

Distribution of Electrons in Quantum Dots Analyzed by Classical Mapping and Molecular Dynamics

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The electron system of arbitrary degeneracy can be mapped onto a classical system where electrons of the same spin are assigned an additional interaction and the effect of degeneracy is taken into account through an imaginative temperature. We apply this method to electrons in quantum dots modeled as two-dimensional electron liquid confined in a finite domain by a harmonic potential. We analyze distribution functions by molecular dynamics instead of solving integral equations which are not so useful in the case without translational invariance.

I. INTRODUCTION

The behavior of electrons in quantum dots is an important subject of theoretical and experimental researches both as a manifestation of many-body effects between electrons and as an element of nano-electronic devices. A simple example of quantum dot can be realized by applying a potential to two-dimensional electron systems at the interface of GaAs/GaAlAs. The first principle theoretical analyses are nevertheless still not simple except for the case where only a few electrons are included.

Recently the classical-map hypernetted-chain method (CHNC) has been developed by Dharma-wardana and Perrot.[1-4] This reproduces the results of the first principle quantum simulations by mapping the quantum system to the classical system with specified temperature and interactions, and enables us to analyze properties of spin polarized two-dimensional electron liquids at finite temperatures.[5] We here apply this method to analyze two-dimensional electron liquids in finite domains such as quantum dots. The natural units are adopted in what follows.

II. CHNC METHOD

The mapping in the CHNC method consists of three elements, (1) the assignment of the “quantum” temperature, (2) the modification of the Coulomb potential to account for the diffraction effect, and (3) the inclusion of the spin-dependent potential (Pauli potential) which accounts for the Fermi statistics for electrons.

A. Quantum temperature

Electron liquids at the temperature T is assigned a temperature T_{cf} given by

$$T_{cf} = \sqrt{T_q^2 + T^2}. \quad (1)$$

Here T_q is the quantum temperature which expresses the effect of degeneracy in terms of the kinetic temperature of classical fluid. In the two-dimensional case, T_q is given by

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

where $r_s = 1/(\pi n)^{1/2}$, E_F is the Fermi energy, $a = 1.470342$, $b = 6.099404$, $c = 0.476465$, and k_B is the Boltzmann constant.[6]

B. Coulomb potential with diffraction effect

In order to take the effect of quantum diffraction into account, the Coulomb potential is replaced by

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

Here $k_{th} = (2\pi m^* T_{cf})^{1/2}$ with $m^* = 1/2$, m^* being the reduced mass of scattering pair of electrons.[7]

C. Pauli potential

In this method an effective potential (Pauli potential), P_{ii} , is assumed between electrons of the same spin in order to take the effect of Fermi statistics for electrons into account. The Pauli potential is determined by

$$g_{ii}^0(r) = \exp[-\beta P_{ii}(r) + h_{ii}^0(r) - c_{ii}^0(r)], \quad (4)$$

where $\beta = 1/k_B T_{cf}$, $g_{ii}^0(r) = h_{ii}^0(r) + 1$ is pair distribution function, $c_{ii}^0(r)$ is direct distribution function, and the superscript 0 denotes the values for the ideal Fermi gas. The pair correlation function for the ideal Fermi gas $h_{ii}^0(r)$ is given by

$$\begin{aligned} h_{ii}^0(r) &= -\frac{1}{n_i^2} \sum_{\mathbf{k}_1, \mathbf{k}_2} n(k_1)n(k_2) \exp[i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{r}] \\ &= -[f_i(r)]^2. \end{aligned} \quad (5)$$

Here n_i is the surface density of species i ($i = 1$ and 2 denote up and down spins, respectively), $n(k)$ is Fermi occupation number at the temperature T and, at $T = 0$, $f_i(r) = 2J_1(k_F^i r)/k_F^i r$ ($J_1(x)$ is the Bessel function and k_F^i is Fermi wave number of species i).

The pair potential between species i and species j , $\phi_{ij}(r)$, is thus given by

$$\phi_{ij}(r) = P_{ii}(r)(1 + \sigma_i \sigma_j) + V_{cou}(r), \quad (6)$$

where $\sigma_i = \pm 1$ denotes the z-component of the spin of i -th electron.

III. APPLICATION TO FINITE SYSTEMS

As a model of quantum dots, we introduce a two-dimensional harmonic potential which confines electrons within a finite two-dimensional domain

$$\sum_i \frac{1}{2} k r_i^2. \quad (7)$$

The strength of confinement is adjusted so as to give average densities of electrons. The Hamiltonian of the system is then given by

$$\begin{aligned} H(\{\mathbf{r}_i\}) &= \sum_i \frac{\mathbf{P}_i^2}{2m_e} + \frac{1}{2} \sum_{i \neq j} V_{cou}(|\mathbf{r}_i - \mathbf{r}_j|) \\ &+ \frac{1}{2} \sum_{i \neq j} P_{ii}(|\mathbf{r}_i - \mathbf{r}_j|)(1 + \sigma_i \sigma_j) + \sum_i \frac{1}{2} k r_i^2, \end{aligned} \quad (8)$$

where \mathbf{P}_i is the momentum of i -th electron.

Since it is not easy to solve the hyper-netted chain(HNC) and similar integral equations in the case of finite systems where we have no translational invariance, we apply the classical molecular dynamics to our system. The latter gives in principle exact results for given interparticle and external potentials.

IV. ONE-BODY AND PAIR DISTRIBUTION FUNCTIONS

Total density of electrons is given by $n = n_1 + n_2$ and the degree of spin polarization ζ is defined by

$$\zeta = \frac{(n_1 - n_2)}{n}. \quad (9)$$

We here consider only the case of $\zeta = 0$.

We apply molecular dynamics to electrons described by the Hamiltonian (8) and obtain one-body and pair distribution functions. The results are shown in Figs.1-8.

Since our systems are classical, they are characterized by the coupling parameter

$$\Gamma = \frac{e^2(\pi n)^{1/2}}{k_B T_{cf}}, \quad (10)$$

when we neglect the effect of the Pauli potential. Thus the quantum system is mapped onto a classical system where Γ is given by

$$\Gamma = \frac{b + c r_s}{1 + a r_s} r_s. \quad (11)$$

As an example, the quantum system with $r_s = 50$, $\zeta = 0$, and $T = 0$ is mapped to a classical system with $\Gamma = 20.1$. The one-body and the pair distribution functions in the classical Coulomb system with $\Gamma = 20.1$ are shown in Figs.9-10, respectively. Comparing Fig.4 with Fig.9, we observe that the effects of diffraction and Pauli potential are not significant and main role is placed by the temperature effect in the mapping.

The quantum Monte Carlo results for the infinite system by Tanatar and Ceperley[8] predicts that crystallization occurs around $r_s = 37$. But this phenomena is not confirmed in our simulation.

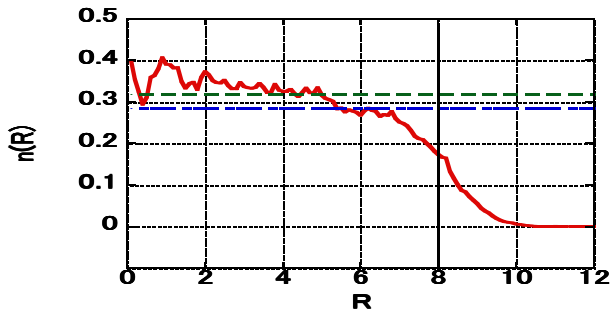


FIG. 1: One-body distribution function for $r_s = 1$ in a finite system. Dotted line is the mean density corresponding to r_s , dashed line is the mean density used to compute the pair distribution function for particles located within the longitudinal solid line.

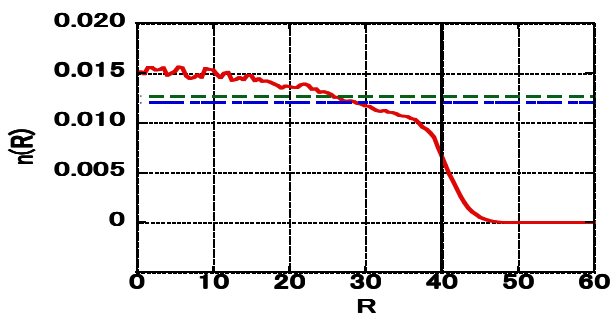


FIG. 2: The same as in Fig.1 for $r_s = 5$.

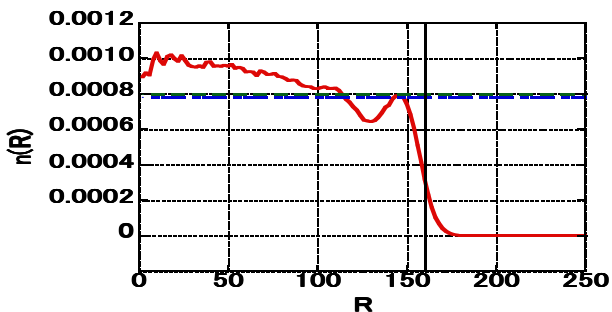


FIG. 3: The same as in Fig.1 for $r_s = 20$.

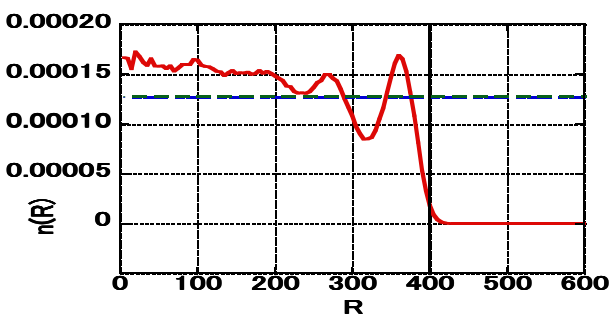


FIG. 4: The same as in Fig.1 for $r_s = 50$.

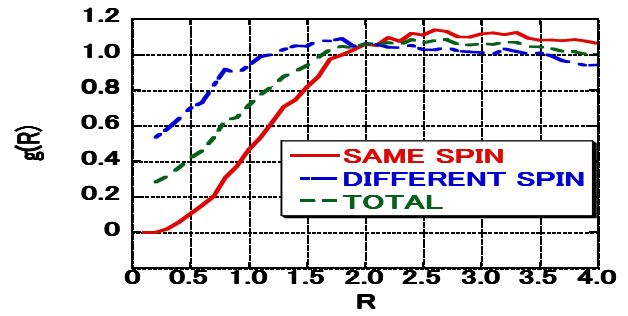


FIG. 5: Pair distribution function for $r_s = 1$ in a finite system.

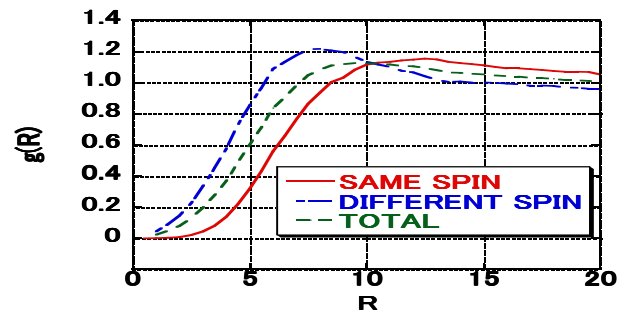


FIG. 6: The same as in Fig.5 for $r_s = 5$.

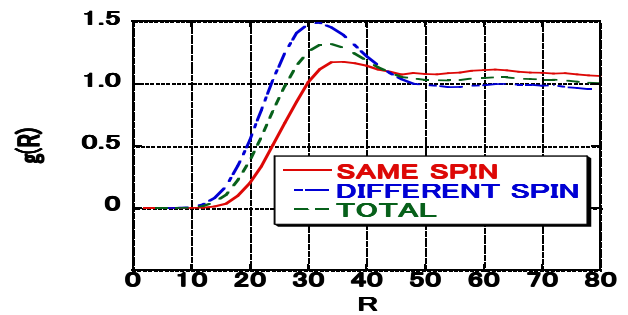


FIG. 7: The same as in Fig.5 for $r_s = 20$.

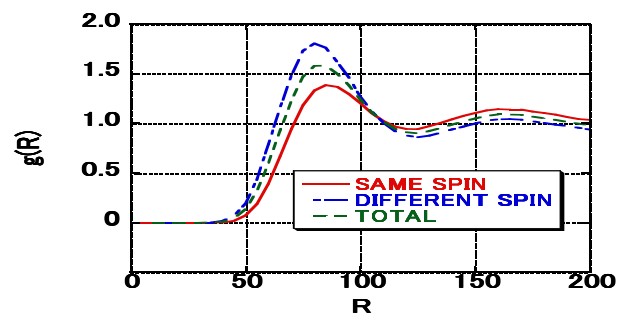


FIG. 8: The same as in Fig.5 for $r_s = 50$.

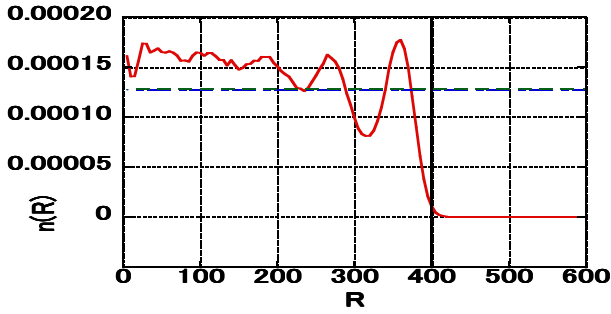


FIG. 9: One-body distribution function for $\Gamma = 20.1$ in a classical system.

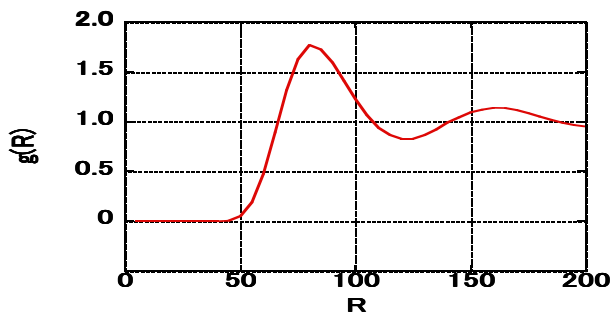


FIG. 10: Pair distribution function for $\Gamma = 20.1$ in a classical system.

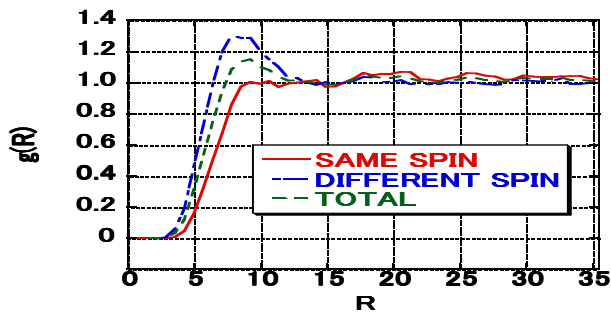


FIG. 11: Pair distribution function for $r_s = 5$ in a uniform system.

These one-body distribution functions indicate that the oscillation in the density starts from outside and the amplitude increases with the increases of r_s . We may regard this phenomenon as similar to the one we observe in classical Coulomb systems confined in finite domains.

In Figs.5-8, we observe the effect of the Pauli potential for electrons of the same spin component as an additional repulsion. On the other hand, the effect on the one-body distribution function is not so clear as described above. In Fig.11, we show the pair distribution function for $r_s = 5$ and $T = 0$ in a uniform system. Comparing this result with those of previous analyses based on quantum Monte Carlo method, we note that our result has more pronounced oscillation. This may suggest that T_q given by Perrot and Dharma-wardana is appropriate for the application of HNC equation but would be somewhat small for the application of the molecular dynamics simulation.

V. CONCLUSION

The behavior of electrons in two-dimensional finite systems is of essential importance in understanding physical properties of quantum dots. It is shown that the combination of the classical mapping and molecular dynamics is useful to obtain this information. It is also shown that the assignment of the temperature derived for analyses by the hypernetted-chain equation seems to need some adjustment for application of molecular dynamics.

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