

Spin Polarization of Two-Dimensional Electron System in a Finite Domain

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We analyze the ground state of the two-dimensional quantum system of electrons confined in a parabolic potential with the system size around 100. We map the system onto a classical system on the basis of the classical-map hypernetted-chain (CHNC) method which has been proven to work in the integral-equation-based analyses of uniform unbounded systems and then apply classical numerical simulations. We find that the confined system undergoes the transition to the spin polarized state with the decrease of the average density and the corresponding critical value is as low as $r_s \sim 0.3$ in terms of the usual r_s parameter estimated for the average density. As the ground state for given value of the r_s parameter, our data give the critical value for the transition around 20 which is consistent with the known possibility. The advantage of our method is a direct applicability to geometrically complex systems which are difficult to analyze by integral equations. The application to the structure like quantum dots reported here is the first example of such applications.

I. INTRODUCTION

The two-dimensional system of electrons is now one of indispensable elements of semiconductor electronic devices and its properties are the basis for the construction of mesoscopic devices such as quantum dots. When the number of electrons is a few or less in these finite systems, the first principle quantum analysis as a molecule can be done as reported by a number of authors. On the other hand, we may apply the results of uniform system in the case of very large number of electrons. In the case where we have electrons of an intermediate number, for example a few hundreds, it is difficult to apply the results of uniform system and it is also difficult to apply the first principle methods.

In this article, we propose to apply the classical numerical simulations based on the mapping between the quantum and classical systems. As the mapping, we adopt the classical-map hypernetted-chain equation (CHNC) method developed by Dharma-wardana and Perrot[1-6]. We perform the Monte Carlo and

molecular dynamics simulations on electrons confined by a two-dimensional parabolic potential and, among various properties, we focus on the spin polarization in the ground state. We use the atomic units and take $k_B = 1$ when necessary, k_B being the Boltzmann constant.

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 quantum diffraction, and (3) the inclusion of the spin-dependent potential (the Pauli potential) which accounts for the Fermi statistics for electrons..

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A. Quantum temperature

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

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

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

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

where $r_s = 1/(\pi n)^{1/2}$, E_F is the Fermi energy, $a = 1.470342$, $b = 6.099404$, $c = 0.476465$ [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 (the Pauli potential), P_{ii} , is additionally assumed between electrons of the same spin in order to take the effect of Fermi statistics 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 $\beta = 1/T_{cf}$, $g_{ii}^0(r) = h_{ii}^0(r) + 1$ is pair distribution function, $c_{ii}^0(r)$ is the direct correlation function, and the superscript 0 denotes the values for the ideal Fermi gas.

The pair correlation function for the two-dimensional 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 the Fermi wave number of species i).

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

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

Here $\sigma_i = \pm 1$ 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 expressed as

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

The Hamiltonian of the system is 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 the i -th electron.

It is not easy to solve the hypernetted-chain (HNC) and similar integral equations in the case of finite systems where we have no translational invariance. Therefore the extension of the integral-equation-based CHNC method to finite systems is not straightforward. On the other hand, numerical simulations can be applied also to finite systems with almost the exact similarity. In order to analyze the system confined by the potential, we thus apply the classical Monte Carlo and molecular dynamics simulations. In principle, the latter gives exact results for given interparticle and external potentials when the sampling is sufficient.

IV. RESULTS AND DISCUSSIONS

When the number of electrons N , the strength of the external confining potential k , and the spin polar-

ization ζ are given, the distribution of electrons is determined within the error inherent in numerical simulations. The free energy is a function of (N, k, ζ) and the ground state is the one with the lowest value. The values of the free energy is obtained by the integration with respect to the coupling as usual. Examples of values are shown in Figs.1-4.

When the confinement is sufficiently strong, the ground state is given by the state with $\zeta = 0$ and when we decrease the confinement, the ground state is taken over by the state with $\zeta = 1$. In Table I, the critical value is expressed in terms of the average density or r_s which is roughly estimated for the density distribution obtained by simulations. Since the range of distribution differs according to the value of ζ , we list two kinds of values corresponding to $\zeta = 0$ and $\zeta = 1$: Due to the Pauli potential, the density for $\zeta = 1$ is lower than for $\zeta = 0$. We observe that we have spin polarized states when the confinement is weak and the critical density is given by $r_s \sim 0.3$.

TABLE I: Total Energy v.s. Coupling Parameter

N	32	64	128
$\zeta = 0$	~ 0.33	~ 0.28	~ 0.22
$\zeta = 1$	~ 0.41	~ 0.35	~ 0.27

The critical density obtained above may seem to be much higher than the possible transition to polarized state at $r_s \sim 27$ in the uniform unbounded system[8-10]. In order to compare our results for confined systems with those for uniform systems, however, it is necessary to regard the free energy as a function of (r_s, ζ) : In confined systems, the value of r_s is a *result* which is to be determined by the average density. The results are shown in Table II and the critical value is around $r_s \sim 20$. Though the estimation of r_s in confined systems has some ambiguity, our data give the results consistent with those for the uniform system.

TABLE II: Total Energy v.s. r_s

N	32	64	128
r_s	~ 23	~ 21	~ 24

The error associated with our results has two main sources; (1) the intrinsic error in the mapping based

on the CHNC method and (2) the estimation of the average density in the confined system and application of the Pauli potential for uniform systems to inhomogeneous systems. Except for the error coming from (1), we roughly estimate the error in the values of r_s in Tables I and II due to (2) to be ± 0.05 and ± 5 , respectively, which is small enough as a first report.

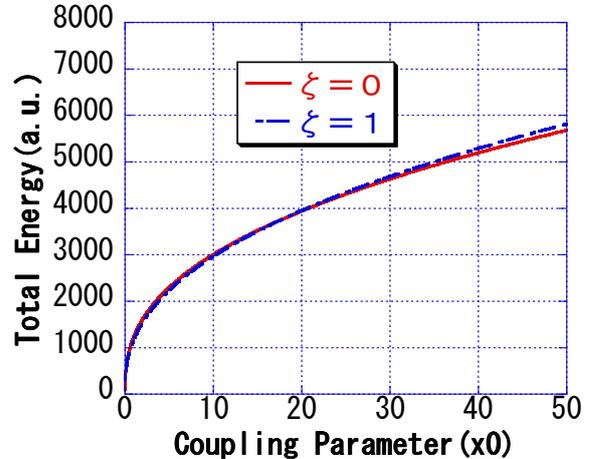
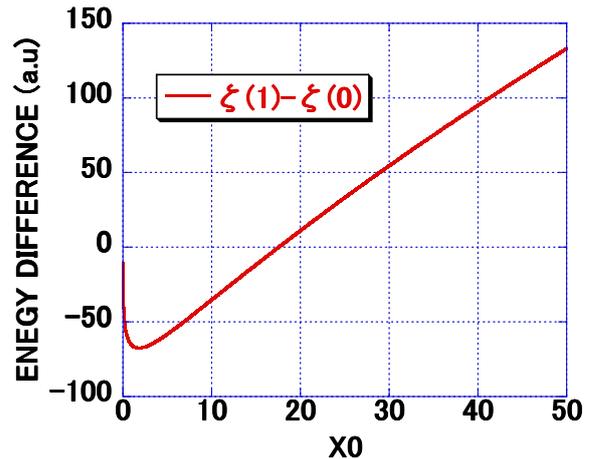


FIG. 1: Total Energy v.s. Coupling Parameter

FIG. 2: Energy difference between $\zeta = 1$ and $\zeta = 0$ in terms of Coupling Parameter.

In conclusion, we have applied the method of classical mapping to confined finite two-dimensional systems of 32-128 electrons and analyzed the spin polarization at zero temperature. It is shown that electrons are polarized when the r_s value for the average density satisfies $r_s > 0.3$. When we regard the r_s value as

a controllable parameter, the spin polarization occurs for $r_s > 20$. The latter critical value is consistent with the known possibility for the uniform system.

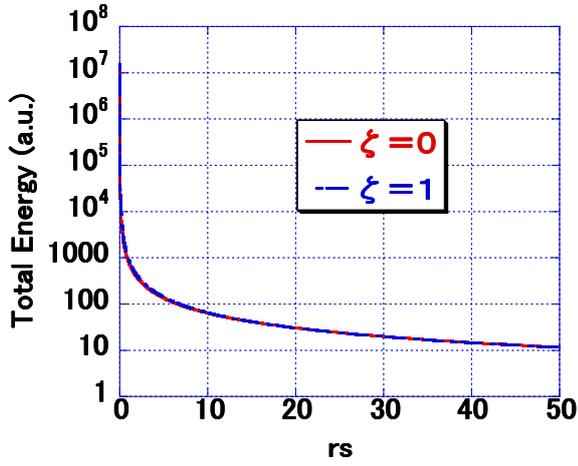


FIG. 3: Total Energy v.s. r_s .

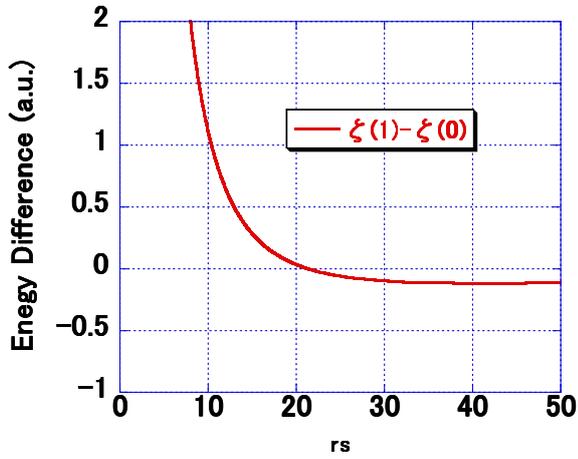


FIG. 4: Energy difference between $\zeta = 1$ and $\zeta = 0$ in terms of r_s .

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