Free Expansion of a Weakly-interacting Dipolar Fermi Gas

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Abstract

We theoretically investigate a polarized dipolar Fermi gas in free expansion. The inter-particle dipolar interaction deforms phase-space distribution in trap and also in the expansion. We exactly predict the minimal quadrupole deformation in the expansion for the high-temperature Maxwell-Boltzmann and zero-temperature Thomas-Fermi gases in the Hartree-Fock and Landau-Vlasov approaches. In conclusion, we provide a proper approach to develop the time-of-flight method for the weakly-interacting dipolar Fermi gas and also reveal a scaling law associated with the Liouville’s theorem in the long-time behaviors of the both gases.
Recent development of trapping and manipulating techniques of atoms enables to realize ultracold dipolar gases of atoms and molecules in several years. In fact, dipolar Bose gases are realized in \(^{52}\text{Cr}\) atoms with magnetic dipole moments \(^{1}\text{[1–3]}\), and dipolar Fermi gases are also realized in heteronuclear \(^{40}\text{K}^{87}\text{Rb}\) molecules with electric dipole moments \(^{4}\text{[4–6]}\). The dipolar gases offer a great infrastructure for quantum many-body physics as new types of actual quantum systems.

The dipolar gases have a tensor-type dipolar interaction \(^{7}\), which depends on not only inter-particle relative position but also directions of the dipole moments. When we suppose the dipolar fermions perfectly polarized in a strong external electric field along the \(z\)-axis of the Cartesian axes as in the actual experiments \(^{4}\text{[4–6]}\), the interaction becomes

\[
v(r) = G_d \frac{1 - 3r_z^2/r^2}{r^3}
\]

with \(r \equiv \{r_x, r_y, r_z\}\), \(r \equiv |r|\), and a positive coupling constant \(G_d \propto d^2\) given later with some scaling units, where the electric dipolar moment \(d\) is experimentally manipulated in \(d \sim 10^{-11\sim 0} e a_B\) by choosing molecular internal states and electric field strength \(^{4}\text{[4–6]}\).

As an important feature, the dipolar Fermi gas is purely dominated by the long-range tensor force because of vanishment of short-range interactions owing to the Pauli blocking effect. The axisymmetric interaction in eq. \(^{1}\) produces anisotropic quantum correlations and density deformation and also makes instability in strong interaction regime \(^{8\sim12}\). Furthermore, differently from the short-range interactions, the long-range dipolar interaction deforms phase-space distribution, which indicates important information for quantum many-body effects in the dipolar gas \(^{11\sim12}\).

Free expansion physics is quite important for the dipolar gas. That is because the expansion is often used to observe the momentum distribution of the trapped gas in the time-of-flight (TOF) method; and the anisotropic momentum deformation directly reflects the phase-space deformation and interaction effects in the dipolar gas. In fact, the dipolar Bose gases are firstly observed in the expansion \(^{1\sim3}\). The dipolar interaction may change the momentum distribution not only in trap but also in the expansion, then we need some corrections to apply the TOF method to obtain the initial momentum distribution differently from the ballistic expansion with a conserved momentum distribution. To obtain the corrections, some people develop the quadrupole scaling method \(^{10\sim12}\); however no work has been done to demonstrate exact time-evolution of the expanding Fermi gas and confirm
validity of the scaling method in the expansion. The expansion problem is one of the most important current issues in theoretical physics on the dipolar gas.

The aim of this work is to reveal the expansion problem, i.e. relationship between the initial and final momentum deformations, in weak interaction regime. Here we exactly evaluate time-evolution of the minimal quadrupole deformation of the expanding gas by developing another scaling ansatz, which reproduces the Liouville’s theorem and perturbation theory from the ballistic expansion. This work must provide a proper correction for the TOF method to detect the quantum many-body effects on the dipolar gas.

Let us define the Hamiltonian of the dipolar gas as

\[ H = \int dr \; \psi^\dagger(r) \left[ -\frac{1}{2} \nabla_r^2 + v_T(r) \right] \psi(r) + H_1 \]  

(2)

with the fermion field operator \( \psi \) and interaction part

\[ H_1 \equiv \int dr \int dr' \psi^\dagger(r') \psi^\dagger(r') v(r - r') \psi(r') \psi(r), \]

(3)

where \( v \) is the dipolar interaction in eq. (1). The trap term is given as \( v_T(r) = \Theta(-t) V_T(r) \) with the step function \( \Theta(x) \) and trap potential \( V_T(r) \) before \( t = 0 \), when we leave the gas. To simplify the notations, we choose units for the reduced Planck constant and mass as \( \hbar = 1 \) and \( m = 1 \) and omit the time parameter \( t \), e.g. \( \psi(r, t) \equiv \psi(r) \).

To treat \( H_1 \) in eq. (2), we apply the time-dependent Hartree-Fock approximation (TDHFA) \[13\], in which the two-body interaction \( H_1 \) is rewritten into one-body interactions with self-consistent mean-fields, the direct (Hartree) and exchange (Fock) terms, reflecting the many-body effects as mean-values. In TDHFA, the field operator satisfies an equation of motion,

\[ i \frac{d\psi(r)}{dt} = -\frac{1}{2} \nabla_r^2 \psi(r) + \int dr' U(r, r') \psi(r'), \]

(4)

with the self-consistent non-local self-energy \( U(r, r') \) given later in eq. (7). Then the Wigner function \[14\],

\[ f(r, p) \equiv \int ds \; e^{-i p \cdot s} \; n \left( r - \frac{s}{2}, r + \frac{s}{2} \right) \]

(5)

with the density matrix \( n(r, r') \equiv \langle \psi^\dagger(r') \psi(r) \rangle \), obeys

\[ \frac{df}{dt} = -p \cdot \nabla_r f + \frac{2}{\hbar} \sin \left[ \frac{\nabla^f \cdot \nabla_r^2 - \nabla_r^f \cdot \nabla_r^2}{2\hbar^{-1}} \right] uf \]

(6)
with the Wigner transformation of \( U(r, r') \),

\[
\begin{align*}
    u(r, p) & \equiv \int ds \, e^{-ip \cdot s} U \left( r + \frac{s}{2}, r' - \frac{s}{2} \right) \\
    & = v_T(r) + u_H(r) + u_F(r, p),
\end{align*}
\]

where \( \nabla^f \) and \( \nabla^u \) act on \( f \) and \( u \), respectively. Here we introduce the Hartree part \( u_H(r) \)

\[
\begin{align*}
    u_H(r) & \equiv \int dr' v(r - r') n(r')
\end{align*}
\]

with the number density \( n(r) \equiv n(r, r) \) and Fock part \( u_F(r, p) \)

\[
\begin{align*}
    u_F(r, p) & \equiv -\int \frac{dq}{(2\pi)^3} V(p - q) f(r, q)
\end{align*}
\]

with the Fourier transformation of \( v(r) \) in eq. (1),

\[
V(p) \equiv \int dr \, e^{-ip \cdot r} v(r) = -\frac{4\pi}{3} G_d \frac{p^2 - 3p_z^2}{p^2},
\]

where \( p \equiv |p| \). We explicitly write \( \hbar (= 1) \) only in eq. (6) for the later explanation.

To treat the quantum dynamics in eq. (6), we use the semi-classical Landau-Vlasov (LV) approach [15]; i.e. expanding the trigonometric function in eq. (6) up to the first order of \( \hbar \).

Then we obtain the LV equation,

\[
\frac{df}{dt} = - \left( p + \nabla p u \right) \cdot \left( \nabla_r f \right) + \left( \nabla_r u \right) \cdot \left( \nabla_p f \right).
\]

As a conclusion of the formulation, we study the expansion by solving the LV equation, eq. (11), with some initial conditions, \( f(r, p; t = 0) = f_0(r, p) \).

Here we emphasize that a feature of the finite-range interaction (e.g. eq. (1)) must be in contribution of the Fock part, i.e. the momentum dependence of \( u \) as shown in eq. (7), so that \( \nabla_p u \) in eq. (11) may give notable contribution in the dipolar gas and should not be omitted.

In this work, we focus on the interaction effects on the time-dependent momentum distribution, \( \rho(p) = \int dr f(r, p) \), which corresponds to the density distribution at long-time limit as

\[
n(r) = \frac{1}{(2\pi t)^3} \rho \left( \frac{r}{t} \right) + O(t^{-1}).
\]

That is because we can pragmatically neglect the interaction after a cut-off time \( t_c \) (\( \rightarrow \infty \) in this theoretical work) [16], when the Wigner function in eq. (11) is regarded as the ballistic solution,

\[
f(r, p) = f_0(\xi, p),
\]
with the Galilei transformation, \( r \rightarrow \xi \equiv r - pt \); then the density distribution at \( t > t_c \) becomes

\[
n(r) = \int \frac{dp}{(2\pi)^3} f_c(r - p(t - t_c), p) = \int \frac{d\xi}{(2\pi t)^2} f_c\left(\xi + pt, \frac{r}{t}\right) + O(t^{-1})
\]

with the Wigner function \( f_c(r, p) \) at \( t = t_c \), where eq. (14) agrees with eq. (12) owing to the conservation of the momentum distribution in the ballistic expansion at \( t > t_c \). Thus the interaction effects appear in the time-evolution before \( t_c \), and one can obtain the final momentum distribution from the density distribution at long-time limit as shown in eq. (12).

Before calculation of the expansion dynamics, we firstly consider the ballistic expansion; i.e. the interaction is neglected only in the expansion process except in the initial states. In the ballistic expansion, the LV equation, eq. (11), becomes

\[
\frac{df}{dt} = -p \cdot \nabla_r f.
\]

Its solution exactly agrees with the ballistic solution in eq. (13). When we assume the initial Wigner function as some function of a parameter \([17]\)

\[
z(r, p) = \sum_{l=x,y,z} (\gamma_l^2 p_l^2 + \omega_l^2 r_l^2),
\]

the dynamics is determined only by a time-dependent parameter \( \bar{z} \equiv z(\xi, p) \), which becomes

\[
\bar{z} = \omega_l^2 p_l^2 t^2 - 2\omega_l^2 r_l p_l t + O(t^0) \quad \text{at the long-time limit.}
\]

In the previous approach \([12]\), the dynamical parameter is approximated as \( \bar{z} \approx z(r', p') \) with \( r_l' \equiv b_l^{-1} r_l \) and \( p_l' \equiv b_l p_l - \dot{b}_l r_l \), where \( b_l \) obeys \( \ddot{b}_l = D_l^2 b_l - 3 \) with \( D_l \equiv \sqrt{\langle p_l^2 \rangle(t = 0)/\langle r_l^2 \rangle(t = 0)} \) and \( b_l(t = 0) = 1 \) and becomes \( b_l = D_l t + 1/(2D_l t) + O(t^{-3}) \) at the long-time limit, after all. Here the cap-dot represents the Newton’s notation for time derivative. Owing to the quadratic Wigner function, \( D_l = \omega_l/\gamma_l \), and \( \bar{z} \approx \omega_l^2 p_l^2 t^2 - 2\omega_l^2 r_l p_l t + O(t^0) \) in the previous ansatz. This result agrees with that of the exact solution. However this agreement is a specific property of the quadratic Wigner function. Our ansatz in this work generally satisfies the ballistic limit beyond the quadratic case and gives the exact solution for the minimal variation from the ballistic expansion as described below.

We now consider the quadrupole deformation of the momentum distribution in the interacting non-ballistic expansion. The quadrupole deformation is the most important deformation owing to the axisymmetric interaction in eq. (1) and reflects not only the initial
deformation in trap but also the additional deformation in the expansion. To describe them, we introduce a time-dependent index parameter: $\lambda_p \equiv \ln(T_z/T_0)$ with $T_z \equiv \langle p_z^2 \rangle$ and $T_0 \equiv (\langle p_x^2 \rangle \langle p_y^2 \rangle \langle p_z^2 \rangle)^{1/3}$; then our interest is just focused on relationship between the initial conditions and $\lambda_p(t \to \infty)$. Eq. (11) leads

$$
\frac{d\lambda_p}{dt} = - \int d\xi \int \frac{dp}{(2\pi)^3} \frac{2p_z}{T_z} \frac{\partial u(\xi + p t, p)}{\partial z} \tilde{f}(\xi, p),
$$

where we define $\tilde{f}(\xi, p) \equiv f(\xi + pt, p)$ and use the partial integral. According to the definition in eq. (7), $u(\xi + pt, p)$ in eq. (17) can be written as

$$
u(\xi, p) = \int d\eta \int \frac{dq}{(2\pi)^3} \bar{v}(\xi - \eta, (p - q)t) \tilde{f}(\eta, q),
$$

where we introduce

$$\bar{v}(x, at) \equiv v(x + at) - V(a)\delta(x + at)
$$

with $q = a + p$ and $\eta = x + \xi$. By substituting eq. (18) into eq. (17) and using exchange symmetry on $\{\xi, p\} \leftrightarrow \{\eta, q\}$, we obtain

$$
\frac{d\lambda_p}{dt} = \int dx \int \frac{da}{(2\pi)^3} a \bar{v}(x, at) \frac{\partial F(x, a)}{\partial x_z}
$$

with

$$
F(x, a) \equiv \int d\xi \int \frac{dp}{(2\pi)^3} \tilde{f}(\xi, p) \tilde{f}(\xi + x, p + a).
$$

We here assume small variation from the ballistic solution in the phase-space distribution and introduce an ansatz for the Wigner function as

$$
\tilde{f}(\xi, p) = f_0(\tilde{\xi}, \tilde{p})
$$

with

$$
\tilde{p}_{x,y} = e^{\lambda/4} (p_{x,y} + \frac{\dot{\lambda}}{4} \xi_{x,y}), \quad \tilde{p}_z = e^{-\lambda/2} (p_z - \frac{\dot{\lambda}}{2} \xi_z),
$$

$$
\tilde{\xi}_{x,y} = e^{-\lambda/4} \xi_{x,y}, \quad \tilde{\xi}_z = e^{\lambda/2} \xi_z,
$$

where $\lambda$ indicates the additional deformation in the expansion, $\lambda_p \simeq \lambda_0 + \lambda$, with $\lambda(t = 0) = 0$. At the ballistic limit, $\lambda = 0$, and it always reproduces the ballistic solution. Furthermore this ansatz exactly satisfies the Liouville’s theorem corresponding to the current equation in the microscopic theory [18, 19].
In this Letter, we consider two general initial conditions: the high-temperature Maxwell-Boltzmann (MB) and zero-temperature Thomas-Fermi (TF) gases in cylindrical harmonic oscillator traps with the small phase-space quadrupole deformation owing to the weak interaction. The initial Wigner function becomes

\[ f_0(r,p) = e^{-(R_c + R_z + P_c + P_z)/2} \] (24)

for the MB gas and

\[ f_0(r,p) = \Theta \left[ 1 - \frac{R_c + R_z + P_c + P_z}{2} \right] \] (25)

for the TF gas with

\[ R_c \equiv e^{(\lambda_0 - \lambda_0)/2}(r_x^2 + r_y^2), \quad R_z \equiv e^{-(\lambda_0 - \lambda_0)}r_z^2, \]
\[ P_c \equiv e^{\lambda_0/2}(p_x^2 + p_y^2), \quad P_z \equiv e^{-\lambda_0}p_z^2, \] (26)

where \( \lambda_0 \equiv \lambda_p(t = 0) \) indicates the initial momentum deformation [20], and \( \Lambda_0 \) indicates sum of the initial density and momentum deformations. In addition, we also determine \( G_d \) in eq. (11) as \( G_d = (k_B T/(\hbar \omega))^{-5/2}N(a_B/\hbar)(m/m_e)(d/(ea_B))^2 \) for the MB gas and \( G_d = (6N)^{1/6}(a_B/\hbar)(m/m_e)(d/(ea_B))^2 \) for the TF gas [21] with the Boltzmann constant \( k_B \), temperature \( T \), particle number \( N \), Bohr radius \( a_B \), electron mass \( m_e \), elementary electric charge \( e \), trap frequency \( \omega \equiv (\omega_\chi \omega_y \omega_\zeta)^{1/3} (= 1 \text{ in this Letter}) \), and oscillator length \( a_{ho} \equiv \sqrt{\hbar/(m \omega)} \). The above formulations reproduce general quadratic descriptions of the MB and TF gases with rescaling [22].

Here we should comment that the interaction effect on \( \Lambda_0 \) in eq. (26) is always cancelled out in the quadrupole deformation owing to conservation of phase-space volume in the Liouville’s theorem. Thus \( \Lambda_0 \) corresponds to the density deformation of a non-interacting gas in the initial trap potential, i.e. \( \Lambda_0 = \ln (\omega_x/\omega_\zeta)^{4/3} = \ln (\omega_y/\omega_\zeta)^{4/3} \).

According to eqs. (22), (24), and (25), \( F(x,a) \) in eq. (21) becomes

\[ F(x,a) = \frac{1}{8} e^{-s^2/4} \] (27)

for the MB gas and

\[ F(x,a) = \frac{\Theta (8 - s^2)}{3\pi} \left[ \arcsin \left( \frac{\sqrt{8 - s^2}}{\sqrt{8}} \right) - \frac{s \sqrt{8 - s^2}}{960} (s^4 - 26s^2 + 264) \right] \] (28)
for the TF gas, where
\[ s \equiv \sqrt{\sum_{j=x,y} A_j + A_z + \sum_{j=x,y} X_j + X_z} \]  
(29)

with
\[
A_j \equiv e^{\lambda_p/2}(a_i + \frac{\dot{\lambda}}{4} x_i)^2, \quad A_z \equiv e^{-\lambda_p}(a_z - \frac{\dot{\lambda}}{2} x_z)^2, \\
X_j \equiv e^{(\Lambda_0 - \lambda_p)/2} x_j^2, \quad X_z \equiv e^{-(\Lambda_0 - \lambda_p)} x_z^2.
\]  
(30)

Substituting eq. (27) or (28) into eq. (20) and expanding up to the first orders of \( \Lambda_0, \lambda_p, \) and \( \dot{\lambda} \), we obtain a time-evolution equation for the minimal deformation:
\[
\dot{\lambda} = G_d \sum_{I=0}^{\infty} \sum_{J=0}^{\infty} \sum_{K=0}^{\infty} \Gamma_{IJK} \Lambda_I^{0} \lambda_p^J \dot{\lambda}^K \\
\simeq G_d \left( \Gamma_{000} + \Gamma_{100} \Lambda_0 + \Gamma_{010} \lambda_p + \Gamma_{001} \dot{\lambda} \right)
\]  
(31)

with the time-dependent coefficients \( \Gamma_{IJK}(t) \) depending on the initial conditions.

After the calculation, we obtain \( \Gamma_{000} = \Gamma_{010} = \Gamma_{001} = 0 \) and
\[
\dot{\lambda} \simeq G_d \Lambda_0 \Gamma_{100}
\]  
(32)
in the both gases. It reveals that the additional deformation \( \lambda \) in the expansion depends only on a conserved quantity \( G_d \Lambda_0 \equiv S \) and exhibits a scaling behavior,
\[
\lambda(t \to \infty) \simeq \gamma_{100} G_d \Lambda_0 = \gamma_{100} S,
\]  
(33)
at long-time limit with \( \gamma_{100} \equiv \int_0^{\infty} dt \Gamma_{100} \). The scaling behavior is due to cancellation of the Hartree and Fock parts determined by the time-developing phase-space distribution with the quadrupole deformation. According to the Liouville’s theorem, the incompressible quadrupole deformation in the momentum space gives strong constraint for the spatial motion as shown in the description of the deformation ansatz, and this constraint provides a source of the cancellation and scaling behavior.

Here it should be noted that the minimal deformation in eq. (32) exactly agrees with that in the first order perturbation theory, which can be obtained by replacing \( F(x, a) \) defined in eq. (20) with that of the ballistic solution, i.e. substituting \( \lambda = 0 \) and \( \dot{\lambda} = 0 \) in eqs. (27) and (28). This agreement is obviously due to the cancellation in the non-perturbative relation in eq. (31) and, after all, indicates that the minimal deformation must be determined only by the first order perturbation according to the scaling behavior.
In addition, we obtain

\[ \Gamma_{100} = \frac{3\gamma_{100}t}{(t^2 + 1)^{5/2}} \]  

(34)

with \( \gamma_{100} = -3/(70\sqrt{\pi}) \approx -0.0242 \) for the MB gas and \( \gamma_{100} \approx -0.00444 \) for the TF gas. Thus the quantum effect, i.e. difference between the MB and TF gases, is in the values of \( \gamma_{100} \) and definitions of \( G_d \). According to the temperature dependence in the MB gas \( (G_d \propto T^{-5/2}) \), the deformation vanishes at the high-temperature limit; in other words, the interaction effect principally appears as the quantum effect.

As a result, according to eq. (32) and \( G_d > 0 \), the interaction slightly reduces (increases) \( \lambda_p \) when \( \Lambda_0 > 0 \) \((< 0)\). It is due to the angular dependence of the dipolar interaction in eq. (1). When \( \Lambda_0 = 0 \), corresponding to the spherical trap, the results reproduce those of the ballistic solution, \( \lambda = 0 \), owing to vanishment of the interaction effect by the angular integration.

Note that \( S \) in eq. (33) can be given by the experimental setup, and \( \lambda_p(\infty) \approx \lambda_0 + \lambda(\infty) \) can be measured from the density distribution at long-time limit according to eq. (12). Thus eq. (33) provides a theoretical approach to obtain the initial momentum deformation \( \lambda_0 \) from the experimental measurement as a proper correction for the TOF method. Because of smallness of \( \gamma_{100} \) for the both gases, the correction is negligible when \( S \) (or the trap anisotropy) is small; otherwise the correction must have important contribution to detect the interaction effects.

Finally we should comment on difference between our and the previous approaches \[10, 12\] to treat the quadrupole deformation in the expansion. These are theoretically same except for choice of the phase-space frames: the expanding frame \( \{\xi, p\} \) in this work and rest frame \( \{r, p\} \) in the previous works. Thus any difference in the results must be due to the frame transformation. The previous ansatz is originally developed to the expanding hydrodynamical Bose gases, and then reproduces agreeable results with the experimental measurements \[23, 24\]. On the other hand, our ansatz is made to reproduce the exact results for the minimal deformation from the ballistic solution in the weak interaction regime and give explicit description of the variation. The both approaches give same results at the ballistic limit for the quadratic Wigner function as discussed above. Thus we find out that the previous ansatz also reproduce our exact results up to the first order perturbation from the ballistic limit in the quadratic case. That is because the exact results depend only on the first order perturbation according to the scaling behavior, and the first order perturbation
is determined by the ballistic solution according to the perturbation theory. This nontrivial
agreement may be a significant property of the quadratic deformed gas associated with the
scaling law.

In conclusion, we reveal that the additional phase-space deformation in the expansion is
negligible when $S$ is small, as shown in eq. (33); as $S$ increases, the deformation linearly
grows and exhibits the scaling law associated with the Liouville’s theorem in the long-
time behaviors of the MB and TF gases. After all, our results give the exact prediction
of the minimal quadrupole deformation in TDHFA and the LV approach, and provide a
proper correction for the TOF method as a fundamental infrastructure for the dipolar gas
physics. At the end, it should be noticed that the scaling law may not be valid for the large
deformation by the strong interaction; then one should directly solve the time-evolution in
the LV equation beyond the quadrupole ansatz to include the other multi-pole contribution.
The expansion problem in the strong interaction regime should be studied in another paper.

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[16] In fact, the effect on $\lambda_p$ decreases as $t^{-3}$ in eqs. (32) and (34). It is due to the $r^{-3}$ dependence of the interaction.

[17] This assumption corresponds to some equilibrium states in harmonic oscillator traps as shown in eqs. (24) and (25); $\gamma_l$ and $\omega_l$ indicate quadratic phase-space deformation of the initial state induced by the interaction and trap.

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[20] In principle, $\lambda_0$ must be determined by $G_d$ and $\Lambda_0$ in the equilibrium states; however we here give no relation between them because it has no influence on the results in this Letter.

[21] $G_d \sim 10^{(-2)\sim(+1)}$ in the actual experiment.

[22] In general, the TF and MB gases with the one-particle self-energy in eq. (7) can be denoted without explicit description of $N$ and $T$ by using scale transformation. Then information of $N$ and $T$ is included only in the scaled parameters ($\tilde{p} = Cp$, $\tilde{r} = Cr$, $\tilde{\mu}$, and $G_d$) depending on the statistics: $C = (6N)^{-1/6}$ and $\tilde{\mu} = (6N)^{-1/3}\mu$ ($= 1$ in eq. (25)) for the TF gas; $C = (k_BT)^{-1/2} \beta^{1/2}$ and $\tilde{\mu} = \ln[N^{-1}\beta^{-3}e^{\beta\mu}]$ ($= 0$ in eq. (24)) for the MB gas.

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