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Particle densities for dilute hard-sphere Bose or Fermi gases in an external potential

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Abstract. We prove that if the diameter of a hard-sphere is much smaller than the size of an external potential, the s-wave pseudopotential reduces to the Huang-Yang s-wave pseudopotential. We obtain the first-order virial expansions of particle densities for dilute hard-sphere Bose or Fermi gases in an arbitrary external potential. In the absence of an external potential, the results reduce to the Huang-Yang-Luttinger and Lee-Yang virial expansions. In the quasi-classical limit, the results reduce to the results of the local density approximation.

PACS. 05.30.-d Quantum statistical mechanics – 05.30.Jp Boson systems – 05.30.Fk Fermion systems and electron gas – 31.15.Bs Statistical model calculations (including Thomas-Fermi and Thomas-Fermi-Dirac models)

1 Introduction

In 1995, Bose-Einstein condensation was observed in the experiments on dilute vapors of rubidium and sodium in which the Bose atoms were confined in magnetic traps and cooled down to extremely low temperatures [1]. These spectacular experimental achievements have stimulated further experimental and theoretical studies [2]. In 1999, the evaporative cooling of dilute Fermi gases was achieved by using the magnetic confinement techniques [3].

The noninteracting quantum gases is a zeroth-order approximation to the real quantum gases. The noninteracting Bose and Fermi gases in d-dimensional harmonic traps are exactly solvable since the single-particle density matrix is available [4,5]. The exact particle and energy densities for the harmonically trapped noninteracting Bose gas in any dimensions have been obtained [6]. The exact particle and energy densities of the harmonically trapped noninteracting Fermi gas in any dimensions have been obtained [6–9]. The density profile for a harmonically trapped noninteracting Fermi gas in any dimensions has been obtained as an asymptotic series in inverse powers of particle number [10,11].

In the 1950s Huang and Yang [12–14] developed a pseudopotential method for a dilute quantum gas in the absence of an external potential. The basic idea is that at low temperatures, only the ground state and the low-lying energy levels of the system are involved. Hence a complete knowledge of N-particle Schrödinger equation is not necessary. At low temperatures, the energies of particles are low. At low energies, usually only the s-wave scattering is important and the s-wave scattering is completely determined by the scattering length a. The eigenvalues and eigenfunctions of the system can be expanded as a power series in a. Hence the actual, complicated N-particle Hamiltonian may be replaced by a much simpler pseudopotential Hamiltonian, which reproduces the ground state and the low-lying energy levels of the system. The thermodynamic quantities may be expanded as a power series in a/λ. Since the current experiments are performed in traps, in this paper, we will apply the pseudopotential method to a dilute quantum hard-sphere gas in an external potential.

This paper is organized as follows. In Section 2, the single-particle Bloch matrix density is given. In Section 3, the validity of the Huang-Yang s-wave pseudopotential is discussed for any external potential. In Section 4, the first-order particle density for a Bose or Fermi gas with spin J in an external potential is obtained. In Section 5, we discuss possible experimental detection. In Section 6, a summary of this paper is given.

2 Single particle bloch density matrix

The single-particle Schrödinger equation reads

$$\left[-\frac{\hbar^2}{2m}\Big(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\Big)+V(\vec{r})\right]\psi_i(\vec{r})=\epsilon_i\psi_i(\vec{r}), \tag{1}$$

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where $V(\vec{r})$ is the external potential, ϵ_i are energy eigenvalues and $\psi_i(\vec{r})$ is a complete set of normalized orthonormal eigenfunctions. The single-particle Bloch density matrix is defined by

$$C(\vec{r},\vec{r'};\beta) = \sum_i \psi_i^*(\vec{r'})\psi_i(\vec{r})e^{-\beta\epsilon_i}, \quad (2)$$

with

$$C(\vec{r},\vec{r'};\beta) = \lambda^{-3}\exp\left[-\frac{(\vec{r}-\vec{r'})^2}{2\hbar^2\beta}\right], \quad (3)$$

for $V(\vec{r}) = 0$, and

$$C(\vec{r},\vec{r'};\beta;\omega_1,\omega_2,\omega_3) = C(x,x';\beta;\omega_1)C(y,y';\beta;\omega_2)C(z,z';\beta;\omega_3), \quad (4)$$

for a harmonic potential $V(\vec{r}) = (m/2)(\omega_1^2x^2 + \omega_2^2y^2 + \omega_3^2z^2)$. Here $\beta = 1/k_BT$, $\lambda = h(2\pi mk_BT)^{-1/2}$ is the thermal wavelength and $C(x,x';\beta;\omega)$ is the Bloch density matrix of a one-dimensional harmonic oscillator [4,5],

$$C(x,x';\beta;\omega) = \left[\frac{m\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}\right]^{1/2} \times\exp\Big\{-\frac{m\omega}{4\hbar}\Big[(x+x')^2\tanh(\beta\hbar\omega/2) + (x-x')^2\coth(\beta\hbar\omega/2)\Big]\Big\}. \quad (5)$$

In the quasi-classical limit, as shown by Landau and Lifshitz [15], $C(\vec{r},\vec{r};\beta)$ may be expanded as a power series in $\hbar$. Using equation (33.13) in [15], we obtain

$$C(\vec{r},\vec{r};\beta) = \lambda^{-3}\left\{1-\frac{\beta^2\hbar^2}{12m}\nabla^2V(\vec{r})+\frac{\beta^3\hbar^2}{24m}\Big[\nabla V(\vec{r})\Big]^2+O(\hbar^4)\right\}e^{-\beta V(\vec{r})}. \quad (6)$$

3 Huang-Yang s-wave pseudopotential

Recently, the s-wave pseudopotential of two quantum particles in isotropic harmonic potential has been determined [16,17]. It was found that for $a/\sqrt{2}a_{ho} \ll 1$, the s-wave pseudopotential reduces to the Huang-Yang s-wave pseudopotential. Here a is the diameter of a hard-sphere and $a_{ho} = (\hbar/m\omega)^{1/2}$.

Define the size L of an external potential $V(\vec{r})$ such that $\hbar^2/mL^2 \sim V(|\vec{r}| = L)$. Let us show that for $a/L \ll 1$, the s-wave pseudopotential of a dilute quantum hard-sphere gas in an external potential reduces to the Huang-Yang s-wave pseudopotential.

Consider the Schrödinger equation of two particles in an external potential $V(\vec{r})$

$$\left[-\frac{\hbar^2}{2m}\Big(\nabla_1^2+\nabla_2^2\Big)+V(\vec{r}_1)+V(\vec{r}_2)\right]\Psi(\vec{r}_1,\vec{r}_2) = E\Psi(\vec{r}_1,\vec{r}_2), \quad |\vec{r}_1-\vec{r}_2| > a, \quad (7)$$

with the boundary condition $\Psi(|\vec{r}_1-\vec{r}_2| = a) = 0$. Introducing center-of-mass coordinates $\vec{R} = (\vec{r}_1+\vec{r}_2)/2$ and relative coordinates $\vec{r} = \vec{r}_1-\vec{r}_2$, equation (7) becomes

$$\left[-\frac{\hbar^2}{4m}\nabla_{\vec{R}}^2-\frac{\hbar^2}{m}\nabla_{\vec{r}}^2+V(\vec{R}+\vec{r}/2)+V(\vec{R}-\vec{r}/2)\right]\Psi(\vec{R},\vec{r}) = E\Psi(\vec{R},\vec{r}), \quad r > a. \quad (8)$$

We may extend equation (8) to the regime $r < a$. To the order a, we may make an approximation $V(\vec{R}+\vec{r}/2) + V(\vec{R}-\vec{r}/2) = 2V(\vec{R}) + O(r^2)$. To this degree approximation, the center-of-mass motion decouples from the relative motion. The relative motion is

$$\left(-\frac{\hbar^2}{m}\nabla_{\vec{r}}^2\right)\Omega(\vec{r}) = E_r\Omega(\vec{r}), \quad r \le a. \quad (9)$$

The s-wave ($l = 0$) solution is

$$\Omega(\vec{r}) = \left[\frac{\sin(kr)}{kr}-\tan(ka)\frac{\cos(kr)}{kr}\right]\left[\frac{\partial(r\Omega)}{\partial r}|_{r\to 0}\right], \quad r \le a. \quad (10)$$

where $k = (mE_r)^{1/2}/\hbar$. So we obtain

$$\left(-\frac{\hbar^2}{m}\nabla_{\vec{r}}^2\right)\Omega(\vec{r}) = E_r\Omega(\vec{r}) - \frac{4\pi\hbar^2}{m}\frac{\tan(ka)}{k}\delta(\vec{r})\frac{\partial(r\Omega)}{\partial r}, \quad r \le a. \quad (11)$$

Since $E_r \sim \hbar^2/mL^2$, we find $ka \sim a/L \ll 1$. So equation (11) becomes

$$\left(-\frac{\hbar^2}{m}\nabla_{\vec{r}}^2\right)\Omega(\vec{r}) = E_r\Omega(\vec{r}) - \frac{4\pi a\hbar^2}{m}\delta(\vec{r})\frac{\partial(r\Omega)}{\partial r}, \quad r \le a. \quad (12)$$

Therefore equations (7) and (12) can be written in one single equation valid for all values of $\vec{r}_1$ and $\vec{r}_2$ [18],

$$\left[-\frac{\hbar^2}{2m}\Big(\nabla_1^2+\nabla_2^2\Big)+V(\vec{r}_1)+V(\vec{r}_2)+\frac{4\pi a\hbar^2}{m}\delta(\vec{r}_1-\vec{r}_2)\frac{\partial}{\partial r_{12}}r_{12}\right]\Psi(\vec{r}_1,\vec{r}_2) = E\Psi(\vec{r}_1,\vec{r}_2). \quad (13)$$

To the order a, equation (13) is exact. Equation (13) contains the desired pseudopotential

$$H = \sum_{i=1}^N\left[-\frac{\hbar^2}{2m}\nabla_i^2+V(\vec{r}_i)\right]+\frac{4\pi a\hbar^2}{m}\sum_{1\le i<j\le N}\delta(\vec{r}_i-\vec{r}_j)\frac{\partial}{\partial r_{ij}}r_{ij}, \equiv H_0+H' \quad (14)$$

where $r_{ij} = |\vec{r}_i-\vec{r}_j|$.

4 Bose or Fermi gas with spin J

The second quantization of H' is

$$H' = \frac{2\pi a\hbar^2}{m} \sum_{i\alpha j\gamma k\theta l\omega} a_{i\alpha}^{\dagger} a_{j\gamma}^{\dagger} a_{l\omega} a_{k\theta} \int d^3r_1 d^3r_2 \times \left[\psi_i^*(\vec{r})\chi_\alpha^\dagger(1)\psi_j^*(\vec{r})\chi_\gamma^\dagger(2)\right]\delta(\vec{r}_1-\vec{r}_2) \times \left[\psi_k(\vec{r})\chi_\theta(1)\psi_l(\vec{r})\chi_\omega(2)\right]$$
$$= \frac{2\pi a\hbar^2}{m} \sum_{i\alpha j\gamma k\theta l\omega} a_{i\alpha}^{\dagger} a_{j\gamma}^{\dagger} a_{l\omega} a_{k\theta}\delta_{\alpha\theta}\delta_{\gamma\omega} \times \int d^3r \psi_i^*(\vec{r})\psi_j^*(\vec{r})\psi_k(\vec{r})\psi_l(\vec{r}), \quad (15)$$

where $a_{i\alpha}^\dagger$, $a_{i\alpha}$ are creation and annihilation operators of bosons or fermions for the single-particle state $\psi_i\chi_\alpha$, respectively. Here χ_α is the spin wave function and $\alpha = -J, -J+1, \cdots, J$. The unperturbed wave function of N bosons or fermions are

$$|\Phi_n\rangle = |\cdots n_{i\alpha}\cdots\rangle, \quad i=1,2,\cdots; \quad \alpha=-J,-J+1,\cdots,J, \quad (16)$$

where $n_{l\alpha}$ represents the occupation number on the single-particle quantum state $\psi_l\chi_\alpha$. We have, for bosons

$$a_{i\alpha}|\cdots n_{i\alpha}\cdots\rangle = \sqrt{n_{i\alpha}}|\cdots n_{i\alpha}-1\cdots\rangle, \quad (17)$$

$$a_{i\alpha}^\dagger|\cdots n_{i\alpha}\cdots\rangle = \sqrt{n_{i\alpha}+1}|\cdots n_{i\alpha}+1\cdots\rangle, \quad (18)$$

and for fermions

$$a_{i\alpha}|\cdots n_{i\alpha}\cdots\rangle = \begin{cases} (-1)^S\sqrt{n_{i\alpha}}|\cdots n_{i\alpha}-1\cdots\rangle, & n_{i\alpha}=1 \\ 0, & n_{i\alpha}=0 \end{cases} \quad (19)$$

$$a_{i\alpha}^\dagger|\cdots n_{i\alpha}\cdots\rangle = \begin{cases} (-1)^S\sqrt{n_{i\alpha}+1}|\cdots n_{i\alpha}+1\cdots\rangle, & n_{i\alpha}=0 \\ 0, & n_{i\alpha}=1 \end{cases} \quad (20)$$

where

$$S = \sum_{l=1}^{i-1}\sum_{\theta=-J}^{\alpha-1} n_{l\theta} + n_{i-1,\alpha} + n_{i,\alpha-1}. \quad (21)$$

Using equations (17)–(20), we obtain the first-order energy [19], for Bose gas

$$\left\langle \Phi_n|H'|\Phi_n\right\rangle = \frac{2\pi a\hbar^2}{m}\sum_{i\alpha j\gamma}\Big[2n_{i\alpha}n_{j\gamma}(1-\delta_{ij}\delta_{\alpha\gamma}) \times (1+\delta_{\alpha\gamma}) + \delta_{ij}\delta_{\alpha\gamma}(n_{i\alpha}^2 - n_{i\alpha})\Big] \times \int d^3r|\psi_i(\vec{r})|^2|\psi_j(\vec{r})|^2, \quad (22)$$

and for Fermi gas,

$$\langle \Phi_n|H'|\Phi_n\rangle = \frac{2\pi a\hbar^2}{m}\sum_{i\alpha j\gamma} 2n_{i\alpha}n_{j\gamma}(1-\delta_{\alpha\gamma}) \times \int d^3r|\psi_i(\vec{r})|^2|\psi_j(\vec{r})|^2. \quad (23)$$

The canonical partition function may be expanded as a power series in a,

$$Q_N = Q_N^{(0)} + Q_N^{(1)} + \cdots, \quad (24)$$

with

$$Q_N^{(1)} = -\beta Tr\left(e^{-\beta H_0}H'\right) = -\beta\sum_n e^{-\beta E_n^{(0)}}\langle\Phi_n|H'|\Phi_n\rangle. \quad (25)$$

Substituting equations (22) and (23) into (25), we obtain, for Bose gas

$$Q_N^{(1)} = -\frac{2\pi a\hbar^2\beta}{m}\sum_{n_{l\theta},\sum n_{l\theta}=N} e^{-\beta\sum_{l\theta}n_{l\theta}\epsilon_l} \times \sum_{i\alpha j\gamma}\Big[2n_{i\alpha}n_{j\gamma}(1-\delta_{ij}\delta_{\alpha\gamma}) \times (1+\delta_{\alpha\gamma}) + \delta_{ij}\delta_{\alpha\gamma}(n_{i\alpha}^2-n_{i\alpha})\Big] \times \int d^3r|\psi_i(\vec{r})|^2|\psi_j(\vec{r})|^2, \quad (26)$$

and for Fermi gas,

$$Q_N^{(1)} = -\frac{2\pi a\hbar^2\beta}{m}\sum_{n_{l\theta},\sum n_{l\theta}=N} e^{-\beta\sum_{l\theta}n_{l\theta}\epsilon_l}\sum_{i\alpha j\gamma}2n_{i\alpha}n_{j\gamma} \times (1-\delta_{\alpha\gamma})\int d^3r|\psi_i(\vec{r})|^2|\psi_j(\vec{r})|^2. \quad (27)$$

The grand partition function may also be expanded as a power series in a,

$$\Xi = \sum_{N=0}^{\infty} z^N Q_N = \sum_{n=0}^{\infty}\left[\sum_{N=0}^{\infty} z^N Q_N^{(n)}\right] = \sum_{n=0}^{\infty}\Xi^{(n)}, \quad (28)$$

so

$$\ln\Xi = \ln\Xi^{(0)} + \frac{\Xi^{(1)}}{\Xi^{(0)}} + \cdots, \quad (29)$$

where $z=\exp(\mu/k_BT)$ is fugacity and μ is chemical potential, and

$$\Xi^{(0)} = \sum_{N=0}^{\infty} z^N \sum_{n_{l\theta},\sum n_{l\theta}=N} e^{-\beta\sum_{l\theta}n_{l\theta}\epsilon_l} = \prod_{l\theta}\left[\sum_{n_{l\theta}}\left(ze^{-\beta\epsilon_l}\right)^{n_{l\theta}}\right], \quad (30)$$

$$\Xi^{(n)} = \sum_{N=0}^{\infty} z^N Q_N^{(n)}. \quad (31)$$

Substituting equations (26) and (27) into (31), we obtain, for Bose gas,

$$\frac{\Xi^{(1)}}{\Xi^{(0)}} = -\frac{2\pi a\hbar^2\beta}{m}\left\{\prod_{l\theta}\left[\sum_{n_{l\theta}=0}^{\infty}\left(ze^{-\beta\epsilon_l}\right)^{n_{l\theta}}\right]\right\}^{-1} \times\sum_{i\alpha j\gamma}\left\{\prod_{l\theta}\left[\sum_{n_{l\theta}=0}^{\infty}\left(ze^{-\beta\epsilon_l}\right)^{n_{l\theta}}\right]\right\} \times\Big[2n_{i\alpha}n_{j\gamma}(1-\delta_{ij}\delta_{\alpha\gamma})(1+\delta_{\alpha\gamma}) +\delta_{ij}\delta_{\alpha\gamma}(n_{i\alpha}^2-n_{i\alpha})\Big]\int d^3r|\psi_i(\vec{r})|^2|\psi_j(\vec{r})|^2$$
$$= -\frac{2\pi a\hbar^2\beta}{m}\sum_{\alpha\gamma}\sum_{ij}\langle n_{i\alpha}\rangle\langle n_{j\gamma}\rangle(1+\delta_{\alpha\gamma}) \times\int d^3r|\psi_i(\vec{r})|^2|\psi_j(\vec{r})|^2$$
$$= -\frac{2\pi a\hbar^2\beta}{m}(2J+1)(2J+2)\int d^3r\Lambda_B(\vec{r})^2, \quad (32)$$

and for Fermi gas,

$$\frac{\Xi^{(1)}}{\Xi^{(0)}} = -\frac{2\pi a\hbar^2\beta}{m}\left\{\prod_{l\theta}\left[\sum_{n_{l\theta}=0,1}\left(ze^{-\beta\epsilon_l}\right)^{n_{l\theta}}\right]\right\}^{-1} \times\sum_{i\alpha j\gamma}\left\{\prod_{l\theta}\left[\sum_{n_{l\theta}=0,1}\left(ze^{-\beta\epsilon_l}\right)^{n_{l\theta}}\right]\right\}2n_{i\alpha}n_{j\gamma}(1-\delta_{\alpha\gamma}) \times\int d^3r|\psi_i(\vec{r})|^2|\psi_j(\vec{r})|^2$$
$$= -\frac{2\pi a\hbar^2\beta}{m}\sum_{\alpha\gamma}\sum_{ij}\langle n_{i\alpha}\rangle\langle n_{j\gamma}\rangle(1-\delta_{\alpha\gamma}) \times\int d^3r|\psi_i(\vec{r})|^2|\psi_j(\vec{r})|^2$$
$$= -\frac{2\pi a\hbar^2\beta}{m}(2J+1)(2J)\int d^3r\Lambda_F(\vec{r})^2, \quad (33)$$

where $\langle\rangle$ denotes ensemble average, for Bose gas

$$\langle n_{l\alpha}\rangle = \frac{\sum_{n_{l\alpha}=0}^{\infty} n_{l\alpha}[ze^{-\beta\epsilon_l}]^{n_{l\alpha}}}{\sum_{n_{l\alpha}=0}^{\infty}[ze^{-\beta\epsilon_l}]^{n_{l\alpha}}} = \frac{ze^{-\beta\epsilon_l}}{1-ze^{-\beta\epsilon_l}}, \quad (34)$$

$$\langle n_{l\alpha}^2\rangle = \langle n_{l\alpha}\rangle + 2\langle n_{l\alpha}\rangle^2, \quad (35)$$

and for Fermi gas

$$\langle n_{l\alpha}\rangle = \frac{\sum_{n_{l\alpha}=0,1} n_{l\alpha}[ze^{-\beta\epsilon_l}]^{n_{l\alpha}}}{\sum_{n_{l\alpha}=0,1}[ze^{-\beta\epsilon_l}]^{n_{l\alpha}}} = \frac{ze^{-\beta\epsilon_l}}{1+ze^{-\beta\epsilon_l}}, \quad (36)$$

Λ_B and Λ_F are defined by

$$\Lambda_B(\vec{r}) = \sum_i|\psi_i(\vec{r})|^2\frac{ze^{-\beta\epsilon_i}}{1-ze^{-\beta\epsilon_i}} = \sum_{n=1}^{\infty}z^nC(\vec{r},\vec{r};n\beta), \quad (37)$$

$$\Lambda_F(\vec{r}) = \sum_i|\psi_i(\vec{r})|^2\frac{ze^{-\beta\epsilon_i}}{1+ze^{-\beta\epsilon_i}} = \sum_{n=1}^{\infty}(-1)^{n+1}z^nC(\vec{r},\vec{r};n\beta). \quad (38)$$

where the power series converge for $z < e^{\beta\epsilon_0}$ with $\epsilon_0 = min(\epsilon_\alpha)$. For $z > e^{\beta\epsilon_0}$, $\Lambda_F(\vec{r})$ has been obtained by a inverse Laplace transform in [9]. Using Theorem 2 and Lemma 2 in [9], we obtain

$$\Lambda_F(\vec{r}) = \sum_{n=0}^{\infty}\Big\{(-1)^n\mathcal{L}_\mu^{-1}\left[\frac{C(\vec{r},\vec{r};\beta')}{\beta'+n\beta}\right] + (-1)^n\mathcal{L}_\mu^{-1}\left[\frac{C(\vec{r},\vec{r};\beta')}{\beta'-n\beta}\right]\Big|_{\mathrm{Re}(\beta'-n\beta)>0} - e^{n\beta\mu}C(\vec{r},\vec{r};n\beta)\Big\}, \quad (39)$$

where

$$\mathcal{L}_x^{-1}h(s) \equiv \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}e^{sx}h(s)ds, \quad x>0, c>0. \quad (40)$$

Using Theorem 5 in [9], we obtain for a isotropic harmonic potential,

$$\Lambda_F(\vec{r}) = \pi^{-3/2}a_{ho}^{-3}\exp(-r^2/a_{ho}^2)\sum_{n=0}^{\infty}(-1)^n \times\sum_{j=0}^{\infty}(-1)^jL_j(2r^2/a_{ho}^2) \times\sum_{k=0}^{\infty}\frac{\Gamma(3/2+k)}{k!\Gamma(3/2)}\Big[e^{-n\beta\hbar\omega(\mu/\hbar\omega-j-2k-3/2)} \times\Theta(\mu/\hbar\omega-j-2k-3/2) - (1-\delta_{n,0})e^{-n\beta\hbar\omega(-\mu/\hbar\omega+j+2k+3/2)} \times\Theta(-\mu/\hbar\omega+j+2k+3/2) + (j\to j+1)\Big], \quad (41)$$

where $a_{ho} = (\hbar/m\omega)^{1/2}$, $L_n(x) \equiv (e^x/n!)d^n(e^{-x}x^n)/dx^n$ are the Laguerre polynomials, $\Theta(x) = 1$ for $x \geq 0$ and $\Theta(x) = 0$ for $x < 0$.

Substituting equations (29), (30), (32), (33) into the thermodynamic relation

$$N = \int d^3r\rho(\vec{r}) = z\frac{\partial}{\partial z}\ln\Xi, \quad (42)$$

we obtain number density

$$\rho_B(\vec{r}) = (2J+1)\left[\Lambda_B(\vec{r}) - (1+J)\frac{4\pi a\hbar^2\beta}{m}z\frac{\partial}{\partial z}\Lambda_B(\vec{r})^2\right] + O\left(a^2\right), \quad (43)$$

$$\rho_F(\vec{r}) = (2J+1)\left[\Lambda_F(\vec{r}) - J\frac{4\pi a\hbar^2\beta}{m}z\frac{\partial}{\partial z}\Lambda_F(\vec{r})^2\right] + O\left(a^2\right). \quad (44)$$

Equations (43) and (44) may be expanded as

$$\rho_B(\vec{r}) = (2J+1)\left[\sum_{n=1}^{\infty} z^n C(\vec{r},\vec{r};n\beta)\right]\left[1-(1+J)\frac{8\pi a\hbar^2\beta}{m} \times \sum_{l=1}^{\infty} z^l l C(\vec{r},\vec{r};l\beta)\right] + O\left(a^2\right), \quad (45)$$

$$\rho_F(\vec{r}) = (2J+1)\left[\sum_{n=1}^{\infty}(-1)^{n+1} z^n C(\vec{r},\vec{r};n\beta)\right]\left[1-J\frac{8\pi a\hbar^2\beta}{m} \times \sum_{l=1}^{\infty}(-1)^{l+1} z^l l C(\vec{r},\vec{r};l\beta)\right] + O\left(a^2\right). \quad (46)$$

Substituting equations (3) into (45) and (46), we obtain the famous Huang-Yang-Luttinger [14] and Lee-Yang [21] virial expansions in the absence of an external potential,

$$\rho_B(\vec{r}) = (2J+1)\lambda^{-3} g_{\frac{3}{2}}(z)\left[1-4(1+J)\frac{a}{\lambda}g_{\frac{1}{2}}(z)\right] + O\left(a^2\right), \quad (47)$$

$$\rho_F(\vec{r}) = (2J+1)\lambda^{-3} g_{\frac{3}{2}}(-z)\left[-1-4J\frac{a}{\lambda}g_{\frac{1}{2}}(-z)\right] + O\left(a^2\right). \quad (48)$$

Substituting equations (6) into (45) and (46), we obtain the virial expansions in the quasi-classical limit,

$$\rho_B(\vec{r}) = (2J+1)\lambda^{-3} g_{\frac{3}{2}}\left(ze^{-\beta V(\vec{r})}\right)\left[1-4(1+J)\frac{a}{\lambda} \times g_{\frac{1}{2}}\left(ze^{-\beta V(\vec{r})}\right)\right] - \frac{(2J+1)\beta^2\hbar^2}{12m\lambda^3} g_{-\frac{1}{2}}\left(ze^{-\beta V(\vec{r})}\right)\bigtriangledown^2 V(\vec{r}) + \frac{(2J+1)\beta^3\hbar^2}{24m\lambda^3} g_{-\frac{3}{2}}\left(ze^{-\beta V(\vec{r})}\right)\left[\bigtriangledown V(\vec{r})\right]^2 + O\left(a^2\right), \quad (49)$$

$$\rho_F(\vec{r}) = (2J+1)\lambda^{-3} g_{\frac{3}{2}}\left(-ze^{-\beta V(\vec{r})}\right)\left[-1-4J\frac{a}{\lambda}g_{\frac{1}{2}} \times \left(-ze^{-\beta V(\vec{r})}\right)\right] + \frac{(2J+1)\beta^2\hbar^2}{24m\lambda^3} g_{-\frac{1}{2}}\left(-ze^{-\beta V(\vec{r})}\right)\bigtriangledown^2 V(\vec{r}) - \frac{(2J+1)\beta^3\hbar^2}{24m\lambda^3} g_{-\frac{3}{2}}\left(-ze^{-\beta V(\vec{r})}\right)\left[\bigtriangledown V(\vec{r})\right]^2 + O\left(a^2\right), \quad (50)$$

where $g_\gamma(z) = \sum_{n=1}^{\infty} z^n n^{-\gamma}$. The first terms are the local-density approximation [20]. The second and third terms are the corrections.

5 Possible experimental detection

For a dilute ultracold Fermi gas, the correction caused by the weak interactions between atoms is small. In order to seek possible experimental detection, let us consider the dilute Fermi gas at absolute zero in an isotropic harmonic trap. From equations (41) and (44) we obtain, for $T = 0$ K,

$$\rho_F(\vec{r}) = (2J+1)\Lambda_F(\vec{r})\left[1-J\frac{8\pi a\hbar^2}{m}\frac{\partial}{\partial\mu}\Lambda_F(\vec{r})\right] + O\left(a^2\right), \quad (51)$$

with

$$\Lambda_F(\vec{r}) = \pi^{-3/2} a_{ho}^{-3}\exp(-r^2/a_{ho}^2)\sum_{j=0}^{\infty}(-1)^j L_j(2r^2/a_{ho}^2) \times \sum_{k=0}^{\infty}\frac{\Gamma(3/2+k)}{k!\Gamma(3/2)} \times \left[\Theta(\mu/\hbar\omega - j - 2k - 3/2) + \Theta(\mu/\hbar\omega - j - 1 - 2k - 3/2)\right]. \quad (52)$$

From equation (38) we obtain, for $T = 0$ K,

$$\Lambda_F(\vec{r}) = \sum_{\epsilon_i<\mu}|\psi_i(\vec{r})|^2, \quad (53)$$

and

$$\int d^3r\Lambda_F(\vec{r}) = \sum_{\epsilon_i<\mu}1 = \sum_{n=0}^{M}(n+1)(n+2)/2 = (M+1)(M+2)(M+3)/6, \quad (54)$$

where $M = Int(\mu/\hbar\omega - 3/2)$.

From equation (52) we obtain

$$\Lambda_F(0) = \pi^{-3/2} a_{ho}^{-3}\sum_{k=0}^{Int(M/2)}\frac{\Gamma(3/2+k)}{k!\Gamma(3/2)}. \quad (55)$$

From equations (52), (54) and (55), we obtain, for $\mu/\hbar\omega \approx M \gg 6$ or equivalently for $N \gg (2J+1)48$,

$$\int d^3r\Lambda_F(\vec{r}) = (\mu/\hbar\omega)^3/6, \quad (56)$$

and

$$\Lambda_F(0) = \frac{4}{3\pi^2}a_{ho}^{-3}(\mu/2\hbar\omega)^{3/2}, \quad (57)$$

and

$$\Lambda_F(r/a_{ho} = \sqrt{2\mu/\hbar\omega}) \sim a_{ho}^{-3}\exp(-2\mu/\hbar\omega) \sim 0. \quad (58)$$

From equations (56)–(58), we see that the local density approximation is valid [10],

$$\Lambda_F(\vec{r}) = \frac{\sqrt{2}}{3\pi^2}\left(\frac{m}{\hbar^2}\right)^{3/2}\left(\mu - m\omega^2 r^2/2\right)^{3/2}. \quad (59)$$

Substituting equations (59) into (51), we obtain, for $N \gg (2J+1)48$ and $T = 0$ K,

$$\rho_F(\vec{r}) = \frac{(2J+1)\sqrt{2}}{3\pi^2} a_{ho}^{-3} \left(\frac{\mu}{\hbar\omega}\right)^{3/2} \left(1 - m\omega^2 r^2/2\mu\right)^{3/2} \times \left[1 - \frac{4\sqrt{2}J(2J+1)}{\pi} \frac{a}{a_{ho}} \left(\frac{\mu}{\hbar\omega}\right)^{1/2} (1 - m\omega^2 r^2/2\mu)^{1/2}\right]. \quad (60)$$

Similarly, for an anisotropic harmonic potential, we obtain, for $N \gg (2J+1)48$ and $T = 0$ K,

$$\Lambda_F(\vec{r}) = \frac{\sqrt{2}}{3\pi^2} \left(\frac{m}{\hbar^2}\right)^{3/2} \left[\mu - m\left(\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2\right)/2\right]^{3/2}, \quad (61)$$

$$\begin{aligned} \rho_F(\vec{r}) = & \frac{(2J+1)\sqrt{2}}{3\pi^2} a_{ho}^{-3} \left(\frac{\mu}{\hbar\omega_{ho}}\right)^{3/2} \\ & \times \left[1 - \frac{m}{2\mu}\left(\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2\right)\right]^{3/2} \\ & - \frac{8J(2J+1)^2}{3\pi^3} a_{ho}^{-3} \left(\frac{\mu}{\hbar\omega_{ho}}\right)^2 \frac{a}{a_{ho}} \\ & \times \left[1 - \frac{m}{2\mu}\left(\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2\right)\right]^2, \end{aligned} \quad (62)$$

$$N = \frac{2J+1}{6} \left(\frac{\mu}{\hbar\omega_{ho}}\right)^3 - J(2J+1)^2 \times \frac{512\sqrt{2}}{315\pi^2} \left(\frac{\mu}{\hbar\omega_{ho}}\right)^{5/2} \frac{a}{a_{ho}}, \quad (63)$$

where $\omega_{ho} = (\omega_1\omega_2\omega_3)^{1/3}$ and $a_{ho} = (\hbar/m\omega_{ho})^{1/2}$.

From equation (62) we see that the expansion parameter is $(\mu/\hbar\omega_{ho})^{1/2} a/a_{ho} \sim N^{1/6} a/a_{ho}$. For the current experiments, we have $a \sim$ 10–100 Å, $\omega_{ho} \sim$ 10–100 Hz, $m \sim 10^{-26}$ kg and $a_{ho} \sim 10^5$ Å, $a/a_{ho} \sim 10^{-3}$–10^{-4}. For $a/a_{ho} = 0.003$ and $J = 1/2$, the density distributions of a dilute Fermi gas at absolute zero in an isotropic harmonic potential are shown in Figure 1 for $N = 10^6, 10^7, 10^8, 10^9$, respectively. We see that for $N < 10^6$, the correction is negligible. For $10^6 < N < 10^{12}$, the correction is small but it is experimentally detectable. For $N > 10^{12}$, the perturbation expansion fails.

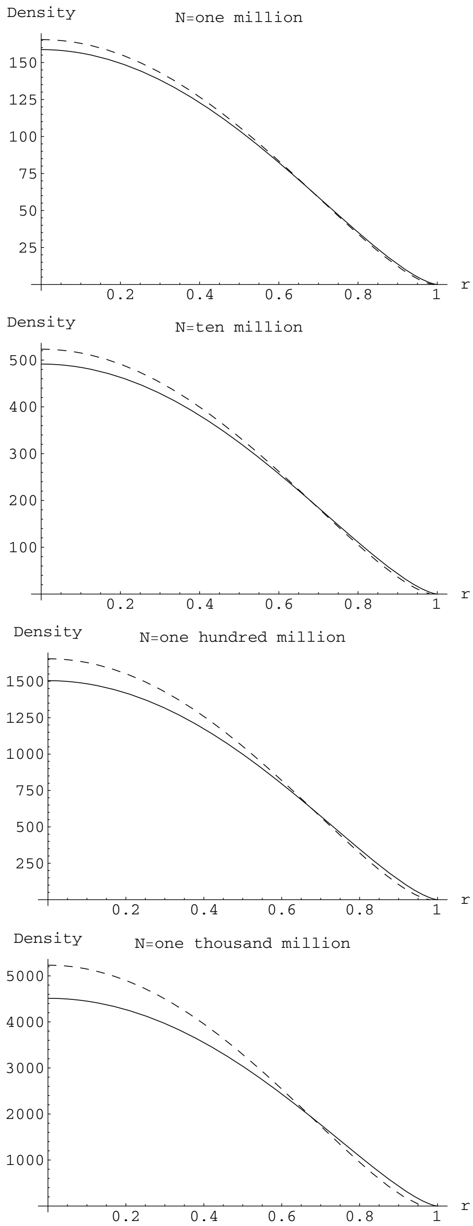

Fig. 1. Density ρ as functions of r for $N = 10^6, 10^7, 10^8, 10^9$. Here $a/a_{ho} = 0.003$. The unit of ρ is a_{ho}^{-3}. The units of r are $17.132a_{ho}, 25.2542a_{ho}, 37.3124a_{ho}, 55.3355a_{ho}$ for $N = 10^6, 10^7, 10^8, 10^9$, respectively. The dashing lines represent the noninteracting cases.

6 Conclusion

We have proved that if the diameter of a hard-sphere is much smaller than the size of an external potential, the s-wave pseudopotential reduces to the Huang-Yang s-wave pseudopotential. We obtain first-order virial expansions of particle densities for dilute hard-sphere Bose or Fermi gases in an arbitrary external potential, which are expressed in terms of the single-particle Bloch density matrix. Since the Bloch density matrix of a harmonic oscillator is known, we obtain explicit results for the gases in a harmonic potential. In the absence of an external potential, the results reduce to the Huang-Yang-Luttinger and Lee-Yang virial expansions. In the quasi-classical limit, the results reduce to the results of the local density approximation.

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