Finite Two-Dimensional Systems of Electrons at Zero and Finite Temperatures: Simulations Based on Classical Map Hypernetted Chain (CHNC) Method

T. MIYAKE, K. NAKANISHI, C. TOTSUJI, K. TSURUTA and H. TOTSUJI

Graduate School of Natural Science and Technology/Faculty of Engineering
Okayama University, Okayama 700-8530, Japan

We analyze two-dimensional quantum systems of electrons on the basis of the classical-map hypernetted-chain (CHNC) method which maps electron systems onto classical systems of charges. This method has been proposed originally for the analyses through the hypernetted chain (HNC) and related integral equations. Confirming the applicability of simulations based on this mapping in homogeneous systems, we perform Monte Carlo and molecular dynamics simulations on two-dimensional finite systems of electrons confined by an external potential such as quantum dots. We emphasize the advantage of simulations over integral-equation-based analyses for systems without the translational invariance. With decreasing strength of confinement, these systems undergo a transition from the spin unpolarized to the spin polarized state accompanying the discontinuous change of the average density. The critical value of r_s estimated from the average density is as low as $r_s \sim 0.4$. For given average density (instead of given strength of confinement), the transition between the spin-unpolarized and spin-polarized states occurs at the critical r_s value around 10 which is closer to the known possibility of polarization at $r_s \sim 27$. We also show the applicability of this method to two-dimensional electron systems at finite temperatures.

Keywords: 2d-electron system, quantum dot, CHNC method, numerical simulation, spin polarization

1. Introduction

Degenerate plasmas have been one of important subjects of plasma physics. Simulations which are useful in analyses of classical systems of charges still have some difficulties in applications to quantum systems and the system sizes of *ab initio* simulations are much smaller than those of classical ones. In this article, we investigate the possibility of classical simulations of quantum systems via the method of mapping.

We take two-dimensional systems of electrons as the target of our analyses. They are one of indispensable elements of semiconductor electronic devices and their properties not only in the bulk but also in finite systems are the basis for the construction of new electronic devices such as quantum dots. For finite systems of electrons with small number of electrons the *ab initio* quantum analyses have been reported by many authors[1, 2] and the number of electrons in recent investigations has increased up to 20 or more. The spin polarization as a function of electron number[3, 4] and the formation of Wigner crystal[5, 6, 7] have been reported.

When we have very large number of electrons, we may apply the results of uniform system[8, 9, 10, 11]. In the case of electrons of intermediate numbers, for example a few hundreds, however, it may not be justified to apply the results of uniform system. It may

be also not easy to apply *ab initio* methods.

We apply the classical numerical simulations to these finite systems of electrons via the mapping between the quantum and classical systems[12]. As the mapping, we adopt the classical-map hypernetted-chain equation (CHNC) method by Dharma-wardana and Perrot originally proposed for the analysis of electron systems through HNC and related integral equations[13, 14, 15, 16]. This method reproduces the known results of *ab initio* quantum simulations in three and two dimensions to a good accuracy and is useful to obtain the spin polarization and other characteristics including the case of finite temperatures[16, 17, 18].

We emphasize that numerical simulations can be applied to finite systems without the translational invariance which are difficult to analyze on the basis of the HNC and similar integral equations. We also note that, we are able to take the contribution of the bridge function automatically into account through resultant distribution functions. Though the bridge function is expected to be approximately evaluated within the framework of the modified HNC approach[19], accurate numerical simulations could be simpler and applicable to cases without translational invariance.

There exists a difficulty in applications to systems where the electron density is a function of the

position: The CHNC method interprets the system into the classical one introducing density dependent quantum temperature and mutual potential. Except for the cases of sufficiently large systems with slowly changing density profile, we have to somehow define the average density to be used in the mapping. In this article, we follow earlier works[20, 21, 6, 7] as described in Section 4.

We first confirm that the classical Monte Carlo and molecular dynamics methods based on the CHNC mapping at $T = 0$ give the results of at least the same accuracy with those of integral-equation-based CHNC method[22]. We then perform the Monte Carlo and molecular dynamics simulations on electrons confined by a two-dimensional parabolic potential with the system size is too large to apply the *ab initio* methods and too small to be regarded as homogeneous system. We mainly focus our attention to the possible spin polarization of the ground state ζ in the domain where the electron density is higher than the critical density for the Wigner lattice formation [5, 6, 7]. We use the atomic units and take $k_B = 1$ when necessary, k_B being the Boltzmann constant.

2. CHNC method

The elements of the mapping in the CHNC method are the assignment of the "quantum" temperature to account for the effect of degeneracy, the modification of the Coulomb potential to account for the quantum diffraction, and the inclusion of an extra potential (the Pauli potential) for electrons of the same spin.

When the electron system is at the temperature T, the corresponding classical system is assigned a temperature T_{cf}

$$T_{cf} = (T_q^2 + T^2)^{1/2}, \qquad (1)$$

where T_q is the "quantum" temperature. Of two proposals for T_q[13, 17] in the two-dimensional case, we adopt the one by Bulutay and Tanatar[17] which gives somewhat better results for small values of r_s [22];

$$T_q = \frac{1 + ar_s}{b + cr_s} E_F, \qquad (2)$$

where $r_s = 1/(\pi n)^{1/2}$, n is the surface density, E_F is the Fermi energy, $a = 1.470342$, $b = 6.099404$, and $c = 0.476465$.

To take the effect of quantum diffraction into account, the Coulomb potential is replaced by [23]

$$V_{cou}(r) = \frac{1}{r}[1 - e^{-rk_{th}}]. \qquad (3)$$

The value of k_{th} is expressed by the thermal de Broglie wave number as $k_{th} = 1.158T_{cf}^{0.103}k_{th}^0$ with $k_{th}^0 = (2\pi m^* T_{cf})^{1/2}$ and $m^* = 1/2$, m^* being the reduced mass of scattering pair of electrons[15].
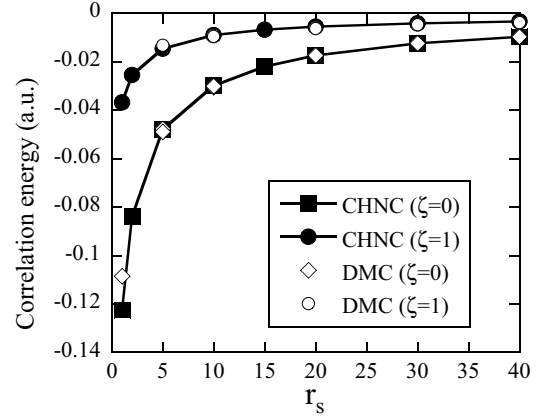

Fig. 1 Correlation energy: CHNC numerical simulation vs. diffusion Monte Carlo (DMC).

The additional potential (the Pauli potential), $P_{\sigma\sigma}$, is determined, within the hypernetted-chain(HNC) approximation, so as to reproduce the pair correlation function of ideal Fermi gas. The pair potential between electrons of spin species σ and σ', $\phi_{\sigma\sigma'}(r)$, is thus given by the sum of (3) and $P_{\sigma\sigma}$.

3. Application to Homogeneous Systems

Before simulation-based applications of the CHNC method, the accuracy of the method needs to be confirmed in the context of simulations. Figure 1 shows the results of Monte Carlo simulations of two-dimensional electron liquids at $T = 0$ in comparison with those of *ab initio* quantum simulations. Simulations based on the CHNC mapping are at least of the same accuracy with the integral-equation-based analyses of the method.

4. Application to Finite Systems

As a model of electrons in quantum dots, we consider N electrons confined by a two-dimensional harmonic potential[2]. Since any confining potential has a parabolic form at least near the center and the electrostatic potential of a uniform distribution of opposite charge in a circle is approximately represented by the harmonic potential to a good accuracy within the radius of distribution[24], we may expect the harmonic potential to be applicable in experiments.

The Hamiltonian of the system is given by

$$\hat{H} = -\sum_i \frac{\hbar^2}{2m_e}\Delta_i + \sum_{i>j}\frac{e^2}{r_{ij}} + \frac{1}{2}k\sum_i r_i^2. \qquad (4)$$

We perform the Monte Carlo and molecular dynamics simulations based on the classical Hamiltonian determined by the CHNC mapping.

Elements of the CHNC method are defined for uniform systems and depends on the density. As men-

tioned in Introduction, we have to determine the average density of the system by some appropriate method and adopt the quantum temperature and the Pauli potential corresponding to the average density in our application to systems which are not uniform. For the distribution $n(r)$, we define the average density $\bar{n}$ by

$$\bar{n} = \frac{\int n^2(r)dS}{\int n(r)dS} \qquad (5)$$

and assign r_s by $r_s = 1/(\pi\bar{n})^{1/2}$ following earlier works on inhomogeneous systems[20, 21, 6, 7]. By iterations, we attain the consistency of resultant r_s with the value used for the quantum temperature and the Pauli potential in simulations.

The average of the Coulomb interaction energy

$$\langle \hat{H}_{int} \rangle = \langle \sum_{i>j} \frac{1}{r_{i,j}} \rangle = \frac{e^2}{a_B} e(N, \zeta, \omega) \qquad (6)$$

is determined for given number of electrons N, the strength of the external confining potential k, and the spin polarization ζ. The dimensionless coupling parameter ω is defined by

$$\omega^2 = \frac{ka_B^3}{e^2} = \frac{\hbar^6 k}{m_e^3 e^8}. \qquad (7)$$

The free energy of our system $F(N, \zeta, \omega)$ is obtained through the integration with respect to the coupling parameter:

$$F(e^2) - F(0) = \frac{\omega}{2} \int_\omega^\infty \frac{d\omega}{\omega^2} e(N, \zeta, \omega). \qquad (8)$$

The difference between states with $\zeta = 0$ and $\zeta = 1$ is shown in Fig.2. When ω is large (strong confinement and resultant high average density), the ground state is not polarized ($\zeta = 0$) and when ω is small (weak confinement and resultant low average density), we have a polarized ground state ($\zeta = 1$). The critical value is $\omega = 2.1$ for $N = 64$ and $\omega = 2.4$ for $N = 128$. Since the confinement is given, we have a jump in the value of r_s around the critical density $r_s \sim 0.4$: With the decrease of the confinement, the system reorganizes itself into the polarized state with larger radius of distribution.

The critical density may seem to be much higher than the value in uniform systems $r_s \sim 27$[9, 10, 11, 15, 16]. We note, however, that when the free energies at given average density are compared as shown in Fig.3, the critical value of r_s is around 10. Though the estimation of r_s in confined systems has some ambiguity, our data give the result close to $r_s \sim 27$ of the known possibility in uniform systems. Since the density of electrons is not uniform, the average density underestimates and overestimates the real density near the center and on the periphery, respectively, and the quantum temperature is underestimated and
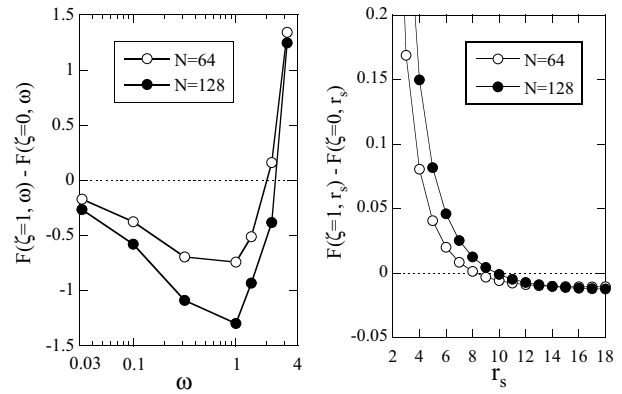

Fig. 2 Difference of ground state energies in unpolarized ($\zeta = 0$) and polarized ($\zeta = 1$) states vs. ω.

Fig. 3 Difference of ground state energies in unpolarized ($\zeta = 0$) and polarized ($\zeta = 1$) states vs. r_s.

overestimated, correspondingly. The Pauli potential has also similar errors. The critical r_s value might be affected these deviations. This possibility, however, needs further investigation and is not conclusive within our present analyses.

5. Application to Systems at Finite Temperatures

One of the merits of our method is the applicability to systems at finite temperatures which have very small number of results of quantum simulations. Integral-equation-based analyses have shown possible existence of the domain of an intermediate spin polarization[16]. We apply the mapping to homogeneous two-dimensional systems of electrons at finite temperatures.

The Pauli potential is a universal function of $k_F^\sigma r$ (k_F^σ being the Fermi wavenumber for species σ), but its behavior at zero and finite temperatures is significantly different: The finite-temperature Pauli potential is short-ranged without the long-range asymptote at $T = 0$

$$\beta P(k_F^\sigma r) \sim \frac{\pi}{k_F^\sigma r}. \qquad (9)$$

As shown in Fig.4, it decays more rapidly on increasing temperature.

At finite temperatures, we obtain the results shown in Fig.5. For given r_s, the differences in the Helmholtz free energies of spin-polarized ($\zeta = 1$) and spin-unpolarized ($\zeta = 0$) states first decrease and then increase with the increase of the temperature. The decrease is significant for $r_s < 10$. As a function of r_s, the difference is still positive but becomes close to zero at low but finite temperatures around $r_s \sim 10$.

In the integral-equation-based CHNC analysis[16] which gives a spin-polarized domain for $27 < r_s$ at
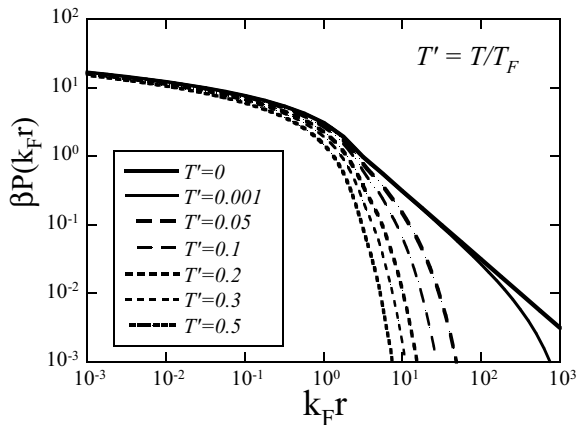
Fig. 4 Pauli potential $P_{\sigma\sigma}(k_F r)$ at zero and finite temperatures as the function of $k_F r$. $T' = T/T_F$.
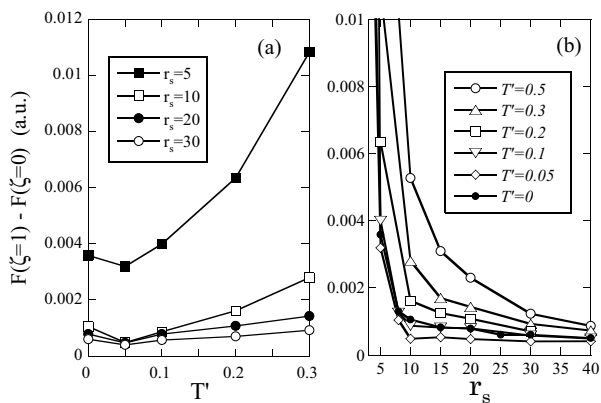

Fig. 5 (a) Difference of Helmholtz free energy in $\zeta = 0$ and $\zeta = 1$ states vs. $T' = T/T_F$ in homogeneous two-dimensional systems. (b) The same as in (a) vs. r_s.

6. Conclusions

After confirming the applicability of the CHNC mapping in numerical-simulation-based analyses of two-dimensional electron systems, we have applied the method to confined finite systems of intermediate sizes (64 and 128 electrons). It is shown that electrons are polarized when the value of r_s for the average density satisfies $r_s > 0.4$. When we regard r_s as a control parameter, the spin polarization occurs for $r_s \sim 10$. The latter critical value is not so far from the known possibility for the uniform system. We have also shown some results obtained by application of the method to homogeneous systems at finite temperatures.

[1] N. F. Johnson, J. Phys. Condens. Matter **7**, 965(1995).
[2] S. M. Reimann and M. Manninen, Rev. Mod. Phys. **74**, 1283(2002).
[3] S. M. Reimann, M. Koskinen, M. Mannine, Phys. Rev. B **62**, 8108(2000).
[4] R. Hanson, L. P. Kouwenhoven, J. R. Petta, S. Tarucha, L. M. K. Vandersypen, Rev. Mod. Phys. **79**, 1217(2007).
[5] A. V. Filinov, M. Bonitz, and Yu. E. Lozovik, Phys. Rev. Lett. **86**, 3851(2001).
[6] A. Ghosal, A. D. Güçlü, C. J. Umirigar, D. Ullmo, H. U. Baranger, Phys. Rev. B **76**, 085341(2007).
[7] A. D. Güçlü, A. Ghosal, C. J. Umirigar, H. U. Baranger, Phys. Rev. B **77**, 041301(2008).
[8] B. Tanatar and D. M. Ceperley, Phys. Rev. B **39**, 5005 (1989).
[9] F. Rapisarda and G. Senatore, Aust. J. Phys. **49**, 161 (1996).
[10] D. Varsano, S. Moroni, and G. Senatore, Europhys. Lett. **53**, 348(2001).
[11] C. Attaccalite, S. Moroni, P. Gori-Giorgi, and G. B. Bachelet, Phys. Rev. Lett. **88**, 256601(2002).
[12] T. Miyake, K. Nakanishi, C. Totsuji, K. Tsuruta, and H. Totsuji, Phys. Lett. A **372**, 6197 (2008).
[13] M. W. C. Dharma-wardana and F. Perrot, Phys. Rev. Lett. **84**, 959(2000).
[14] F. Perrot and M. W. C. Dharma-wardana, Phys. Rev. B **62**, 16536(2000).
[15] F. Perrot and M. W. C. Dharma-wardana, Phys. Rev. Lett. **87**, 206404(2001).
[16] M. W. C. Dharma-wardana and F. Perrot, Phys. Rev. Lett. **90**, 136601(2003).
[17] C. Bulutay and B. Tanatar, Phys. Rev. B **65**, 195116(2002).
[18] N. Q. Khanh and H. Totsuji, Solid State Com. **127**, 37(2004); N. Q. Khanh and H. Totsuji, Phys. Rev. B **69**, 165110(2004).
[19] Y. Rosenfeld and N. W. Ashcroft, Phys. Rev. A **20**, 1208(1979).
[20] M. W. C. Dharma-wardana, Phys. Rev. B **72**, 125339(2005).
[21] P. Gori-Giorgi and A. Savin, Phys. Rev. A **71**, 032513(2005).
[22] C. Totsuji, T. Miyake, K. Nakanishi, K. Tsuruta, and H. Totsuji, *unpublished*.
[23] H. Minoo, M. M. Gombert, and C. Deutsch, Phys. Rev. A **23**, 924(1981).
[24] O. Ciftja, J. Computer-Aided Mater. **14**, 37(2007).

$T = 0$, it has been shown that the boundary of the polarized domain first decreases from 27 and then increases to larger values with the increase of the temperature. Our results shown in Fig.5 are consistent with this behavior.

The system approaches to the classical one with the increase of the temperature. Since the spin polarization is a quantum effect (the exchange effect) coming from the correlation between electrons of the same spin, the domain of spin polarization is expected to decrease. The above result (the increase of the polarized domain at low but finite temperatures) indicates that the approach to the classical system is not monotonous. In our method, the exchange effect is represented by the Pauli potential and we expect its behavior at finite temperatures shown in Fig.4 may naturally have some relation to the above behavior. The detail, however, is not yet clear and needs further analyses. The analyses of finite electron systems are also in progress.