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## A new real-space correlated-basis-functions approach for electron correlations of the semiconductor inversion layer

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**Abstract.** Based on the real-space correlated-basis-functions theory and the collective oscillation behaviour of the electron gas with effective Coulomb interaction, the many-body wavefunction is obtained for the quasi-two-dimensional electron system in the semiconductor inversion layer. The pair-correlation function and the correlation energy of the system have been calculated by the integro-differential method in this paper. A comparison with other previous theoretical results is also made. The new theoretical approach and its numerical results show that the pair-correlation functions are definitely positive and satisfy the normalisation condition.

### 1. Introduction

In the past two decades, many contributors became very interested in the area of two-dimensional (2D) and quasi-two-dimensional (Q2D) electron systems [1–8]. The representative many-body theories for treating the correlations of such systems are, for example, the random-phase approximation (RPA), the Hubbard approximation (HA), the self-consistent STLS approximation [7] of Singwi *et al*, the Monte Carlo method [4], and the coupled-cluster method (CCM) [8]. From the calculations of these theories for the pair-correlation function, which is a very important key to the many-particle problem, we can find the following facts.

(i) Most of the calculations are carried out in the momentum space, which is very similar to the three-dimensional (3D) system. The usual theoretical approaches are firstly focused on the calculation of the static structure factor, which is defined as

$$S(Q) = \langle \rho_Q \rho_{-Q} \rangle / N \quad (1)$$

where  $\rho_Q$  is the fluctuation density operator. The pair-correlation function  $g(R)$  can then be obtained through the Fourier transformation

$$g(R) = 1 + \frac{1}{2\pi n} \int_0^\infty Q \, dQ J_0(QR) [S(Q) - 1] \quad (2)$$

where  $J_0(x)$  is the zeroth-order Bessel function, and  $n$  is the electron density.

It is true that it is more convenient to obtain analytic expressions in momentum space than in the real space when we deal with the homogeneous electron system but, if we wish to carry out further numerical work, serious errors will be introduced into the calculation because of the cut-off approximation for the infinite integral in the momentum space. It is well known that the function

$$h(R) = g(R) - 1 \quad (3)$$

which satisfies the normalisation condition

$$-n \int h(\mathbf{R}) d\mathbf{R} = 1 \quad (4)$$

is a rapidly converging short-range factor. In real space, we can use it as a strongly automatic cut-off factor naturally, but in the momentum space, its Fourier transform,  $S(Q) - 1$ , is, however, only a weakly converging function.

(ii) The numerical results of the pair-correlation functions in many previous theories may appear to be negative values when the two electrons are very close in the case of a low electron density. Although many workers have tried to eliminate these imperfections, they still have not found the mathematical proof to show that their theory will obtain definite positive values for the pair-correlation function irrespective of how close the two particles are and how low the electron density is.

(iii) Few contributors have shown the oscillating behaviour of the pair-correlation function in the region of large  $R$ , the distance between the two electrons. Careless use of these results will lose much physical information.

Recently Feng and Sun [9, 10] developed a new systematic many-particle theory, the real-space correlated-basis-functions (RSCBF) method, to treat the electron correlation for both inhomogeneous and homogeneous electron systems. The starting point of the theory is to calculate the pair-correlation function directly in real space, i.e. coordinate space. The theory was first used in the case of metal surfaces [9, 10] and the 3D uniform metallic electron system [11]. Later it was extended to the 2D electron gas [12, 13], and one-dimensional (1D) and quasi-one-dimensional (Q1D) electron systems [14, 15]. By the integro-differential and variational method, the RSCBF theory can obtain the many-body wave function, one-particle profile (for the inhomogeneous system), the pair-correlation function and the correlation energy simultaneously. The remarkable advantage of the RSCBF theory is that the calculated pair-correlation functions are positive definite and satisfy the normalisation condition. The main approximation of the theory is the convolution approximation (CA) [16–18], although it leads to a very complicated form for the correlation energy equation and introduces errors into the real calculation. The previous numerical results seem very good for the long-range Coulomb interaction, but these studies cannot estimate the errors caused by CA and show why the CA is good enough for the calculation of the electron correlation energy and some other physical quantities.

In this paper, we shall improve the previous RSCBF research work by presenting an exact but very simple variational correlation energy expression. As an application of the new theoretical approach, we have dealt with the Q2D electron system of the inversion layer of the semiconductor.

## 2. Effective Hamiltonian of a Q2D electron system and many-body wavefunction

The Q2D electron can be regarded as a bounded 3D system; the electrons move freely in the  $x$ - $y$  plane and are tightly bounded in the  $z$  direction as in the real case of the semiconductor inversion layer.

To demonstrate the motion in the  $z$  direction for the semiconductor inversion layer, in [2, 7, 8] the form of the Fang–Howard variational wavefunction was adopted:

$$\xi(z) = (b^3/2)^{1/2} z \exp(-bz/2) \quad (5)$$

where  $b$  is a variational parameter, which was chosen by minimising the total single-particle energy [7]

$$b = (48\pi e^2 m_e / K_{sc} \hbar^2) (N_{depl} + \frac{11}{32} N_{inv}). \quad (6)$$

Here  $N_{depl} = 7.6 \times 10^{10} \text{ cm}^{-2}$  is the electron concentration in the depletion layer and  $N_{inv}$  is the electron concentration in the inversion layer. The consequent effective Coulomb interaction for the Q2D electron then reads [7]

$$V_{\text{eff}}(R) = \frac{1}{2\pi} \int_0^\infty Q \, dQ J_0(QR) v(Q) F(Q) \quad (7)$$

the inverse Fourier transform of which is

$$v_{\text{eff}}(Q) = v(Q) F(Q) \quad (8)$$

where  $v(Q) = 2\pi e^2 / \bar{K} q$  is the Fourier transform obtained in the 2D electron system. The dielectric constant  $\bar{K}$  is  $(K_{sc} + K_{ins})/2$ , where  $K_{sc}$  and  $K_{ins}$  are the dielectric constants in the semiconductor and insulator, respectively. For the inversion layer of silicon–metal–oxide, the introduced function  $F(Q)$  is given by

$$F(Q) = (1 + K_{ins}/K_{sc}) \left[ \frac{3}{16}(1 + Q/b)^{-1} + \frac{3}{16}(1 + Q/b)^{-2} + \frac{1}{8}(1 + Q/b)^{-3} \right] + \frac{1}{2}(1 - K_{ins}/K_{sc})(1 + Q/b)^{-6} \quad (9)$$

where  $K_{sc} = 11.8$  and  $K_{ins} = 3.8$  [7]. When  $F(Q) = 1$ , it reduces to the ideal case of the 2D electron system.

The model Hamiltonian for the Q2D system is written as

$$H = \int d\mathbf{R} \psi^\dagger(\mathbf{R}) T \psi(\mathbf{R}) + \frac{\lambda^2}{2} \iint d\mathbf{R} d\mathbf{R}' \psi^\dagger(\mathbf{R}) \psi^\dagger(\mathbf{R}') V_{\text{eff}}(|\mathbf{R} - \mathbf{R}'|) \psi(\mathbf{R}') \psi(\mathbf{R}). \quad (10)$$

Note that we have introduced a strength parameter  $\lambda$  into the Hamiltonian. When  $\lambda = 0$ , it describes the non-interacting free-electron system; in the full strength limit  $\lambda = 1$ , it just demonstrates the Q2D effective Coulomb interaction system.

Define the density fluctuation operator as

$$\rho_Q = \sum_j \exp(-i\mathbf{Q} \cdot \mathbf{R}_j). \quad (11)$$

Equation (10) can be rewritten as

$$H = \sum_j \frac{\hbar k_j^2}{2m^*} + \frac{\lambda^2}{2A} \sum_{Q \neq 0} v_{\text{eff}}(Q) (\rho_Q^\dagger \rho_Q - N) \quad (12)$$

where  $m^* = 0.9m_e$  is the effective mass in the 2D plane.

According to the Bohm–Pines theory [19], for a suitable choice of a wavevector  $Q_c$ , the density fluctuations for  $Q < Q_c$  display essentially collective behaviour and oscillate at a frequency near to the collective plasma frequency and for  $Q > Q_c$  they represent single-particle behaviour. Separating the part of  $Q < Q_c$  in equation (12) and carrying out the canonical transformation [19], we obtain a ground-state wavefunction for the Q2D system as follows:

$$\begin{aligned}\Psi(\lambda) &= D[\varphi] \exp\left(-\frac{\lambda}{A} \sum_{Q < Q_c} v_{\text{eff}}(Q) \frac{\rho_Q^\dagger \rho_Q}{2\hbar\omega_p(Q)}\right) \\ &= D[\varphi] \exp\left(-\frac{\lambda}{A} \sum_{Q < Q_c} \sum_{j \neq l} v_{\text{eff}}(Q) \frac{\exp(i\mathbf{Q} \cdot \mathbf{R}_{jl})}{2\hbar\omega_p(Q)}\right)\end{aligned}\quad (13)$$

where  $D[\varphi]$  denotes the Slater determinant combined with a complete set of single-electron orbital wavefunctions, and  $\omega_p(Q)$  is the collective oscillation plasma frequency:

$$\omega_p(Q) = \sqrt{nQ^2 v_{\text{eff}}(Q)/m^*} \quad (14)$$

which can be easily obtained by differentiating twice over the density fluctuation operator  $\rho_Q$  with respect to the time. Let

$$c(Q) = -2v_{\text{eff}}(Q)\theta(Q_c - Q)/\hbar\omega_p(Q) \quad (15)$$

where  $\theta(x)$  denotes the step function:

$$\theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0. \end{cases} \quad (16)$$

Then the many-body wavefunction changes to

$$\Psi(\lambda) = D[\varphi] \exp\left(\frac{\lambda}{4A} \sum_{Q < Q_c} c(Q)(\rho_Q^\dagger \rho_Q - N)\right). \quad (17)$$

Returning to the real space by taking the inverse Fourier transformation, we finally obtain the  $\lambda$ -dependent variational wavefunction in the Jastrow–Feenberg form often used in CBF theory:

$$\Psi(\lambda) = F(\lambda)D[\varphi] \quad (18)$$

where

$$F(\lambda) = \exp\left(\frac{\lambda}{2} \sum_{i < j} u(R_{ij})\right) \quad (19)$$

and  $u(R)$  is called the correlation factor, which is the Fourier transform of function  $c(Q)$ :

$$u(R) = \frac{1}{2\pi} \int_0^\infty Q \, dQ J_0(QR)c(Q) \quad (20)$$

and  $Q_c$  in  $c(Q)$  can be determined by minimising the energy of Q2D electron system.

### 3. Equations for the variational energy and the pair-correlation function

The  $\lambda$ -dependent ground-state energy of the Q2D electron system is simply defined as the expectation value of the Hamiltonian in the ground state:

$$E(\lambda) = \langle \Psi(\lambda) | H(\lambda) | \Psi(\lambda) \rangle / \langle \Psi(\lambda) | \Psi(\lambda) \rangle. \quad (21)$$

Substituting equation (10) for the Hamiltonian in equation (21), we find after differentiating and integrating over  $E(\lambda)$  with respect to  $\lambda$ , that

$$E(\lambda) = E(0) + E_{xc}(\lambda). \quad (22)$$

The first term in equation (22) is just the ground-state energy of a non-interacting Q2D electron gas, which satisfies

$$T | \Psi(0) \rangle = E(0) | \Psi(0) \rangle. \quad (23)$$

The second term is the so-called exchange–correlation energy in terms of the integral of the  $\lambda$ -dependent pair-correlation function  $g(R|\lambda)$  with the effective interaction potential

$$E_{xc}(\lambda) = 2\pi n N \int_0^\lambda \lambda' d\lambda' \int_0^\infty R dR V_{\text{eff}}(R) [g(R|\lambda') - 1]. \quad (24)$$

The correlation energy is then easily calculated by subtracting the exchange energy from it:

$$E_c(\lambda) = 2\pi n N \int_0^\lambda \lambda' d\lambda' \int_0^\infty R dR V_{\text{eff}}(R) [g(R|\lambda') - g(R|0)]. \quad (25)$$

The pair-correlation function  $g(R|\lambda)$  is defined as

$$g(R|\lambda) \equiv g(R_{12}|\lambda) \equiv [N(N-1)/n^2] \left[ \int |\Psi(\lambda)|^2 d\mathbf{R}_3 d\mathbf{R}_4 \dots d\mathbf{R}_N / \int |\Psi(\lambda)|^2 d\mathbf{R}_1 d\mathbf{R}_2 \dots d\mathbf{R}_N \right] \quad (26)$$

When  $\lambda = 0$ , it describes the Hartree–Fock pair correlation function. Differentiating  $g(R|\lambda)$  with respect to  $\lambda$ , and again integrating over it, we can obtain a closed non-linear integral equation for the pair-correlation function in the CA:

$$g(R|\lambda) = g(R|0) \exp \left( \int_0^\lambda d\lambda' \frac{B(R|\lambda')}{g(R|\lambda')} \right). \quad (27)$$

In this equation,

$$B(R|\lambda) = g(R|\lambda)\gamma(R|\lambda) + 2\delta(R|\lambda) + \zeta(R|\lambda) \quad (28)$$

where  $\gamma(R|\lambda)$  is given by

$$\gamma(R|\lambda) = u(R) + 2\gamma_1(R|\lambda) + \gamma_2(R|\lambda). \quad (29)$$

Here

$$\gamma_1(R|\lambda) \equiv \gamma_1(R_{12}|\lambda) = n \int d\mathbf{R}_3 h(R_{13}|\lambda) u(R_{32}) \quad (30)$$

$$\gamma_2(R|\lambda) = n \int d\mathbf{R}_3 h(R_{13}|\lambda) \gamma_1(R_{32}|\lambda) \quad (31)$$

and

$$\delta(R|\lambda) = n \int d\mathbf{R}_3 h(R_{13}|\lambda) \gamma(R_{13}|\lambda) h(R_{32}|\lambda) \quad (32)$$

$$\zeta(R|\lambda) = n \int d\mathbf{R}_3 h(R_{13}|\lambda) \delta(R_{32}|\lambda). \quad (33)$$

Thus the pair-correlation function  $g(R|\lambda)$  can be solved from equations (27)–(33) by numerical iteration.

#### 4. Numerical results and discussion

In order to compare with the previous theoretical results, we take all the relevant parameters as chosen in [7, 8]. For the convenience of the numerical calculation, we introduce dimensionless variables into all the integral expressions presented in section 3.  $R$  is in units of  $k_F^{-1}$  and  $Q$  in units of  $k_F$ . For a Q2D electron system, the Fermi vector  $k_F$  is of the form

$$k_F = \sqrt{2}/r_s a_B^* \quad (34)$$

where  $a_B^*$  is the effective Bohr radius defined as

$$a_B^* = \bar{K}\hbar^2/m^*e^2. \quad (35)$$

For the correlation energy, we let it be in units of effective Rydberg energy:

$$1R^* = m^*e^4/2\bar{K}\hbar^2. \quad (36)$$

In the Hartree–Fock approximation, the pair-correlation function is given by [12, 13]

$$g(R|0) = 1 - 0.5[2J_1(k_F R)/k_F R]^2 \quad (37)$$

where  $J_1(x)$  is the first-order Bessel function.

Using the above-introduced parameters and the Hartree–Fock pair-correlation function, and choosing a trial variational parameter  $Q_c$  in units of  $k_F$ , we then get the pair-correlation function after solving equation (27). By minimising the energy, we can finally determine the optimum parameter  $Q_c(r_s)$ , the pair-correlation function  $g(R; r_s)$ , the correlation energy  $E_c(r_s)$  and the many-body wavefunction simultaneously.

Figure 1 shows the numerical results of the pair-correlation function for  $r_s = 2, 4, 8$  and 16. In order to display the quantum oscillation behaviour clearly, we have had  $g(R)$  enlarged for large  $R$  in the small rectangular inset in figure 1.

In table 1, we present the results of the correlation energies for different densities. For comparison, we have also presented other previous typical theoretical results [7, 8]. In figure 2, we plotted the pair-correlation function results for  $r_s = 16$  from different theories.

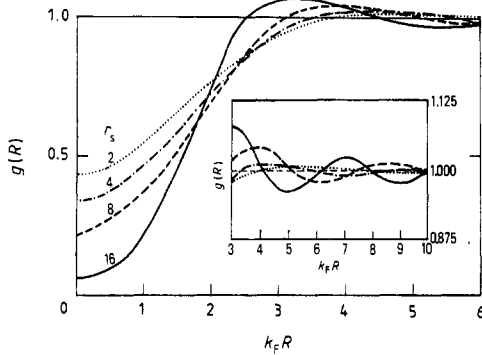
From the numerical results of this paper, we find that the proved RSCBF approach for the Q2D system has its own advantages.

(i) It ensures that the pair-correlation function is definitely positive without the limitation of the distance between the two particles and of the densities of the electron system, which is considered below. As we know from equation (37), the correct results given by the Pauli principle should always have

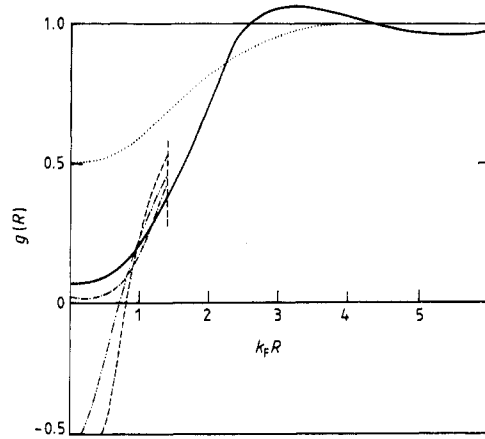
$$g(R|0) \geq \frac{1}{2}. \quad (38)$$

On the other hand, we know from equations (28)–(33) that the function  $B(R|\lambda)$  is a convergent real number, since all the integral functions are definite convergent. Thus equation (27) ensures that  $g(R|\lambda)$  will never be negative if the solution exists.

(ii) The pair-correlation function satisfies the normalisation condition in equation (4) extremely well. The average errors of our results are less than  $10^{-3}$ . This is because the CA still keeps the normalisation condition as shown in [18].



**Figure 1.** The pair-correlation functions of a Q2D system for different electron densities where  $R$  is in units of  $k_F^{-1}$ .



**Figure 2.** Comparison of the pair-correlation functions for  $r_s = 16$ : —, present result; — — —, STLS approximation; - - - -, HA; - · - · -, RPA; · · · · ·, Hartree-Fock approximation. The relevant parameters are the same as in figure 1.

**Table 1.** The exchange and correlation energies for a Q2D electron system.

| $r_s$ | $Q_c$<br>( $k_F$ ) | $E_x/N$ (Ryd*)  |            | $E_c/N$ (Ryd*)  |         |        |          |         |
|-------|--------------------|-----------------|------------|-----------------|---------|--------|----------|---------|
|       |                    | Present results | Jonson [7] | Present results | RPA [7] | HA [7] | STLS [7] | CCM [8] |
| 0.5   | 0.6                | -1.379          | -1.382     | -0.069          | -0.077  | -0.061 | -0.060   | -0.0610 |
| 1     | 0.8                | -0.749          | -0.751     | -0.064          | -0.079  | -0.061 | -0.060   | -0.0591 |
| 2     | 0.9                | -0.405          | -0.407     | -0.051          | -0.078  | -0.060 | -0.058   | -0.0546 |
| 4     | 1.1                | -0.222          | -0.222     | -0.048          | -0.076  | -0.058 | -0.049   | -0.0492 |
| 8     | 1.3                | -0.122          | -0.122     | -0.040          | -0.074  | -0.057 | -0.044   | -0.0446 |
| 16    | 1.6                | -0.067          | -0.067     | -0.033          | -0.070  | -0.055 | -0.034   | -0.0393 |

(iii) The oscillation behaviour of the pair-correlation function is described well.

(iv) The expression for the correlation energy is simple and exact compared with the previous results. The simple formula can easily be extended to other dimensional electron systems. As adopted in [13], we can also use the complicated form with the CA to calculate the correlation energy. The results of the CA are very close to the present results only with errors of  $10^{-3}$  in the units of  $R^*$ . This tells us that the CA is a good approximation for the long-range Coulomb interacting system.

In passing we point out that the coupling parameter  $\lambda$ , which describes the strength of the Coulomb interaction of the Q2D electron system appearing in the many-body wavefunction in equations (18) and (19) is just the same as the strength parameter introduced in the Hamiltonian in equation (10), the pair-correlation function in equation (27), and the correlation energy in equation (25). This important connection makes calculation much easier than in the previous CBF methods [11, 13, 15]. To our knowledge this is the first time that this connection has been presented in the CBF approach.



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