomic gases is considered in presence of a waveguide and in the vicinity of a Feshbach resonance. The interaction between atoms and the coupling with the Feshbach molecules is modeled by using a quantitative separable two-channel model. The scattering phase-shift in a atomic waveguide is defined. This permits to extend the Beth-Uhlenbeck formula for the second order virial coefficient to this inhomogeneous case.

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INTRODUCTION

The use of magnetic Feshbach resonances permits one to achieve the unitary regime in atomic gases where universal thermodynamic properties such as the Equation Of State (EOS) are expected [1, 2]. Dramatic progress in cold atoms experiments make it possible to achieve precise measurement of the EOS for two-component fermions in the BEC-BCS crossover [3–7]. More recently the EOS for the strongly interacting Bose gas has been also subject to intensive studies [8–10]. However even in the non-degenerate regime, large three-body atomic losses prevent one to achieve a global thermal equilibrium in the Bose gas [8]. In the resonant scattering regime, due to a large scale separation between the short range of the interatomic forces and the large scattering length, few-body systems have also universal properties exemplified by the Efimov effect [11]. In this context, the virial expansion where the n^{th} order term is known from the solution of the n -body problem, achieves a remarkable bridge between the few- and the many-body problems [12]. For non degenerate gases and for sufficiently small densities and high temperature, the fugacity is a small parameter and the virial expansion is thus a way to derive an accurate EOS. Consequently the virial expansion is subject of current interest for the two-component Fermi gas [13–23] and also for the Bose gas where the Efimov effect plays an important role [24, 25]. Concerning the Bose gas, the momentum distribution has been measured recently [10] and a law at second order in the fugacity including both elastic and inelastic processes has been derived [9]. Based on single channel models, there are now very accurate evaluations of the third and even of the fourth virial coefficients [26] in homogeneous strongly interacting gases. Currently there are three methods to derive the virial coefficients from a given model: the harmonic oscillator method [15–17, 20], the diagrammatic method [18] and the T -matrix method [19, 27]. At the second order of the expansion, Beth and Uhlenbeck showed that

the contribution of the interaction to the virial coefficient can be expressed in terms of the scattering phase-shifts for all partial waves [28]. In the context of cold atoms, collisions are dominated by two-body s -wave scattering and the second virial coefficient can be thus expressed as a function of the s -wave scattering phase-shift. non-interacting In current experiments it is also possible to trap cold atoms in highly anisotropic external harmonic potential. This permits one to achieve one-dimensional (1D) or two-dimensional (2D) systems in the limit where all the characteristic energies, including the temperature, are smaller than the atomic zero-point energy of the tight direction(s) of the trap [29]. This way the 2D EOS for the two-component resonant Fermi gas has been measured [30, 31]. On the theoretical side, highly anisotropic traps can be modeled by considering harmonic atomic waveguides where interatomic collisions are well known in the low energy limit [32–34]. The first terms of the virial expansions for strictly 1D or 2D gases using single channel approach have also been studied and the Beth-Uhlenbeck formula for system in pure 2D or 1D systems is well established [35, 36].

In this paper, we aim at answering two issues: first, how the molecular state contributes to the Beth-Uhlenbeck formula near a Feshbach resonance and second, how this formula can be generalized when one considers atomic waveguides where several transverse modes are populated, thus when the dimensionality of the system is between the strict 1D or 2D and the three dimensional limit. This last issue is especially relevant for atomic wave guides where few transversal mode are populated. One can wonder how the low dimensional limit is reached in a regime where the Local Density Approximation (LDA) does not apply.

In this paper, we extend the Beth-Uhlenbeck relation for the second order virial term to the case of atoms coherently coupled with diatomic molecules in a 2D or a 1D harmonic waveguide. To this end, we use a two-channel modeling of the Feshbach resonance. Our main results

are as follows: first, we define the notion of scattering phase-shift in atomic waveguide in Eq. (84); second, we calculate the second order virial coefficient in Eq. (101) by using the T -matrix and the diagrammatic approaches.

The structure of the paper is as follows. In sec. IA and sec. IB we introduce the notations for atoms and molecules in atomic waveguides and consider the thermodynamic equilibrium. This permits us to define the cumulant, cluster and virial expansions in sec. IC, sec. ID and sec. IE. The link between the two expansions is done with the cluster expansion in sec. ID. We then consider the non-interacting gas in sec. II which makes it possible to define the domain of validity of the LDA in the thermodynamic limit. In sec. IIIA we introduce a separable two-channel model already used for bosons or fermions in the vicinity of a magnetic Feshbach resonance [37–42]. We then obtain the full T -matrix of the model in sec. IIIB and define in sec. IIIC the notion of scattering phase-shift in a waveguide. In sec. IIID we use the T -matrix formalism to deduce the Beth-Uhlenbeck relation. Eventually in sec. IV, we adapt the method of Ref. [18] to the two-channel model and deduce the Beth-Uhlenbeck formula from modified Feynman diagrams.

I. VIRIAL AND CUMULANT EXPANSIONS IN ATOMIC WAVEGUIDES

A. Harmonic waveguides

In this paper we consider structureless particles (atoms or molecules) in one-dimensional ($D = 1$) or two-dimensional ($D = 2$) waveguides. Our formalism includes also the case where there is no external potential ($D = 3$). For $D = 2$, the waveguide is a harmonic oscillator in the z direction and for $D = 1$, it is an isotropic harmonic oscillator in the $x - y$ plane. The molecules are created from pairs of atoms by the means of the Feshbach mechanism. We denote the trap frequency of the harmonic waveguides by ω and we assume that it is the same for atoms and molecules considered in this paper (see the discussion in appendix B of Ref. [37]). The threshold of the energy continuum in the open channel is denoted by E_0 :

$$E_0 = \frac{(3 - D)\hbar\omega}{2}. \quad (1)$$

The internal quantum numbers of the species are labeled by η : $\eta = b$ for the atomic bosons in the open channel, $\eta = \uparrow, \downarrow$ for the two-component fermions in the open channel and $\eta = m$ for the diatomic molecules in the closed channel. The mass of the species η is then denoted by m_η . For convenience, we denote also the mass of the bosonic and \uparrow fermionic species by $m = m_b = m_\uparrow$. The quantum numbers for the single particles are denoted by α and the one-body energy for the species $\eta = b, \uparrow, \downarrow$ is denoted by ϵ_η^α . For example in 2D waveguides $\alpha = (k_x, k_y, n_z)$ where (k_x, k_y) are the wavenumbers for the free directions (x, y)

and n_z is the quantum number of the harmonic oscillator associated with the trap along z and

$$\epsilon_\eta^\alpha = \frac{\hbar^2}{2m_\eta}(k_x^2 + k_y^2) + \hbar\omega \left(n_z + \frac{1}{2} \right) \quad (2)$$

We also introduce for convenience, the index $\eta = r$ to denote the relative particle associated with two bosons in the Bose gas (or of a pair $\uparrow\downarrow$ in the Fermi gas) with the relative mass $m_r = m/2$ (or $m_r = \frac{m_\downarrow}{1+m_\downarrow/m}$). The center of mass of such a pair is denoted by the index $\eta = c$ with the mass $m_c = 2m$ for bosons and $m_c = m + m_\downarrow$ for fermions. The molecular state has an internal energy with respect to the 3D open channel continuum denoted by E_m . The one-body energy of the molecular state is thus

$$\epsilon_m^\alpha = \epsilon_c^\alpha + E_m \quad (3)$$

B. Thermodynamics at equilibrium

We adopt a grand canonical description of the system at equilibrium at temperature T with the grand potentials denoted by Ω_B (respectively Ω_F) for the Bose gas (respectively for the Fermi gas). The chemical potential for each species η is denoted by μ_η and the fugacity is denoted by $z_\eta = e^{\beta\mu_\eta}$ where $\beta = 1/(k_B T)$. To perform the thermodynamic limit, we assume periodic boundary conditions in the free direction(s) of the atomic waveguides by introducing a D -dimensional box of length L . We then consider arbitrarily large values of L for a fixed temperature and chemical potentials. We then assume that the summation over a wavenumber, say along the direction z is continuous: $\sum_{k_z} \equiv L \int \frac{dk_z}{(2\pi)}$. The thermodynamic equilibrium between molecules and atoms implies in the Bose gas

$$\mu_m = 2\mu_b \quad ; \quad z_m = (z_b)^2 \quad (4)$$

and in the Fermi gas

$$\mu_m = \mu_\uparrow + \mu_\downarrow \quad ; \quad z_m = z_\uparrow z_\downarrow. \quad (5)$$

Consequently, the mean conserved numbers of particles are obtained from the grand potentials by

$$\langle \hat{N}_b \rangle + 2\langle \hat{N}_m \rangle = -\frac{\partial \Omega_B}{\partial \mu_b} \quad ; \quad \langle \hat{N}_{\uparrow/\downarrow} \rangle + \langle \hat{N}_m \rangle = -\frac{\partial \Omega_F}{\partial \mu_{\uparrow/\downarrow}}. \quad (6)$$

Another important thermodynamic quantity is the D -dimensional spatial density of the species η defined by

$$\rho_D^\eta = \frac{\langle \hat{N}_\eta \rangle}{L^D}. \quad (7)$$

For a 2D (respectively, 1D) atomic waveguide ρ_D^η is the areal (respectively, the linear) density of species η . In what follows, we use the one-body canonical partition

function in the atomic D -dimensional waveguide for the species $\eta = b$ and \uparrow

$$Q = \frac{(L/\lambda)^D}{[2 \sinh(\beta\hbar\omega/2)]^{3-D}} \quad (8)$$

where λ is the de Broglie wavelength

$$\lambda = \sqrt{\frac{2\pi\beta\hbar^2}{m}}. \quad (9)$$

C. Cumulant expansion

Instead of considering directly the expansion of the grand potential in terms of the densities, it is easier to deal with the expansion in terms of the fugacities. Both expansions are sometimes called virial expansion, however we make a distinction between the two by denoting the second one as the cumulant expansion [24]. Following Ref. [20], we define the cumulants b_n (respectively $b_{n,p}$) for the Bose gas (respectively the Fermi gas) with

$$\Omega_B = -\frac{Q}{\beta} \sum_{n \geq 1} b_n (z_b)^n; \Omega_F = -\frac{Q}{\beta} \sum_{\substack{n,p \geq 0 \\ n+p \neq 0}} b_{n,p} (z_\uparrow)^n (z_\downarrow)^p. \quad (10)$$

The cumulants can be thus deduced from the mean conserved numbers of particles by using Eq. (6). For the Bose gas one obtains

$$\langle \hat{N}_b \rangle + 2\langle \hat{N}_m \rangle = Q \sum_{n \geq 1} n b_n (z_b)^n \quad (11)$$

and for the Fermi gas

$$\langle \hat{N}_\uparrow \rangle + \langle \hat{N}_m \rangle = Q \sum_{n,p \geq 0} n b_{n,p} (z_\uparrow)^n (z_\downarrow)^p \quad (12)$$

$$\langle \hat{N}_\downarrow \rangle + \langle \hat{N}_m \rangle = Q \sum_{n,p \geq 0} p b_{n,p} (z_\uparrow)^n (z_\downarrow)^p. \quad (13)$$

D. Cluster expansion

In the Bose gas we define the cluster of order n as the set of eigenstates of the many-body Hamiltonian composed of N_b bosons and N_m molecules such that $N_b + 2N_m = n$. The canonical partition function for this cluster is denoted by Q_n . In the Fermi gas, the cluster of order (n,p) is the set of eigenstates of the many-body Hamiltonian composed of N_\uparrow fermions \uparrow , N_\downarrow fermions \downarrow and N_m molecules such that $N_\uparrow + N_m = n$ and $N_\downarrow + N_m = p$. The canonical partition function for this cluster is denoted by $Q_{n,p}$. Using Eqs. (4) and (5),

the cluster expansion for the grand potentials are

$$\Omega_B = \frac{-1}{\beta} \ln \left(1 + \sum_{n \geq 1} Q_n (z_b)^n \right) \quad (14)$$

$$\Omega_F = \frac{-1}{\beta} \ln \left(1 + \sum_{\substack{n,p \geq 0 \\ n+p \neq 0}} Q_{n,p} (z_\uparrow)^n (z_\downarrow)^p \right) \quad (15)$$

for small fugacities:

$$\Omega_B = \frac{-1}{\beta} \left\{ Q_1 z_b + \left[Q_2 - \frac{(Q_1)^2}{2} \right] (z_b)^2 + \dots \right\} \quad (16)$$

$$\Omega_F = \frac{-1}{\beta} \left\{ Q_{1,0} z_\uparrow + Q_{0,1} z_\downarrow + (Q_{1,1} - Q_{1,0} Q_{0,1}) z_\uparrow z_\downarrow + \left[Q_{2,0} - \frac{(Q_{1,0})^2}{2} \right] z_\uparrow^2 + \left[Q_{0,2} - \frac{(Q_{0,1})^2}{2} \right] z_\downarrow^2 + \dots \right\} \quad (17)$$

We have $Q_{1,0} = Q_1 = Q$. The cumulants of Eq. (10) can be thus expressed in terms of canonical partition function for the Bose gas

$$b_1 = 1 \quad ; \quad b_2 = \frac{Q_2}{Q} - \frac{Q}{2} \quad (18)$$

and for the Fermi gas

$$b_{1,0} = 1 \quad ; \quad b_{0,1} = \frac{Q_{0,1}}{Q} \quad ; \quad b_{2,0} = \frac{Q_{2,0}}{Q} - \frac{Q}{2} \quad (19)$$

$$b_{0,2} = \frac{Q_{0,2} - (Q_{0,1})^2/2}{Q} \quad ; \quad b_{1,1} = \frac{Q_{1,1}}{Q} - Q_{0,1}. \quad (20)$$

E. Virial expansion

As a consequence of the interchannel coupling, the number of atoms or molecules are not conserved quantities. Thus, as the virial expansion is a polynomials in terms of densities, we define it in this context by taking into account the conservation laws for $\hat{N}_b + 2\hat{N}_m$ and $\hat{N}_{\uparrow/\downarrow} + \hat{N}_m$. Moreover, due to the presence of a D -dimensional atomic waveguide we perform the virial expansion in terms of the densities ρ_D^η in Eq. (7):

$$\Omega_B = -\frac{Q}{\beta} \sum_{n \geq 1} (\lambda)^{nD} a_n (\rho_D^b + 2\rho_D^m)^n \quad (21)$$

$$\Omega_F = -\frac{Q}{\beta} \sum_{\substack{n,p \geq 0 \\ n+p \neq 0}} (\lambda)^{(n+p)D} a_{n,p} (\rho_D^\uparrow + \rho_D^m)^n \times (\rho_D^\downarrow + \rho_D^m)^p. \quad (22)$$

In Eq. (21) [respectively Eq. (22)], a_n (respectively $a_{n,p}$) are the virial coefficients for the Bose gas (respectively

for the Fermi gas). In this expression the ratio ρ_D^m/ρ_D^η for $\eta \in \{b, \uparrow, \downarrow\}$ is an important quantity which does not appear in usual one-channel models. It can be evaluated for a two-channel model by using the Hellman-Feynmann theorem [37]. The general relation of the molecular density in terms of the contact permits one to conclude that for a broad resonance ρ_D^m is also negligible with respect to the particle density(ies) in the open channel [43]. In this last regime, one thus recovers the usual virial expansion.

Combining virial and cumulant expansion of the grand potential together with the relation between the D -dimensional density and the cumulants from Eqs. (7), (11), (12) and (13), one finds the relation between the virial coefficients and the cumulants :

$$a_1 = \frac{L^D}{\lambda^D Q} ; a_2 = -\frac{L^{2D} b_2}{\lambda^{2D} Q^2} \quad (23)$$

$$a_{1,0} = a_{0,1} = \frac{L^D}{\lambda^D Q} ; a_{1,1} = \frac{-L^{2D} b_{1,1}}{\lambda^{2D} Q^2 b_{0,1}} \quad (24)$$

$$a_{2,0} = -\frac{L^{2D} b_{2,0}}{\lambda^{2D} Q^2} ; a_{0,2} = -\frac{L^{2D} b_{0,2}}{\lambda^{2D} Q^2 (b_{0,1})^2}. \quad (25)$$

II. GAS WITHOUT INTERACTION

A. Cumulants

We consider the limit of a large box in the free direction(s) ($L \rightarrow \infty$). The mean total number of species ($\eta \in \{b, \uparrow, \downarrow, m\}$) is given at equilibrium by

$$\langle \hat{N}_\eta \rangle (\mu_\eta, T) = \sum_\alpha n_\eta (\epsilon_\eta^\alpha - \mu_\eta). \quad (26)$$

In Eq. (26), depending on the statistics considered, n_η is the Bose-Einstein or the Fermi-Dirac distribution (the molecules considered here are bosons). In this section, we formally assume the thermodynamic equilibrium between atoms and molecules without any interaction by imposing the relations in Eq. (4) or in Eq. (5). For convenience, in what follows we introduce the variable $\chi_\eta = \pm 1$ depending on the statistics of the species η :

$$\chi_b = \chi_m = 1 ; \chi_\uparrow = \chi_\downarrow = -1. \quad (27)$$

We can thus write the occupation number in the following form:

$$n_\eta(E - \mu_\eta) = \frac{z_\eta e^{-\beta E}}{1 - \chi_\eta z_\eta e^{-\beta E}}. \quad (28)$$

To achieve the virial expansion for the non-interacting gas we expand Eq. (28) in power of the fugacity:

$$n_\eta(E - \mu_\eta) = \sum_{n \geq 1} (\chi_\eta)^{n+1} (z_\eta e^{-\beta E})^n. \quad (29)$$

Using Eq. (29) in Eqs. (26) and (11), one obtains the cumulants of the non-interacting Bose gas denoted $b_n^{(0)}$:

$$b_{2p+1}^{(0)} = \frac{f_D^b(2p+1)}{Q} ; b_{2p}^{(0)} = \frac{f_D^b(2p) + f_D^m(p) e^{-p\beta E_m}}{Q}, \quad (30)$$

where the function f_D^η is given by

$$f_D^\eta(n) = \frac{L^D}{\lambda_\eta^D [2 \sinh(n\beta\hbar\omega/2)]^{3-D}} \times \frac{1}{n^{1+D/2}}. \quad (31)$$

In Eq. (31), λ_η is the de Broglie wavelength of the particle η

$$\lambda_\eta = \sqrt{\frac{2\pi\beta\hbar^2}{m_\eta}}. \quad (32)$$

Similarly, the expressions of the cumulants for the non-interacting Fermi gas denoted by $b_{n,p}^{(0)}$ are deduced from Eqs. (29), (12) and (13):

$$b_{n,0}^{(0)} = (-1)^{n+1} \frac{f_D^\uparrow(n)}{Q} ; b_{0,n}^{(0)} = (-1)^{n+1} \frac{f_D^\downarrow(n)}{Q} \quad (33)$$

$$b_{n,n}^{(0)} = \frac{f_D^m(n)}{Q} e^{-n\beta E_m} ; b_{n,p}^{(0)} = 0 \quad \text{otherwise.} \quad (34)$$

In the particular case where $n = p = 1$, one finds a result independent of the trap frequency:

$$b_{1,1}^{(0)} = \left(1 + \frac{m_\downarrow}{m_\uparrow}\right)^{\frac{D}{2}} e^{-\beta E_m} \quad (35)$$

B. 3D dominated regime

In the limit where $\beta\hbar\omega \ll 1$, the particles occupy high energy transverse modes of the waveguide and the system has thus a 3D character. In this 3D dominated regime, the function in Eq. (31) can be approximated by

$$f_D^\eta(n) \simeq \frac{L^D}{\lambda_\eta^D (\beta\hbar\omega)^{3-D} n^{4-D/2}}. \quad (36)$$

The mean number of particles for each species is then

$$\langle \hat{N}_\eta \rangle = \frac{\chi_\eta L^D g_{3-D/2}(\chi_\eta z_\eta)}{\lambda_\eta^D (\beta\hbar\omega)^{3-D}} \quad (37)$$

where $g_\alpha(t) = \sum_{n \geq 1} t^n / n^\alpha$. One can verify that, as expected, it is possible to derive Eq. (37) after spatial integration of the 3D density approximated in the LDA by using

$$\langle \hat{N}_\eta \rangle = \int d^3 r \int \frac{d^3 k}{(2\pi)^3} n_\eta \left(\frac{\hbar^2 k^2}{2m_\eta} - \mu_\eta - V_{\text{trap}}(\mathbf{r}) \right) \quad (38)$$

where V_{trap} is the transverse harmonic potential of frequency ω .

In the 3D dominated regime $\frac{f_D^\eta(n)}{Q} \sim \frac{\lambda^D}{\lambda_\eta^D n^{4-D/2}}$ and the second order cumulant for the Bose gas is

$$b_2^{(0)} \simeq \frac{1}{2^{4-D/2}} + 2^{\frac{D}{2}} e^{-\beta E_m} \quad (39)$$

and for the Fermi gas, the second order cumulants are

$$b_{2,0}^{(0)} \sim -\frac{1}{2^{4-D/2}}; \quad b_{0,2}^{(0)} \sim -\frac{1}{2^{4-D/2}} \left(\frac{m_\downarrow}{m_\uparrow} \right)^{\frac{D}{2}}. \quad (40)$$

These can be compared with the virial coefficients of the homogeneous 3D problem without molecules: for the Bose gas $b_2^{(\text{hom})} = 1/(4\sqrt{2})$ and for the two-components Fermi gas $b_{2,0}^{(\text{hom})} = b_{0,2}^{(\text{hom})} = -1/(4\sqrt{2})$. These results coincide with the analysis of Ref. [14] adapted for a D -dimensional waveguide, which gives $b_2 = 2^{(D-3)/2} b_2^{(\text{hom})}$ and for $m_\uparrow = m_\downarrow$, $b_{2,0} = b_{0,2} = 2^{(D-3)/2} b_{2,0}^{(\text{hom})}$.

We introduce the total number of atoms, including the bounded atoms of the molecular state: $N = \langle \hat{N}_b \rangle + 2\langle \hat{N}_m \rangle$ for bosons and $N = \langle \hat{N}_\uparrow \rangle + \langle \hat{N}_\downarrow \rangle + 2\langle \hat{N}_m \rangle$ for fermions. In the 3D dominated regime, we see from Eq. (37) that the dimensionless quantity

$$N \left(\frac{\lambda}{L} \right)^D \times (\beta \hbar \omega)^{3-D} \quad (41)$$

has a finite limit when $N \rightarrow \infty$, $L \rightarrow \infty$ and $\omega \rightarrow 0$. This defines the thermodynamic limit of the problem where the LDA can be applied.

C. Low dimensional regime

In the low dimensional regime the temperature is sufficiently small that the particles populate only the lowest transverse state of the harmonic waveguide. This regime is achieved in the limit $\beta \hbar \omega \gg 1$ and one can use the approximation from (31):

$$f_D^\eta(n) \sim \frac{L^D}{\lambda_\eta^D} \times \frac{\exp(-n\beta E_0)}{n^{1+D/2}}. \quad (42)$$

In this regime the mean number of particles for each species is given by

$$\langle \hat{N}_\eta \rangle(\mu, T) = \chi_\eta \frac{L^D}{\lambda_\eta^D} g_{\frac{D}{2}} \left(\chi_\eta e^{\beta \mu'_\eta} \right), \quad (43)$$

where for $\eta = b, \uparrow, \downarrow$ we have introduced the shifted chemical potential $\mu'_\eta = \mu_\eta - E_0$ and for $\eta = m$, $\mu'_m = \mu_m - E_0 - E_m$. We thus recover the same result as for a strictly D dimensional homogeneous system with a chemical potential shifted by the zero point motion of the transverse potential. The cumulant $b_n^{(0)}$ for the Bose gas (respectively $b_{n,p}^{(0)}$ for the Fermi gas) differs from the ones

of the strictly homogeneous D dimensional system by a factor $\exp(-n\beta E_0)$ [respectively $\exp(-(n+p)\beta E_0)$]. The thermodynamic limit in the low dimensional regime $\langle \hat{N}_\eta \rangle \rightarrow +\infty$, $L \rightarrow +\infty$ is obtained as expected for fixed values of β , and μ'_η .

III. BETH-UHLENBECK FORMULA IN ATOMIC WAVEGUIDES

A. Separable two-channel model

The atom-atom interaction and the atom-molecule coupling are described by using the separable two-channel model introduced for the two-component Fermi gas in Ref. [37] and for identical bosons in Refs. [38–42]. Atoms evolve in the open channel and molecules in the closed channel. In this simplified model, atoms and molecules are structureless particles and we consider only a single diatomic molecular state. The Feshbach mechanism corresponds to the coherent coupling between the molecular state and a pair of atoms of reduced mass μ and total mass M . We denote the free Hamiltonian for a pair of atoms by \hat{H}_0^a and the free Hamiltonian for a single molecule \hat{H}_0^m . The Hamiltonians \hat{H}_0^a and \hat{H}_0^m include the external potential if it exists. For convenience, we adopt a matrix formalism. The free Hamiltonian for the two-body problem is

$$[\hat{H}_0] = \begin{bmatrix} \hat{H}_0^a & 0 \\ 0 & \hat{H}_0^m \end{bmatrix}. \quad (44)$$

In this paper, we assume the separability between the relative and the center of mass motions. This is the case for the harmonic waveguides considered in this paper. The quantum numbers of the eigenstates of \hat{H}_0^a are denoted by (α_c) for the center of mass and (α_r) for the relative particle. They are denoted by (α_m) for the eigenstates of \hat{H}_0^m :

$$[\hat{H}_0] \begin{bmatrix} |\alpha_r, \alpha_c\rangle \\ |\alpha_m\rangle \end{bmatrix} = \begin{bmatrix} (\epsilon_c^{\alpha_c} + \epsilon_r^{\alpha_r}) |\alpha_r, \alpha_c\rangle \\ \epsilon_m^{\alpha_m} |\alpha_m\rangle \end{bmatrix}. \quad (45)$$

To model the direct interaction and the Feshbach coupling, we introduce the operator

$$\hat{A}_\epsilon = \hat{1}_{\text{Com}} \otimes \langle \delta_\epsilon | \quad (46)$$

where $\hat{1}_{\text{Com}}$ is the identity operator in the Hilbert space associated with the center of mass of a pair of atoms or of a molecule and the bra $\langle \delta_\epsilon |$ acts on the states associated with the relative particle of a pair. In Eq. (46) the state $|\delta_\epsilon\rangle$ belongs to the Hilbert space of the relative motion for two particles in the open channel and permits one to introduce a cut-off in the model. For convenience we choose a Gaussian shape and in configuration space and the momentum representation one has

$$\langle \mathbf{r} | \delta_\epsilon \rangle = \frac{\exp(-r^2/\epsilon^2)}{\epsilon^{3\pi/2}}; \quad \langle \mathbf{k} | \delta_\epsilon \rangle = \exp(-k^2 \epsilon^2/4). \quad (47)$$

In Eq. (47), ϵ is the short range parameter of the model. It is of the order of the characteristic radius of the actual potential experienced by atoms or of the size of the actual molecular states (i.e. of the order of few nanometers). Using these notations, the direct interaction between two atoms is given by a separable pairwise potential characterized by the strength g :

$$\hat{V}^a = g\hat{A}_\epsilon^\dagger\hat{A}_\epsilon. \quad (48)$$

The coherent coupling between a pair of atoms in the open channel and a molecule is

$$\hat{V}^{\text{ma}} = \Lambda\hat{A}_\epsilon \quad (49)$$

where Λ is a real parameter. Previous studies showed that using the same state $|\delta_\epsilon\rangle$ in the direct interaction and in the inter-channel coupling is sufficient to obtain a quantitative description of two-body scattering and shallow bound states [38]. The Hamiltonian of the two-body problem is denoted by

$$[\hat{H}] = [\hat{H}_0] + [\hat{V}], \quad (50)$$

where we have used a matrix notation for the potential of the two-channel model:

$$[\hat{V}] = \begin{bmatrix} \hat{V}^a & \hat{V}^{\text{am}} \\ \hat{V}^{\text{ma}} & 0 \end{bmatrix} \quad (51)$$

and $\hat{V}^{\text{am}} = (\hat{V}^{\text{ma}})^\dagger$.

B. Transition operator for the two-channel model

In what follows, we obtain the transition operator of the model by using the resolvent method. For this purpose we introduce the resolvent for a non-interacting pair of atoms (denoted \hat{G}_0^a) and the resolvent for a molecule (denoted \hat{G}_0^{m}):

$$\hat{G}_0^a(s) = \frac{1}{s - \hat{H}_0^a} \quad ; \quad \hat{G}_0^{\text{m}}(s) = \frac{1}{s - \hat{H}_0^{\text{m}}}. \quad (52)$$

The resolvent of the free two-body Hamiltonian is

$$[\hat{G}_0(s)] = \begin{bmatrix} \hat{G}_0^a(s) & 0 \\ 0 & \hat{G}_0^{\text{m}}(s) \end{bmatrix}. \quad (53)$$

The transition operator has a matrix form

$$[\hat{T}(s)] = \begin{bmatrix} \hat{T}^a(s) & (\hat{T}^{\text{ma}}(s))^\dagger \\ \hat{T}^{\text{ma}}(s) & \hat{T}^{\text{m}}(s) \end{bmatrix} \quad (54)$$

and verifies the Lippmann-Schwinger equation

$$[\hat{T}(s)] = [\hat{V}] + [\hat{V}][\hat{G}_0(s)][\hat{T}(s)]. \quad (55)$$

One finds the following matrix elements for the transition operator:

$$\begin{aligned} \hat{T}^a(s) &= \hat{V}^a + \hat{V}^{\text{am}}\hat{G}_0^{\text{m}}(s)\hat{V}^{\text{ma}} + \hat{V}^a\hat{G}_0^a(s)\hat{T}^a(s) \\ &\quad + \hat{V}^{\text{am}}\hat{G}_0^{\text{m}}(s)\hat{V}^{\text{ma}}\hat{G}_0^a(s)\hat{T}^a(s). \end{aligned} \quad (56)$$

$$\hat{T}^{\text{ma}}(s) = \hat{V}^{\text{ma}} + \hat{V}^{\text{ma}}\hat{G}_0^a(s)\hat{T}^a(s) \quad (57)$$

$$\hat{T}^{\text{m}}(s) = \hat{V}^{\text{ma}} \left[\hat{G}_0^a(s) + \hat{G}_0^a(s)\hat{T}^a(s)\hat{G}_0^a(s) \right] \hat{V}^{\text{am}}. \quad (58)$$

Using the separable form of the potentials in Eqs. (48) and (49) one finds

$$\hat{T}^a(s) = \frac{\hat{A}_\epsilon^\dagger\hat{A}_\epsilon}{\frac{1}{\hat{g}_\epsilon^{\text{eff}}(s)} - \hat{A}_\epsilon\hat{G}_0^a(s)\hat{A}_\epsilon^\dagger} \quad (59)$$

$$\hat{T}^{\text{ma}}(s) = \frac{\hat{V}^{\text{ma}}}{1 - \hat{g}_\epsilon^{\text{eff}}(s)\hat{A}_\epsilon\hat{G}_0^a(s)\hat{A}_\epsilon^\dagger} \quad (60)$$

$$\hat{T}^{\text{m}}(s) = \frac{|\Lambda|^2\hat{A}_\epsilon\hat{G}_0^a(s)\hat{A}_\epsilon^\dagger}{1 - \hat{g}_\epsilon^{\text{eff}}(s)\hat{A}_\epsilon\hat{G}_0^a(s)\hat{A}_\epsilon^\dagger}, \quad (61)$$

where we have introduced the operator

$$\hat{g}_\epsilon^{\text{eff}}(s) = g + |\Lambda|^2\hat{G}_0^{\text{m}}(s). \quad (62)$$

The eigenvalues of the operator $\hat{g}_\epsilon^{\text{eff}}(s)$ in Eq. (62) are given by

$$\hat{g}_\epsilon^{\text{eff}}(s)|\alpha_c\rangle = g^{\text{eff}}(s_{\alpha_c}^{\text{rel}})|\alpha_c\rangle \quad (63)$$

$$s_{\alpha_c}^{\text{rel}} = s - \epsilon_c^{\alpha_c} \quad (64)$$

$$g^{\text{eff}}(s_{\alpha_c}^{\text{rel}}) = g + \frac{|\Lambda|^2}{s_{\alpha_c}^{\text{rel}} - E_{\text{m}}}. \quad (65)$$

Due to the separability, one can define the T matrix of the relative degree of freedom:

$$\langle\alpha'_r|\hat{T}^a(s)|\alpha_r, \alpha_c\rangle = \langle\alpha'_r|\hat{T}^{\text{rel}}(s_{\alpha_c}^{\text{rel}})|\alpha_r\rangle\langle\alpha'_c|\alpha_c\rangle. \quad (66)$$

One then recovers the expression of the T -matrix used in Ref. [42]:

$$\langle\alpha'_r|\hat{T}^{\text{rel}}(s_{\alpha_c}^{\text{rel}})|\alpha_r\rangle = \frac{\langle\alpha'_r|\delta_\epsilon\rangle\langle\delta_\epsilon|\alpha_r\rangle}{\frac{1}{g^{\text{eff}}(s_{\alpha_c}^{\text{rel}})} - \langle\delta_\epsilon|\hat{G}_0^{\text{rel}}(s_{\alpha_c}^{\text{rel}})|\delta_\epsilon\rangle}. \quad (67)$$

where we have introduced the resolvent \hat{G}_0^{rel} for the non-interacting relative motion:

$$H_0^{\text{rel}}|\alpha_r\rangle = \epsilon_r^{\alpha_r}|\alpha_r\rangle \quad (68)$$

$$\hat{G}_0^{\text{rel}}(s) = \frac{1}{s - \hat{H}_0^{\text{rel}}}. \quad (69)$$

Using these notations, the diagonal part of the T -matrix for the molecule can be written as

$$\langle\alpha'_c|\hat{T}^{\text{m}}(s)|\alpha_c\rangle = \frac{|\Lambda|^2\langle\delta_\epsilon|\hat{G}_0^{\text{rel}}(s_{\alpha_c}^{\text{rel}})|\delta_\epsilon\rangle\langle\alpha'_c|\alpha_c\rangle}{1 - g^{\text{eff}}(s_{\alpha_c}^{\text{rel}})\langle\delta_\epsilon|\hat{G}_0^{\text{rel}}(s_{\alpha_c}^{\text{rel}})|\delta_\epsilon\rangle}. \quad (70)$$

The expression of the T -matrix in Eq. (67) can be expressed in terms of the scattering parameters such as the scattering length in presence of a 2D or 1D atomic waveguide [42].

C. Scattering in atomic waveguides

1. Multimode scattering regime

We consider the scattering problem for the relative particle of a pair of bosons or of a pair of \uparrow and \downarrow fermions in a D -dimensional atomic waveguide characterized by the length

$$l_{\text{ho}} = \sqrt{\frac{\hbar}{m_r \omega}}. \quad (71)$$

For the 2D waveguides, the eigenfunctions of the harmonic trap, are denoted by $\phi_n(z)$:

$$\phi_n(z) \equiv \langle z|n\rangle = \frac{e^{-\frac{z^2}{2l_{\text{ho}}^2}}}{\pi^{1/4} \sqrt{2^n n! l_{\text{ho}}}} H_n(z/l_{\text{ho}}). \quad (72)$$

For the 1D waveguides we use in this section, the cylindrical quantum numbers are $\alpha_r \equiv (k, n, m)$, where n is the radial wavenumber of the transverse harmonic oscillator and $m\hbar$ is the angular momentum along the axis z . The single particle energy of the relative particle is thus

$$\epsilon_r^{(k, n, m)} = \frac{\hbar^2 k^2}{2m_r} + \hbar\omega(2n + |m| + 1) \quad (73)$$

and the eigenfunction of the transverse harmonic oscillator are given by

$$\langle \rho|n, m\rangle = \frac{1}{l_{\text{ho}}} \left[\frac{\pi(n + |m|)!}{n!} \right]^{-1/2} \left(\frac{\rho}{l_{\text{ho}}} \right)^{|m|} e^{im\theta} \times e^{-\frac{1}{2}(\rho/l_{\text{ho}})^2} L_n^{(|m|)}(\rho^2/l_{\text{ho}}^2), \quad (74)$$

where $L_n^{(\alpha)}$ is the generalized Laguerre polynomial and $\rho = (\rho, \theta)$ are the polar coordinates in the $x - y$ plane.

As a consequence of the separable form of the atomic T -matrix where $|\delta_\epsilon\rangle$ is a s -wave state, scattering occurs only for s waves in the free space, for even transverse states in 2D waveguides, and for transverse states with zero angular momentum ($m = 0$) in 1D waveguides. Thus for a given collisional energy E , the number of transverse states that can be populated is given by:

$$N_D(E) = \left\lfloor \frac{E}{2\hbar\omega} - \frac{1}{2D} \right\rfloor \quad (75)$$

where $\lfloor \cdot \rfloor$ gives the integer part. For $E > \hbar\omega(2 + 1/D)$, there are thus several accessible transverse modes for the incoming and outgoing waves in a scattering process.

a. 2D scattering from a single mode incoming state – For a given collisional energy, we define the $N_D(E)$ positive wavenumbers k_p of the asymptotic scattering states from the energy conservation:

$$E = \frac{\hbar^2 k_p^2}{2m_r} + \hbar\omega \left(2p + \frac{1}{2} \right). \quad (76)$$

We consider the scattering state $|\Psi_p^{2D}\rangle$ where the incoming wave occupies only one transverse mode: it is characterized by the quantum numbers $\alpha_r = (k_p \hat{e}_x, 2p)$ where $p \leq N_2(E)$. In the limit of large inter-particle distances ($\rho \gg l_{\text{ho}}$) one has [42]:

$$\langle \rho, z|\Psi_p^{2D}\rangle = \langle z|2p\rangle e^{ik_p \hat{e}_x \cdot \rho} - \frac{m_r}{\hbar^2} \sum_{p'=0}^{N_2(E)} \phi_{2p'}(z) \times \frac{e^{i(k_{p'} \rho + \frac{\pi}{4})}}{\sqrt{2\pi k_{p'} \rho}} \langle k_{p'} \hat{e}_\rho, 2p'|\hat{T}^{\text{rel}}(E + i0^+)|k_p \hat{e}_x, 2p\rangle, \quad (77)$$

where \hat{e}_ρ is the unitary vector ρ/ρ .

b. 1D scattering from a single mode incoming state –

For a transverse mode ($n, m = 0$), analogously to the 2D case, we define the wavenumber k_n from the energy conservation:

$$E = \frac{\hbar^2 k_n^2}{2m_r} + \hbar\omega(2n + 1) \quad (78)$$

and consider the scattering state $|\Psi_n^{1D}\rangle$ where the incoming wave is characterized by the quantum numbers $\alpha_r = (k_n \hat{e}_z, n, 0)$ where $n \leq N_1(E)$. In the limit of large inter-particle distances ($z \gg l_{\text{ho}}$), the scattering wave function verifies:

$$\langle \rho, z|\Psi_n^{1D}\rangle = \langle \rho|n, 0\rangle e^{ik_n z} - \frac{im_r}{\hbar^2} \sum_{n'=0}^{N_1(E)} \frac{e^{ik_{n'}|z|}}{k_{n'}} \times \langle \rho|n', 0\rangle \langle k_{n'}, n', 0|\hat{T}^{\text{rel}}(E + i0^+)|k_n, n, 0\rangle. \quad (79)$$

2. Scattering phase shift

For a given value of the dimension D of the waveguide and $N_D > 1$, the outgoing state in Eq. (77) or in Eq. (79) occupies several transverse modes whereas the incoming state occupies only one transverse mode. This prevents to define the notion of scattering phase shift by using this type of scattering state. To circumvent this problem, we now consider the incoming state $|\Psi_D^E\rangle$ of relative energy E , such that the probability of occupation in each transverse mode is conserved in the scattering process. Moreover, as the interaction acts only in the s -wave sector, we consider only states which are rotationally invariant with respect to $0z$ in 2D and are even function of z in 1D. We expand $|\Psi_D^E\rangle$ over the basis $|\Psi_p^{2D}\rangle$ or $|\Psi_p^{1D}\rangle$. In the limit of large inter-particle distances one has for the 2D waveguide:

$$\langle \rho, z|\Psi_2^E\rangle = \int \frac{d\theta}{2\pi} \sum_{p=0}^{N_2(E)} \alpha_p \langle \rho, z|\Psi_p^{2D}\rangle \quad (80)$$

and for the 1D waveguide

$$\langle \rho, z|\Psi_1^E\rangle = \sum_{p=0}^{N_1(E)} \frac{\beta_p}{2} (\langle \rho, z|\Psi_p^{1D}\rangle + \langle \rho, -z|\Psi_p^{1D}\rangle) \quad (81)$$

We first consider the scattering phase-shift in the 2D waveguide. After projection over $\langle z|2p\rangle$, one obtains in the limit for large values of ρ :

$$\int dz \langle 2p|z\rangle \langle \rho, z | \Psi_2^E \rangle = \sqrt{2} \alpha_p \frac{\sin(k_p \rho + \frac{\pi}{4})}{\sqrt{\pi k_p \rho}} - \frac{m_r}{\hbar^2} \times \frac{e^{i(k_p \rho + \frac{\pi}{4})}}{\sqrt{2\pi k_p \rho}} \sum_{p'=0}^{N_2(E)} \alpha_{p'} \langle k_p \hat{\mathbf{e}}_\rho, 2p | \hat{T}^{\text{rel}}(E+i0^+) | k_{p'} \hat{\mathbf{e}}_x, 2p' \rangle. \quad (82)$$

It is now possible to introduce the notion of scattering phase-shift denoted $\delta(E)$ by identifying Eq. (82) with the asymptotic form expected in 2D scattering:

$$\int dz \phi_{2p}(z) \langle \rho, z | \Psi_2^E \rangle = \frac{\alpha_p \sqrt{2} e^{i\delta(E)}}{\sqrt{\pi k_p \rho}} \times \sin \left[k_p \rho + \delta(E) + \frac{\pi}{4} \right]. \quad (83)$$

Remarkably, one finds the same expression as in the free space:

$$\delta(E) = \arg \left[\frac{1}{g_{\text{eff}}(E)} - \langle \delta_\epsilon | \hat{G}_0^{\text{rel}}(E+i0^+) | \delta_\epsilon \rangle \right] \quad (84)$$

and

$$\alpha_p = K \left(\frac{1-\eta}{1+\eta} \right)^p \phi_{2p}(0) \exp(-k_p^2 \epsilon^2/4), \quad (85)$$

where $\eta = \epsilon^2/(2l_{\text{ho}}^2)$ and K is an arbitrary multiplicative constant.

The scattering phase-shift in a 1D waveguide is obtained along the same lines as above. One searches for the coefficients β_n in Eq. (81) such that at large inter-particle distances

$$\int d^2 \rho \langle n, m=0 | \rho \rangle \langle \rho, z | \Psi_1^E \rangle = \beta_n e^{i\delta(E)} \times \sin \left[k_n |z| + \delta(E) + \frac{\pi}{2} \right]. \quad (86)$$

One finds the same expression for the phase shift as in Eq. (84) (but with a different resolvent \hat{G}_0^{rel}) and

$$\beta_n = K \left(\frac{1-\eta}{1+\eta} \right)^n \frac{\exp(-k_n^2 \epsilon^2/4)}{k_n}. \quad (87)$$

D. Second order virial coefficient

The second order virial coefficient is related to the resolvent of the two-channel model

$$[\hat{G}(s)] = \frac{1}{s - [\hat{H}]} \quad (88)$$

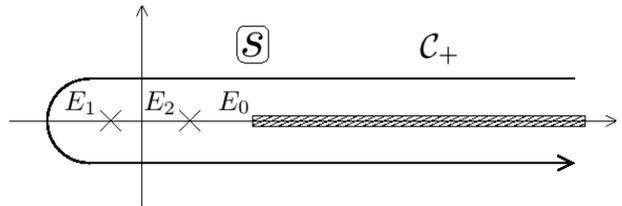


FIG. 1: Example of contour of integration in Eq. (89) where E_1 and E_2 are the energies of two-bound states.

through the identity

$$\text{Tr} \left\{ e^{\beta[\hat{H}]} \right\} = \int_{\mathcal{C}_+} \frac{ds e^{-\beta s}}{2i\pi} \text{Tr} \left\{ [\hat{G}(s)] \right\} \quad (89)$$

where \mathcal{C}_+ is a counter clockwise contour from $\infty + i0^+$ to $\infty - i0^+$ in a loop which encompasses all the poles of the integrand and the cut of the energy continuum on the real axis. An example of such a contour is plotted in Fig. (1). Using the relation between the transition operator and the resolvent of the Hamiltonian

$$[\hat{G}(s)] - [\hat{G}_0(s)] = [\hat{G}_0(s)][\hat{T}(s)][\hat{G}_0(s)], \quad (90)$$

one finds the contribution of the interaction to the second order virial coefficient for the two-component Fermi gas $\Delta b_{1,1} = b_{1,1} - b_{1,1}^{(0)}$ [23, 27]:

$$\Delta b_{1,1} = \frac{1}{Q} \int_{\mathcal{C}_+} \frac{ds e^{-\beta s}}{2i\pi} \text{Tr} \left\{ [\hat{G}_0(s)][\hat{T}(s)][\hat{G}_0(s)] \right\}. \quad (91)$$

The trace in Eq. (91) can be decomposed in the atomic and molecular sectors:

$$\Delta b_{1,1} = \frac{1}{Q} \int_{\mathcal{C}_+} \frac{ds e^{-\beta s}}{2i\pi} \text{Tr} \left\{ \hat{G}_0^{\text{a}}(s) \hat{T}^{\text{a}}(s) \hat{G}_0^{\text{a}}(s) + \hat{G}_0^{\text{m}}(s) \hat{T}^{\text{m}}(s) \hat{G}_0^{\text{m}}(s) \right\}. \quad (92)$$

The correction to the second virial coefficient is then

$$\Delta b_{1,1} = \frac{1}{Q} \int_{\mathcal{C}_+} \frac{ds e^{-\beta s}}{2i\pi} \left\{ \sum_{\alpha_r, \alpha_c} \frac{\langle \alpha_r | \hat{T}^{\text{rel}}(s_{\alpha_c}^{\text{rel}}) | \alpha_r \rangle}{[s_{\alpha_c}^{\text{rel}} - \mathcal{E}_r(\alpha_r)]^2} + \sum_{\alpha_c} \frac{\langle \alpha_c | \hat{T}^{\text{m}}(s) | \alpha_c \rangle}{(s_{\alpha_c}^{\text{rel}} - E_m)^2} \right\}. \quad (93)$$

It is then fruitful to use the identity

$$\sum_{\alpha_r} \frac{|\langle \alpha_r | \delta_\epsilon \rangle|^2}{[s_{\alpha_c}^{\text{rel}} - \mathcal{E}_r(\alpha_r)]^2} = -\frac{d}{ds_{\alpha_c}^{\text{rel}}} \langle \delta_\epsilon | \hat{G}_0^{\text{rel}}(s_{\alpha_c}^{\text{rel}}) | \delta_\epsilon \rangle, \quad (94)$$

which permits one to obtain

$$\frac{\langle \alpha_c | \hat{T}^{\text{m}}(s) | \alpha_c \rangle}{(s_{\alpha_c}^{\text{rel}} - E_m)^2} + \sum_{\alpha_r} \frac{\langle \alpha_r | \hat{T}^{\text{rel}}(s_{\alpha_c}^{\text{rel}}) | \alpha_r \rangle}{[s_{\alpha_c}^{\text{rel}} - \mathcal{E}_r(\alpha_r)]^2} = \frac{d}{ds_{\alpha_c}^{\text{rel}}} \ln \left[1 - g^{\text{eff}}(s_{\alpha_c}^{\text{rel}}) \langle \delta_\epsilon | \hat{G}_0^{\text{rel}}(s_{\alpha_c}^{\text{rel}}) | \delta_\epsilon \rangle \right]. \quad (95)$$

By making the change of variable $s = s_{\alpha_c}^{\text{rel}} + \epsilon_c^{\alpha_c}$ in the integral of Eq. (93), one can then perform the summation over α_c with

$$\sum_{\alpha_c} e^{-\beta \epsilon_c^{\alpha_c}} = \left(\frac{m_c}{m_{\uparrow}} \right)^{\frac{D}{2}} Q, \quad (96)$$

which gives the contribution of the center of mass degree of freedom. Equation (93) can be then expressed as:

$$\Delta b_{1,1} = \left(\frac{m_c}{m_{\uparrow}} \right)^{\frac{D}{2}} \int_{C_+} \frac{ds e^{-\beta s}}{2i\pi} \left\{ \frac{d}{ds} \ln [g^{\text{eff}}(s)] + \frac{d}{ds} \ln \left[\frac{1}{g^{\text{eff}}(s)} - \langle \delta_{\epsilon} | \hat{G}_0^{\text{rel}}(s) | \delta_{\epsilon} \rangle \right] \right\}. \quad (97)$$

One recognizes in the second term of the integral of Eq. (97) the denominator of the relative T -matrix of Eq. (67). As shown in Ref. [42], for the separable two-channel model used in this paper there are at most two dimers in atomic waveguides. Their energies denoted by E_1 , and E_2 are thus simple poles of this second term. This last term has also a pole at $s = E_m - \frac{|\Lambda|^2}{g}$. The first term in the integral of Eq. (97) has a pole at $s = E_m$ and a pole at $s = E_m - \frac{|\Lambda|^2}{g}$. The two residues at $s = E_m - \frac{|\Lambda|^2}{g}$ cancel each other and one finds:

$$\Delta b_{1,1} = \left(\frac{m_c}{m_{\uparrow}} \right)^{\frac{D}{2}} \left\{ -e^{-\beta E_m} + \sum_i e^{-\beta E_i} - \int_{E_0}^{\infty} \frac{ds}{2i\pi} \times e^{-\beta s} \frac{d}{ds} \ln \left[\frac{1}{g^{\text{eff}}(s)} - \langle \delta_{\epsilon} | \hat{G}_0^{\text{rel}}(s + i0^+) | \delta_{\epsilon} \rangle \right] \right\}, \quad (98)$$

where E_0 is the threshold for the continuum of the energy spectrum given in Eq. (1). From Eq. (69), the resolvent verifies:

$$\langle \delta_{\epsilon} | \hat{G}_0^{\text{rel}}(s - i0^+) | \delta_{\epsilon} \rangle = \langle \delta_{\epsilon} | \hat{G}_0^{\text{rel}}(s + i0^+) | \delta_{\epsilon} \rangle^* \quad (99)$$

and one thus obtains from the expression of the scattering phase-shift in Eq. (84)

$$\frac{1}{g^{\text{eff}}(s)} - \langle \delta_{\epsilon} | \hat{G}_0^{\text{rel}}(s + i0^+) | \delta_{\epsilon} \rangle = e^{-2i\delta(s)}. \quad (100)$$

This permits one to extend of the Beth-Uhlenbeck formula to the case of harmonic atomic waveguides

$$\Delta b_{1,1} = \left(1 + \frac{m_{\downarrow}}{m_{\uparrow}} \right)^{\frac{D}{2}} \left\{ -e^{-\beta E_m} + \sum_i e^{-\beta E_i} + \int_{E_0}^{\infty} \frac{ds}{\pi} e^{-\beta s} \frac{d\delta(s)}{ds} \right\}. \quad (101)$$

Remarkably, the explicit molecular contribution in Eq. (101) exactly cancels the one in the non-interacting virial coefficient of Eq. (35). For the Bose gas, the correction $\Delta b_2 = b_2 - b_2^{(0)}$ is derived along the same lines as above. The corresponding Beth-Uhlenbeck formula is obtained from Eq. (101) by making the substitution $m_{\uparrow} \rightarrow m$ and $\Delta b_{1,1} \rightarrow \Delta b_2$.

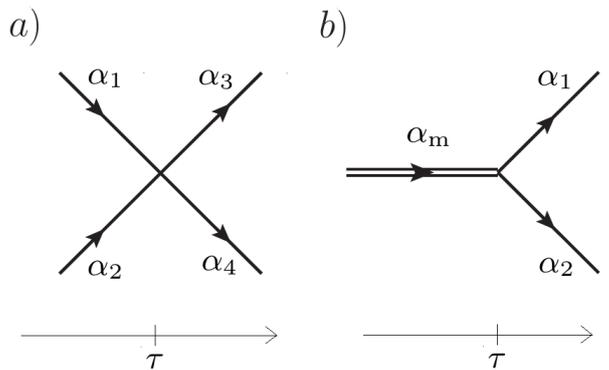


FIG. 2: a) Vertex associated with the direct interaction in the finite temperature formalism : $g \langle \alpha_1 \alpha_2 | \hat{A}_{\epsilon}^{\dagger} \hat{A}_{\epsilon} | \alpha_3 \alpha_4 \rangle \delta(\tau)$; b) idem for the interchannel coupling : $\Lambda \langle \alpha_m | \hat{A}_{\epsilon} | \alpha_1 \alpha_2 \rangle \delta(\tau)$.

IV. DIAGRAMMATIC METHOD IN ATOMIC WAVEGUIDES

A. Green's functions

An alternative way of obtaining the virial coefficients is to deduce them from the population of the different atomic and molecular species by using Eqs. (11), (12) and (13). The diagrammatic method introduced in Ref. [18] permits one to obtain the populations and thus the virial coefficients from a systematic expansion of the Green's function in powers of the fugacities. In this part, the diagrammatic method is adapted for the two-channel model in presence of an atomic waveguide.

We introduce the creation operator $\hat{a}_{\eta,\alpha}^{\dagger}$ for a particle of the species $\eta \in \{\uparrow, \downarrow, b, m\}$ and having the external quantum number denoted by α . Depending on the statistics of the particles η and η' , $\hat{a}_{\eta,\alpha}$ and $\hat{a}_{\eta',\alpha}^{\dagger}$ verify the standard commutation/anti-commutation relations.

The populations of the different species are related to the Green's functions at finite temperature $G_{\eta}(\alpha, \tau) = -\langle T_{\tau} \hat{a}_{\eta,\alpha}(\tau) \hat{a}_{\eta,\alpha}^{\dagger}(0) \rangle$ via the well known formula $\langle \hat{N}_{\eta} \rangle = -\chi_{\eta} \sum_{\alpha} G_{\eta}(\alpha, \tau = 0^-)$. As in standard diagrammatic methods, we then introduce the free Green's function:

$$G_{\eta}^0(\alpha, \tau) = -e^{-(\epsilon_{\eta}^{\alpha} - \mu_{\eta})\tau/\hbar} [\theta(\tau) + \chi_{\eta} n_{\eta}(\epsilon_{\eta}^{\alpha} - \mu_{\eta})] \quad (102)$$

where $\theta(\tau)$ is the Heaviside's function. In the diagrammatic expansions we introduce a solid line for the atomic Green's functions, a double solid line for the molecular Green's functions. The bare vertices for the direct interaction in Eq. (48) and for the interchannel coupling in Eq. (49) are depicted in Fig. (2). Following Ref. [18], we perform the expansion of the Green's function in

Eq. (102) in terms of the fugacity

$$G_\eta^0(\alpha, \tau) = e^{\mu_\eta \tau / \hbar} \left[G_\eta^{(0,0)}(\alpha, \tau) + G_\eta^{(0,1)}(\alpha, \tau) z_\eta + G_\eta^{(0,2)}(\alpha, \tau) z_\eta^2 + \dots \right]. \quad (103)$$

In Eq. (103), $G_\eta^{(0,0)}(\alpha, \tau)$ corresponds to the high temperature limit of the Green's function in vacuum where the fugacity is zero. An important fact for the diagrammatic approach is that it is a purely retarded function :

$$G_\eta^{(0,0)}(\alpha, \tau) = -\theta(\tau) e^{-\epsilon_\eta^\alpha \tau / \hbar}. \quad (104)$$

The other orders in Eq. (103) are given by

$$G_\eta^{(0,n)}(\alpha, \tau) = -(\chi_\eta)^n e^{-\epsilon_\eta^\alpha (n\beta + \tau / \hbar)}. \quad (105)$$

We then introduce the modified Feynman diagrams of Ref. [18] for the diagrammatic expansions in terms of the

fugacities: a n -slashed line (or double line) is associated with the functions $G_\eta^{(0,n)}(\alpha, \tau)$ and by definition a solid non-slashed line corresponds to the function $G_\eta^{(0,0)}(\alpha, \tau)$.

B. Two-particle vertex in the high temperature limit

In what follows, we show how the two-particle vertex in the high temperature limit is simply related to the two-body T -matrix. We consider the fermionic case. The high temperature limit corresponds to a low density limit, where two particle collisions are obtained in the ladder approximation. For the two-particle vertex function, we thus consider the diagrammatic expansion in Fig. (3). The vertex for the atom-atom interaction is then given by the Bethe-Salpeter equation:

$$\begin{aligned} \langle \alpha_1, \alpha_2 | \hat{\Gamma}^a(\tau_2 - \tau_1) | \alpha_3, \alpha_4 \rangle &= \langle \alpha_1, \alpha_2 | \hat{V}^a | \alpha_3, \alpha_4 \rangle \delta(\tau_2 - \tau_1) - \frac{1}{\hbar} \sum_{\alpha_m} \langle \alpha_1, \alpha_2 | \hat{V}^{\text{am}} | \alpha_m \rangle G_m^0(\alpha_m, \tau_2 - \tau_1) \langle \alpha_m | \hat{V}^{\text{ma}} | \alpha_3, \alpha_4 \rangle \\ &- \frac{1}{\hbar} \int_0^{\beta \hbar} d\tau_3 \sum_{\alpha'_1, \alpha'_2} \langle \alpha_1, \alpha_2 | \hat{\Gamma}^a(\tau_3 - \tau_1) | \alpha'_1, \alpha'_2 \rangle G_\uparrow^0(\alpha'_1, \tau_2 - \tau_3) G_\downarrow^0(\alpha'_2, \tau_2 - \tau_3) \langle \alpha'_1, \alpha'_2 | \hat{V}^a | \alpha_3, \alpha_4 \rangle \\ &+ \frac{1}{\hbar^2} \int_0^{\beta \hbar} d\tau_3 \int_0^{\beta \hbar} d\tau_4 \sum_{\alpha'_1, \alpha'_2, \alpha_m} \langle \alpha_1, \alpha_2 | \hat{\Gamma}^a(\tau_3 - \tau_1) | \alpha'_1, \alpha'_2 \rangle G_\uparrow^0(\alpha'_1, \tau_4 - \tau_3) G_\downarrow^0(\alpha'_2, \tau_4 - \tau_3) \\ &\times \langle \alpha'_1, \alpha'_2 | \hat{V}^{\text{am}} | \alpha_m \rangle G_m^0(\alpha_m, \tau_2 - \tau_4) \langle \alpha_m | \hat{V}^{\text{ma}} | \alpha_3, \alpha_4 \rangle. \quad (106) \end{aligned}$$

In the high temperature limit, the free particle Green's functions are given by the first term in the expansion of Eq. (103). Consequently, in this limit there are only retarded functions and there is no β dependence in Eq. (106). We can thus replace the upper limit of the integration interval for the intermediate times by $+\infty$. We also factorize the global time imaginary dependence to extract the vacuum contribution:

$$\lim_{\{z_\eta\} \rightarrow 0} \hat{\Gamma}^a(\tau_2 - \tau_1) = e^{(\mu_\uparrow + \mu_\downarrow)(\tau_2 - \tau_1)} \hat{\Gamma}_{\text{vac}}^a. \quad (107)$$

We then use the separability of the two-channel model that permits one to decouple the center of mass from the relative degree of freedom with identity

$$\begin{aligned} \sum_{\alpha'_1, \alpha'_2} |\alpha'_1, \alpha'_2\rangle G_\downarrow^{(0,0)}(\alpha'_1, \tau) G_\uparrow^{(0,0)}(\alpha'_2, \tau) \langle \alpha'_1, \alpha'_2 | \\ = \sum_{\alpha_r, \alpha_c} |\alpha_r, \alpha_c\rangle \langle \alpha_r, \alpha_c | e^{-\hat{H}_0^a \tau} \theta(\tau). \quad (108) \end{aligned}$$

The atomic part of the T -matrix is the Laplace transform of the vacuum vertex function:

$$\hat{T}^a(s) = \int_0^\infty d\tau e^{s\tau / \hbar} \hat{\Gamma}_{\text{vac}}^a(\tau) \quad (109)$$

$$\hat{\Gamma}_{\text{vac}}^a(\tau) = \int_{\mathcal{C}_\gamma} \frac{ds}{2i\pi\hbar} e^{-s\tau / \hbar} \hat{T}^a(s). \quad (110)$$

The contour \mathcal{C}_γ in the inverse Laplace transform of Eq. (110) is the vertical line in the complex plane $\Re(s) = \gamma \in \mathbb{R}$, oriented from $\gamma - i\infty$ to $\gamma + i\infty$ and such that the integrand is an analytical function on the left hand side of the contour. In the high temperature limit of Eq. (106), the functions in the integrands are retarded and the intermediate imaginary times are thus ordered. This permits one to simplify the calculation of the Laplace transform in Eq. (109). For example the contribution of the third term in the right hand side of Eq. (106) where we set $\tau_1 = 0$, can be evaluated by using

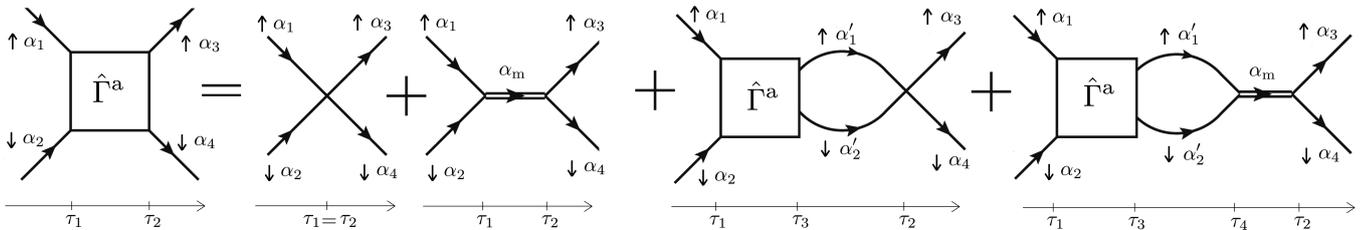


FIG. 3: Diagrammatic form of the Bethe-Salpeter equation for the atom-atom vertex $\hat{\Gamma}^a$.

the following change of variable

$$\begin{aligned} & \int_0^\infty d\tau_2 e^{s\tau_2/\hbar} \int_0^\infty d\tau_3 \hat{\Gamma}_{\text{vac}}^a(\tau_3) e^{-\hat{H}_0^a(\tau_2 - \tau_3)/\hbar} \theta(\tau_2 - \tau_3) \\ &= \int_0^\infty d\tau e^{(s - \hat{H}_0^a)\tau/\hbar} \int_0^\infty d\tau_3 e^{s\tau_3/\hbar} \hat{\Gamma}_{\text{vac}}^a(\tau_3). \end{aligned} \quad (111)$$

We use the same type of change of variable in the fourth term in the right hand side of Eq. (106) and eventually

$$\begin{aligned} \langle \alpha_m | \hat{\Gamma}^m(\tau_2 - \tau_1) | \alpha'_m \rangle &= \sum_{\alpha_1, \alpha_2} \langle \alpha_m | \hat{V}^{\text{ma}} | \alpha_1, \alpha_2 \rangle G_\uparrow^0(\alpha_1, \tau_2 - \tau_1) G_\downarrow^0(\alpha_2, \tau_2 - \tau_1) \langle \alpha_1, \alpha_2 | \hat{V}^{\text{am}} | \alpha'_m \rangle \\ &\quad - \frac{1}{\hbar^2} \int_0^{\beta\hbar} d\tau_3 \int_0^{\beta\hbar} d\tau_4 \sum_{\alpha_1, \alpha_2, \alpha_3, \alpha_4} \langle \alpha_m | \hat{V}^{\text{ma}} | \alpha_1, \alpha_2 \rangle G_\uparrow^0(\alpha_1, \tau_3 - \tau_1) G_\downarrow^0(\alpha_2, \tau_3 - \tau_1) \\ &\quad \times \langle \alpha_1, \alpha_2 | \hat{\Gamma}^a(\tau_4 - \tau_3) | \alpha_3, \alpha_4 \rangle G_\uparrow^0(\alpha_3, \tau_2 - \tau_4) G_\downarrow^0(\alpha_4, \tau_2 - \tau_4) \langle \alpha_3, \alpha_4 | \hat{V}^{\text{am}} | \alpha'_m \rangle, \end{aligned} \quad (112)$$

In the high temperature limit, we introduce the vacuum contribution $\hat{\Gamma}_{\text{vac}}^m$ along the same lines as was done for the atomic part and one recovers the molecular part of the T -matrix in Eq. (70) with

$$\hat{T}^m(s) = - \int_0^\infty d\tau e^{s\tau/\hbar} \hat{\Gamma}_{\text{vac}}^m(\tau). \quad (113)$$

Equation (112) can then be transformed into Eq. (58) and eventually one recovers Eq. (61).

C. The Beth-Uhlenbeck formula from the diagrammatic method

In this part, we evaluate the second order virial coefficient for the two-spin component Fermi gas by using the diagrammatic method. We denote the second order term in the expansion of Eq. (12) by $\delta^{(2)}\langle \hat{N}_\uparrow \rangle + \delta^{(2)}\langle \hat{N}_m \rangle$. The second order virial coefficient is then obtained from the identity

$$\Delta b_{1,1} = \frac{1}{z_\uparrow z_\downarrow Q} \left(\delta^{(2)}\langle \hat{N}_\uparrow \rangle + \delta^{(2)}\langle \hat{N}_m \rangle \right) \quad (114)$$

we obtain the Lippmann-Schwinger equation (56). The expression of the atomic part of the transition matrix in Eq. (59) follows directly from this last equation. Notice that this result could have been also obtained in the zero temperature formalism in vacuum.

Concerning the molecular part, we introduce the operator $\hat{\Gamma}^m$ analogous to $\hat{\Gamma}^a$ with the diagrammatic expansion given in Fig. (4). We thus obtain the Bethe-Salpeter like equation:

and we can express it in terms of the Feynman and blocks diagrams introduced in sec. IV A and sec. IV B in Fig. (5). The corresponding equation is:

$$\begin{aligned} \Delta b_{1,1} &= \frac{1}{\hbar Q} \int_0^{\beta\hbar} d\tau_1 \int_0^{\beta\hbar} d\tau_2 \left[\sum_{\alpha_1, \alpha_2} G_\uparrow^{(0,0)}(\alpha_1, \tau_1) \right. \\ &\quad \times G_\downarrow^{(0,1)}(\alpha_2, \tau_1 - \tau_2) G_\uparrow^{(0,1)}(\alpha_1, 0^- - \tau_2) \\ &\quad \times \langle \alpha_1, \alpha_2 | \hat{\Gamma}_{\text{vac}}^a(\tau_2 - \tau_1) | \alpha_1, \alpha_2 \rangle - \sum_{\alpha_m} G_m^{(0,0)}(\alpha_m, \tau_1) \\ &\quad \left. \times G_m^{(0,1)}(\alpha_m, 0^- - \tau_2) \langle \alpha_m | \hat{\Gamma}_{\text{vac}}^m(\tau_2 - \tau_1) | \alpha_m \rangle \right]. \end{aligned} \quad (115)$$

By using the same type of simplification as in Eq. (108) and performing the change of variable $\tau_2 = \tau + \tau_1$ one finds

$$\begin{aligned} \Delta b_{1,1} &= \frac{-1}{\hbar Q} \int_0^\infty d\tau_1 \int_0^\infty d\tau \theta(\beta\hbar - \tau_1 - \tau) \\ &\quad \times \text{Tr} \left[e^{-\hat{H}_0^a(\beta - \tau/\hbar)} \hat{\Gamma}_{\text{vac}}^a(\tau) + e^{-\hat{H}_0^m(\beta - \tau/\hbar)} \hat{\Gamma}_{\text{vac}}^m(\tau) \right] \end{aligned} \quad (116)$$

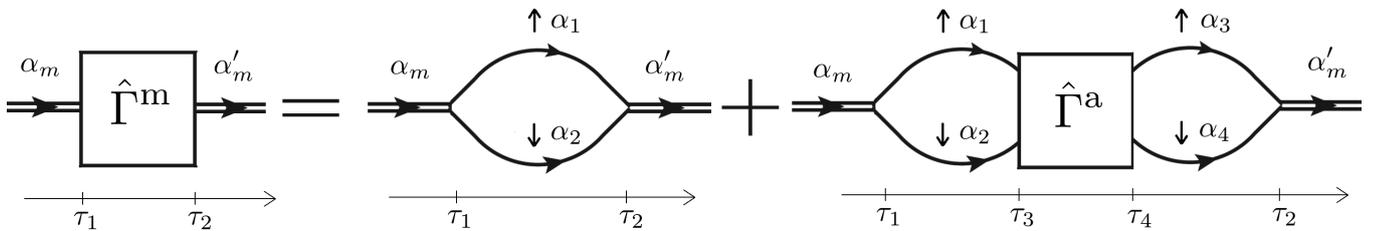
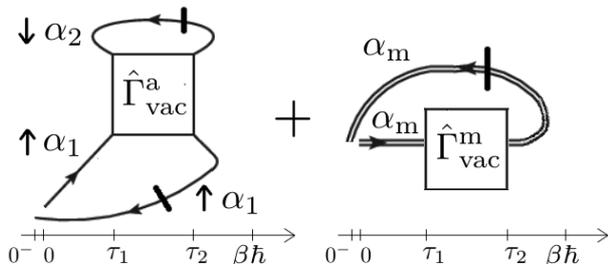


FIG. 4: Diagrammatic form of Eq. (112).

FIG. 5: The two diagrams contributing to $\Delta b_{1,1}$, see Eqs. (114), (115).

and the integration over τ_1 yields

$$\Delta b_{1,1} = \frac{-1}{\hbar Q} \int_0^\infty d\tau (\beta\hbar - \tau) \theta(\beta\hbar - \tau) \times \text{Tr} \left[e^{-\hat{H}_0^a(\beta - \tau/\hbar)} \times \hat{\Gamma}_{\text{vac}}^a(\tau) + e^{-\hat{H}_0^m(\beta - \tau/\hbar)} \hat{\Gamma}_{\text{vac}}^m(\tau) \right]. \quad (117)$$

Equation (117) is a product of convolution of retarded functions evaluated at the imaginary time $\beta\hbar$. It can be thus expressed as the inverse Laplace transform of a product of two Laplace transforms:

$$\Delta b_{1,1} = - \int_{C_\gamma} \frac{ds}{2i\pi} \frac{e^{-\beta s}}{Q} \text{Tr} \left[\frac{\hat{T}^a(s)}{(s - \hat{H}_0^a)^2} + \frac{\hat{T}^m(s)}{(s - \hat{H}_0^m)^2} \right]. \quad (118)$$

Using the analyticity of the integrand, the Bromwich contour C_γ can be deformed into the contour C_+ with an opposite direction and one finds Eq. (92).

CONCLUSIONS

In this paper, we use two methods to derive an explicit formula for the second order virial coefficient for

Bose and Fermi atomic gases in atomic waveguides in the vicinity of a Feshbach resonance. We use a quantitative two-channel model which permits us to explicitly take into account the Feshbach mechanism. Our analysis reveals deep correspondences between two different methods which can be extended to the evaluation of higher order in the virial expansion.

As a consequence of the separability of the model, there is formally no change for the expression of the phase-shift and for the usual Beth-Uhlenbeck formula with respect to the homogeneous case and in absence of Feshbach coupling. However as shown in Ref. [42], the presence of an atomic waveguide and of the inter-channel coupling deeply change the low energy properties with respect to the 3D and single channel results. This way without using the LDA, our formalism permits also to obtain quantitative results in regimes where the systems cannot be considered as purely 1D or 2D.

Previous studies focused on the universal character of the virial expansion near resonance. Our results permits to take into account quantitatively non resonant contributions in two-body scattering. This thus provides a quantitative basis for analysis of experiments where one expects deviations from universal laws due to the presence of an atomic waveguide and/or a finite detuning from resonance.

One can notice that the present formalism can be adapted to evaluate the spectral densities of atomic gases in waveguides including the closed channel by expanding the self energy in terms of the fugacity [36, 44, 45].

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