Lower Bounds for Thermodynamic Quantities of Classical Ionic Mixtures

Hiroo TOTSUJI[*]

Synopsis

Exact lower bounds are given for thermodynamic quantities of ionic mixtures in the uniform background in d dimensions with three-dimensional (1/r) Coulomb interaction (d=2 and 3) and with d-dimensional Coulomb interaction (d=1, 2, and 3). It is shown that these lower bounds improve upon known ones and give values close to experimental results which are available in the case of d=3.

1. Introduction

Exact bounds for thermodynamic quantities are useful for systems where we have no well-defined methods to calculate these quantities. We here investigate one of such systems, the strongly coupled system of charged particles in the uniform background of opposite charges which is important as the simplest system with the long range interaction and also as a model of some real plasmas.

There are two classes of these systems of charged particles, d-dimensional systems with three-dimensional (1/r) Coulomb interaction and d-dimensional systems with d-dimensional Coulomb interaction. To the first belong usual three-dimensional plasmas and two-dimensional ones which have recently become available on the surface of liquid helium or in the metal-oxide-semiconductor (MOS) inversion layer, and

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* Department of Electronics

to the second, three-dimensional plasmas and systems of charged rods
(d=2) and of charged sheets (d=1) where interaction potentials are
logalithmic and linear functions of the distance, respectively.

We have recently given exact lower bounds for thermodynamic
quantities of one-component plasmas (OCP's) in d dimensions with three
dimensional (1/r) Coulomb interaction (d=2 and 3) [1] and of those in
d dimensions with d-dimensional Coulomb interaction (d=1, 2, and 3)
[2], and have shown that these lower bounds improve upon known ones
giving values close to available experimental [3, 4, 5] or exact values
[6, 7]. Here we extend these lower bounds to cases of ionic mixtures
composed of s kinds of ions ($\alpha = 1, 2, \cdots, s$) in the uniform background
of opposite charges. We denote the charge, the total number, the
number density of α - th species of ions by e_α, N_α, and n_α, respectively.

2. Correlation Energy

The correlation energy per particle e_c of our system is given by

$$e_c = (1/2n) \int d\underset{\sim}{r} \sum_{\alpha,\beta} e_\alpha e_\beta n_\alpha n_\beta h^{\alpha\beta}(\underset{\sim}{r}) \phi(r). \qquad (2.1)$$

Here

$$n = \sum_\alpha n_\alpha \ , \qquad (2.2)$$

and $\phi(r)$ denotes the d-dimensional Coulomb interaction [2] whose zero
level is taken as $\phi(r=\ell)=0$ with $\ell=\infty$ for d>2 and $\ell=0$ for d<2;

$$\phi(r) = (2\pi)^{-d} \int d\underset{\sim}{k} \phi(k) \left[\exp(i\underset{\sim}{k} \cdot \underset{\sim}{r}) - \begin{Bmatrix} \theta(2-d) \\ \exp(i\underset{\sim}{k} \cdot \underset{\sim}{\ell}) \end{Bmatrix} \right] = \begin{cases} r^{2-d}/(d-2) & (d \neq 2) \\ -\ell n(r/\ell) & (d=2) \end{cases} \qquad (2.3)$$

where $d\underset{\sim}{k}$ denotes the d-dimensional volume integral in the Fourier space,

$$\phi(k) = 2\pi^{d/2} \Gamma(d/2)^{-1} k^{-2}, \qquad (2.4)$$

and $\theta(x)$ is the unit step function. We also introduced the pair
correlation function of ions α and ions β, $h^{\alpha\beta}(\underset{\sim}{r})$, defined by

$$n_\alpha n_\beta [h^{\alpha\beta}(\underset{\sim}{r})+1]=\int d\underset{\sim}{r}'<\sum_{i=1}^{N_\alpha}\sum_{j=1}^{N_\beta}\delta[\underset{\sim}{r}+\underset{\sim}{r}'-\underset{\sim}{r}_{(i,\alpha)}]\delta[\underset{\sim}{r}'-\underset{\sim}{r}_{(j,\beta)}]$$

$$-\delta_{\alpha\beta}\delta(\underset{\sim}{r})\sum_{i=1}^{N_\alpha}\delta[\underset{\sim}{r}'-\underset{\sim}{r}_{(i,\alpha)}]>/\int d\underset{\sim}{r}', \qquad (2.5)$$

where (i, α) denotes i-th particle of α-th species, $\underset{\sim}{r}_{(i,\alpha)}$ its position, and $< >$ the statistical average. Other thermodynamic quantities are easily derived from the correlation energy.

We define the structure factors by

$$S^{\alpha\beta}(\underset{\sim}{k})=<\rho_{\underset{\sim}{k}}^\alpha\rho_{-\underset{\sim}{k}}^\beta>/(N_\alpha N_\beta)^{1/2}, \qquad (2.6)$$

$$\rho_{\underset{\sim}{k}}^\alpha=\sum_{i=1}^{N_\alpha}\exp[-i\underset{\sim}{k}\cdot\underset{\sim}{r}_{(i,\alpha)}]. \qquad (2.7)$$

For d-dimensional ionic mixtures with d-dimensional Coulomb interaction, the correlation energy is expressed by the structure factors as

$$e_c=(1/2)\overline{e^2}(2\pi)^{-d}\int d\underset{\sim}{k}\phi(k)[\sum_{\alpha,\beta}(e_\alpha e_\beta/\overline{e^2})(n_\alpha n_\beta/n^2)^{1/2}S^{\alpha\beta}(\underset{\sim}{k})-1$$

$$+\left\{\begin{matrix}\theta(2-d)\\ \exp(i\underset{\sim}{k}\cdot\underset{\sim}{\ell})\end{matrix}\right\}] \quad \left\{\begin{matrix}(d\neq2)\\ (d=2)\end{matrix}\right. \qquad (2.8)$$

and for those with three-dimensional Coulomb interaction as

$$e_c=(1/2)\overline{e^2}(2\pi)^{-d}\int d\underset{\sim}{k}\phi_3(k)[\sum_{\alpha,\beta}(e_\alpha e_\beta/\overline{e^2})(n_\alpha n_\beta/n^2)^{1/2}S^{\alpha\beta}(\underset{\sim}{k})-1].$$

Here we used the relations

$$(n_\alpha n_\beta)^{1/2}h^{\alpha\beta}(\underset{\sim}{r})=(2\pi)^{-d}\int d\underset{\sim}{k}[S^{\alpha\beta}(\underset{\sim}{k})-\delta_{\alpha\beta}]\exp(i\underset{\sim}{k}\cdot\underset{\sim}{r}), \qquad (2.10)$$

$$\int d\underset{\sim}{r}(n_\alpha n_\beta)^{1/2}h^{\alpha\beta}(\underset{\sim}{r})=-\delta_{\alpha\beta}, \qquad (2.11)$$

the notation $\overline{Q^m}$ defined by

$$\overline{Q^m}=\sum_\alpha n_\alpha Q_\alpha^m/n, \qquad (2.12)$$

and the d-dimensional Fourier transform of three-dimensional Coulomb interaction $\phi_3(k)$ given by [1]

$$\phi_3(k)=\int d\underset{\sim}{r}\exp(i\underset{\sim}{k}\cdot\underset{\sim}{r})/r=(2\pi^{1/2})^{d-1}\Gamma[(d-1)/2]k^{1-d}. \qquad (2.13)$$

3.   Generalization of Ideas due to Mermin and Onsager

The inequality for the structure factor of the three-dimensional classical OCP due to Mermin [8] has been generalized to cases of d-dimensional OCP with d-dimensional Coulomb interaction [2]. Here we further generalize the inequality to cases of classical ionic mixtures as shown in Appendix. In these cases multiplicity of components gives some variety to inequalities of this type. For the fluctuations of charge density we have

$$\sum_{\alpha,\beta} (e_\alpha e_\beta/\overline{e^2})(n_\alpha n_\beta/n^2)^{1/2} S^{\alpha\beta}(\underset{\sim}{k}) \geq (\overline{e^{1+m}}^2/\overline{e^{2m}}\ \overline{e^2}) k^2/(k^2+k_m^2), \tag{3.1}$$

where k_m denotes the wave number defined by

$$k_m^2 = 2\pi^{d/2}\Gamma(d/2)^{-1} n\overline{e}\ \overline{e^{1+2m}}/\overline{e^{2m}} T, \tag{3.2}$$

T the temperature in energy units, and m an arbitrary parameter. We have also

$$\sum_{\alpha,\beta} (e_\alpha e_\beta/\overline{e^2})(n_\alpha n_\beta/n^2)^{1/2} S^{\alpha\beta}(\underset{\sim}{k}) \geq (n_\delta/n) e_\delta^2 k^2/(k^2+k_\delta^2) \tag{3.3}$$

for any component δ where

$$k_\delta^2 = 2\pi^{d/2}\Gamma(d/2)^{-1} n\overline{e}\ e_\delta/T. \tag{3.4}$$

Here we note that in the random phase approximation (RPA) the structure factors and the fluctuations of charge density are given by

$$S_{RPA}^{\alpha\beta}(\underset{\sim}{k}) = \delta_{\alpha\beta} - (n_\alpha n_\beta/n^2)^{1/2}(e_\alpha e_\beta/\overline{e^2})/(k^2+k_D^2), \tag{3.5}$$

$$\sum_{\alpha,\beta} (e_\alpha e_\beta/\overline{e^2})(n_\alpha n_\beta/n^2)^{1/2} S^{\alpha\beta}(\underset{\sim}{k}) = k^2/(k^2+k_D^2), \tag{3.6}$$

where k_D is the Debye wave number defined by

$$k_D^2 = 2\pi^{d/2}\Gamma(d/2)^{-1} n\overline{e^2}/T. \tag{3.7}$$

The inequality (3.1) with m=1 and Eq.(2.8) lead to an exact lower bound for the correlation energy e_c

$$e_c/T \geq [e_c(RPA)/T](\varepsilon_1) = \begin{cases} \varepsilon_1/2 & (d=1) \\ -(\varepsilon_1/4)[2\gamma + \ln(\varepsilon_1/2) + \ln(\overline{e^3}\overline{e}/\overline{e^2}^2) + \ln(\pi n \ell^2)] & (d=2) \\ -\varepsilon_1/2 & (d=3) \end{cases}$$ (3.8)

where $\gamma = 0.5772\cdots$ and $[e_c(RPA)/T](\varepsilon_1)$ is the RPA value for OCP at the plasma parameter

$$\varepsilon_1 = \overline{e^2} k_1^{d-2}/T .$$ (3.9)

For $d<2$ inequalities (3.1) with $m \neq 1$ and (3.3) also give lower bounds

$$e_c/T \geq (1/2)(\overline{e^{1+m^2}}/\overline{e^{2m}})/k_m T \qquad (d=1) ,$$ (3.10)

$$e_c/T \geq (1/2)(n_\delta/n) e_\delta^2/k_\delta T \qquad (d=1) ,$$ (3.11)

respectively. The random phase approximation, Eqs.(3.5) and (3.6), gives $[e_c(RPA)/T](\varepsilon)$ where

$$\varepsilon = \overline{e^2} k_D^{d-2}/T$$ (3.12)

which satisfies the lower bound conditions (3.8), (3.10), and (3.11) due to the Schwarz inequality

$$\overline{Q^{2p}} \; \overline{Q^{2q}} \geq \overline{Q^{p+q}}^2 .$$ (3.13)

Lower bounds for the correlation energy of OCP due to Onsager's idea [9~11] can also be generalized to cases of ionic mixtures in d dimensions with d-dimensional Coulomb interaction including the case of d=3 given in Ref.13. The results are

$$e_c \geq -[d^2/2(d^2-4)]\overline{e^{1+2/d}} \; \overline{e^{1-2/d}} \; a^{2-d} \qquad (d \neq 2)$$

$$e_c \geq -(\overline{e^2}/4)[3/2 - \ln(\overline{e^2}/\overline{e}^2) + \ln(\pi n \ell^2)] \qquad (d=2)$$ (3.14)

where a is defined by

$$n \int_{r \leq a} dr = 1 .$$ (3.15)

As in the case of OCP [1,2], lower bounds (3.8), (3.10), and (3.11) are effective in the domain of low density and the lower bound (3.14) in the domain of high density.

4.   D-Dimensional Ionic Mixtures with D-Dimensional Coulomb Interaction

In cases of ionic mixtures in d dimensions with d-dimensional Coulomb interaction, we make use of the relation (3.1) or (3.3) and the relations

$$h^{\alpha\beta}(\underset{\sim}{r}) \geq -1 \ , \tag{4.1}$$

and

$$e_\alpha e_\beta > 0 \ . \tag{4.2}$$

With a function $f(k,t)$ which satisfies the conditions

$$\phi(k) = \int_0^\infty dt f(k,t) = (\int_0^G + \int_G^\infty) dt f(k,t) \tag{4.3}$$

$$f(k,t) \geq 0 \quad \text{and} \quad f(\underset{\sim}{r},t) = (2\pi)^{-d} \int d\underset{\sim}{k} f(k,t) \exp(i\underset{\sim}{k}\cdot\underset{\sim}{r}) \geq 0 \tag{4.4}$$

we rewrite the correlation energy as [2]

$$e_C = (\overline{e^2}/2)(2\pi)^{-d} \int d\underset{\sim}{k} \int_0^G dt f(k,t) [\sum_{\alpha,\beta} (e_\alpha e_\beta/\overline{e^2})(n_\alpha n_\beta/n^2)^{1/2} S^{\alpha\beta}(\underset{\sim}{k}) - \underline{S}]$$

$$+ (1/2n) \int d\underset{\sim}{r} \int_G^\infty dt f(r,t) \sum_{\alpha,\beta} e_\alpha e_\beta n_\alpha n_\beta [h^{\alpha\beta}(\underset{\sim}{r}) + 1] + B_1[f,G] \ , \tag{4.5}$$

where $\underline{S}$ denotes the right hand side of (3.1) or (3.3) and $B_1[f,G]$ is given by

$$B_1[f,G] = -(\overline{e^2}/2)(2\pi)^{-d} \int d\underset{\sim}{k} [\int_0^G dt f(k,t)(1-\underline{S}) - \phi(k) \begin{Bmatrix} \theta(2-d) \\ \exp(i\underset{\sim}{k}\cdot\underset{\sim}{\ell}) \end{Bmatrix}]$$

$$- (n\overline{e^2}/2) \int_G^\infty dt f(k=0,t) . \quad \begin{cases} (d \neq 2) \\ (d = 2) \end{cases} \tag{4.6}$$

Noting Eqs.(3.1), (3.3), (4.1), (4.2), and (4.4), we have

$$e_C \geq B[f,G] . \tag{4.7}$$

When $G = \infty$ this lower bound reduces to Eq.(3.8), (3.10), or (3.11).
When we use Eq.(3.1) with $m=1$ and take

$$\tilde{f}(k,t) = (\text{function of } k/t) \times 2t^{-3} , \tag{4.8}$$

as the function $f(k,t)$, $B_1[f,G]$ is written as

$$B_1[f,G]/T = [e_c(RPA)/T](\varepsilon_1) + (\overline{ee^2}/\overline{e^3})\{(\overline{e^3}/\overline{ee^2})\varepsilon_1 2^{-1}(2\pi)^{-d}\int_{\sim}dk\int_{G/k_1}^{\infty}dt\times$$

$$\times\tilde{f}(k,t)/(k^2+1) - 2^{-1}[2\pi^{d/2}\Gamma(d/2)^{-1}]^{-1}\int_{G/k_1}^{\infty}dt\tilde{f}(k=0,t)\} \qquad (4.9)$$

and the values of this lower bound are obtained from values of the
first and second terms at ε_1 and at $(e^3/\overline{e}\ \overline{e^2})\varepsilon_1$ for OCP [2].

In the case of three-dimensional OCP, $f_0(k,t) = 2\pi\exp(-k^2/4t^2)t^{-3}$
gives effective lower bound among several simple functions which
satisfy the conditions (4.3) and (4.4) [1]. For three-dimensional
ionic mixtures we also take f_0 as $f(k,t)$ and compare in Table the
lower bound thus obtained with the results of numerical experiments
[12,13] and other lower bounds, Eqs.(3.8) and (3.14). When $\varepsilon_1 \ll 1$ and
$\varepsilon_1 \gg 1$, this lower bound reduces to

$$e_c/T \geq -(1/2)\varepsilon_1 + (1/2\pi)(\overline{e^3}/\overline{ee^2})\varepsilon_1^2, \qquad (\varepsilon_1 \ll 1) \qquad (4.10)$$

$$e_c/T \geq -(3/2)(3/4\pi)^{1/3}(\overline{ee^2})^{2/3}/aT + (1/2)(\overline{ee^2}/\overline{e^3}), \quad (\varepsilon_1 \gg 1) \qquad (4.11)$$

respectively. The lower bound $B_1[f_0,G]$ improves upon other lower bounds
in the domains of low and intermediate density and gives values close
to experimental results. Thus the approximation $h^{\alpha\beta}(\underset{\sim}{r}) = -1$ in the
short range domain and the random phase approximation in the long range
domain (the difference between k_1 and k_D being assumed small) with the
division of the integration into real and Fourier spaces by an appro-
priate function $f(k,t)$ are useful also for ionic mixtures in spite of
simplicity of the approximations.

Table Experimental values and lower bounds for the correlation energy
of classical ionic mixtures. ($e_1 = e_0$, $e_2 = 2e_0$, and $s=2$)

$(4\pi n/3)^{1/3}e_0^2/T$	n_1/n	n_2/n	$e_c/T^{*\dagger}$	B_1/T	(3.8)	(3.14)	
1	1/2	1/2	-1.645*	-1.932	-3.558	-2.123	*Ref.13
1	5/6	1/6	-0.907†	-1.082	-1.686	-1.279	†Ref.12
5	1/2	1/2	-9.715*	-10.84	-39.77	-10.61	
5	5/6	1/6	-5.601†	-6.396	-18.85	-6.397	
10	1/2	1/2	-20.13*	-22.06		-21.23	
10	5/6	1/6	-11.73†	-13.13		-12.79	
20	1/2	1/2	-41.19*	-44.51		-42.46	
20	5/6	1/6	-24.18†	-26.63		-25.59	

5.   D-Dimensional Ionic Mixtures with Three-dimensional Coulomb Interaction

For d-dimensional ionic mixtures with three-dimensional Coulomb interaction, we have no relations like Eq. (3.1) or (3.3) except for the case of d=3 and we use instead the relation

$$\sum_{\alpha,\beta} e_\alpha e_\beta (n_\alpha n_\beta/n^2)^{1/2} S^{\alpha\beta}(\underset{\sim}{k}) = \langle |\sum_\alpha e_\alpha \rho^\alpha_{\underset{\sim}{k}}|^2\rangle / \sum_\alpha N_\alpha \geq 0 \ . \tag{5.1}$$

With a function f(k,t) which satisfies the conditions (4.4) and

$$\phi_3(k) = \int_0^\infty dt f(k,t) = (\int_0^G + \int_G^\infty) dt f(k,t), \tag{5.2}$$

we rewrite the correlation energy e_c as [1]

$$e_c = (1/2)(2\pi)^{-d} \int d\underset{\sim}{k} \int_0^G dt f(k,t) \langle |\sum_\alpha e_\alpha \rho^\alpha_{\underset{\sim}{k}}|^2\rangle / \sum_\alpha N_\alpha$$

$$+ (1/2n) \int d\underset{\sim}{r} \int_G^\infty dt f(r,t) \sum_{\alpha,\beta} e_\alpha e_\beta n_\alpha n_\beta [h^{\alpha\beta}(\underset{\sim}{r})+1] + B[f,G], \tag{5.3}$$

where

$$B[f,G] = -(\overline{e^2}/2)\int_0^G dt f(r=0,t) - (n\overline{e^2}/2)\int_G^\infty dt f(k=0,t). \tag{5.4}$$

We thus obtain

$$e_c \geq B[f,G]. \tag{5.5}$$

When we take f(k,t)=(function of k/t)/t^d (f(r,t)=(function of rt) in the real space), we have

$$e_c \geq -\pi^{1/2}[d/2(d-1)][\Gamma(d/2+1)\int d\underset{\sim}{r} f(r)/f(r=0)]^{1/d} f(r=0) (\overline{e^2}/\overline{e^2})^{1/d} \overline{e^2}/a, \tag{5.6}$$

where the factor e^2 in the case of OCP [1] is replaced by $(\overline{e^2}/\overline{e^2})^{1/d}\overline{e^2}$.

Appendix

Here we generalize the derivation of the inequality (3.1) for three-dimensional OCP due to Mermin [8] based on the Schwarz inequality

$$<|A|^2> \; \geq \; |<\underset{\sim}{A}^*\underset{\sim}{B}>|^2/<|\underset{\sim}{B}|^2> \; . \tag{A1}$$

As the functions A and $\underset{\sim}{B}$ we now take

$$A = \sum_\alpha e_\alpha A^\alpha, \qquad A^\alpha = \sum_{i=1}^{N_\alpha} \psi[\underset{\sim}{r}_{(i,\alpha)}] \tag{A2}$$

and

$$\underset{\sim}{B} = \sum_\alpha e_\alpha^m \underset{\sim}{B}^\alpha, \qquad \underset{\sim}{B}^\alpha = \sum_{i=1}^{N_\alpha} \{ \varphi[\underset{\sim}{r}_{(i,\alpha)}][\partial/\partial\underset{\sim}{r}_{(i,\alpha)}]U - T[\partial/\partial\underset{\sim}{r}_{(i,\alpha)}]\varphi[\underset{\sim}{r}_{(i,\alpha)}] \}, \tag{A3}$$

where U denotes the interaction energy, and obtain

$$<\underset{\sim}{B}^\alpha A^{\beta*}> = \delta_{\alpha\beta} T \sum_{i=1}^{N_\alpha} <\varphi[\underset{\sim}{r}_{(i,\alpha)}][\partial/\partial\underset{\sim}{r}_{(i,\alpha)}]\psi^*[\underset{\sim}{r}_{(i,\alpha)}]>, \tag{A4}$$

$$<\underset{\sim}{B}^\alpha \cdot \underset{\sim}{B}^{\beta*}> = T \sum_{i=1}^{N_\alpha}\sum_{j=1}^{N_\beta} \{ <\varphi[\underset{\sim}{r}_{(i,\alpha)}]\varphi^*[\underset{\sim}{r}_{(j,\beta)}][\partial/\partial\underset{\sim}{r}_{(i,\alpha)}]\cdot[\partial/\partial\underset{\sim}{r}_{(j,\beta)}]U$$

$$+ \delta_{\alpha\beta}\delta_{ij} T <|[\partial/\partial\underset{\sim}{r}_{(i,\alpha)}]\varphi|^2> \} \; . \tag{A5}$$

We note that

$$[\partial/\partial\underset{\sim}{r}_{(i,\alpha)}]^2 U = -2\pi^{d/2}\Gamma(d/2)^{-1} e_\alpha \rho[\underset{\sim}{r}_{(i,\alpha)}] \tag{A6}$$

and

$$[\partial/\partial\underset{\sim}{r}_{(i,\alpha)}]\cdot[\partial/\partial\underset{\sim}{r}_{(j,\beta)}]U = 2\pi^{d/2}\Gamma(d/2)^{-1} e_\beta \rho^{(i,\alpha)}[\underset{\sim}{r}_{(j,\beta)}] \quad \text{for } \delta_{\alpha\beta}\delta_{ij} = 0 \; . \tag{A7}$$

Here $\rho[\underset{\sim}{r}_{(i,\alpha)}]$ is the charge density at the position $\underset{\sim}{r}_{(i,\alpha)}$ due to other particles (and their periodic images when the periodic boundary condition is used) and the uniform charge density $-\sum_\alpha e_\alpha n_\alpha$ of the background and $\rho^{(i,\alpha)}(\underset{\sim}{r})$ is the charge density at the position $\underset{\sim}{r}$ due to the particle (i,α) (and its periodic images). We thus have

$$<|\underset{\sim}{B}|^2> = 2\pi^{d/2}\Gamma(d/2)^{-1} n T \bar{e} \sum_\alpha e_\alpha^{1+2m} \sum_{i=1}^{N_\alpha} <|\varphi[\underset{\sim}{r}_{(i,\alpha)}]|^2>$$

$$+ T^2 \sum_\alpha e_\alpha^{2m} \sum_{i=1}^{N_\alpha} <|[\partial/\partial\underset{\sim}{r}_{(i,\alpha)}]\varphi[\underset{\sim}{r}_{(i,\alpha)}]|^2>. \tag{A8}$$

Taking $\varphi(\underset{\sim}{r}) = \psi(\underset{\sim}{r}) = \exp(i\underset{\sim}{k}\cdot\underset{\sim}{r})$ in the case of the periodic boundary condition we have the inequality (3.1) where k_m is defined by Eq.(3.2). We also obtain (3.1) in the case of the inpenetrable wall boundary condition by modifying $\varphi(\underset{\sim}{r})$ in the same way as in the case of three-dimensional OCP [8].

When we take

$$B = B^{\delta}$$
$$\underset{\sim}{B} = \underset{\sim}{B}^{\delta} \qquad\qquad\qquad (A9)$$

as the function $\underset{\sim}{B}$, similar arguments lead to the inequality (3.3).

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