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Exact evaluation of the second-order exchange energy of a two-dimensional electron fluid

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A new rigorous method is presented for the evaluation of the second-order exchange energy of a two-dimensional electron fluid. The resulting energy 0.2287 Ry is significant in the correlation energy, in contrast to the three-dimensional case. The present method is applicable to three dimensions.

I. INTRODUCTION

The evaluation of the correlation energy of an electron gas in three dimensions (3D) has been attempted by many investigators since the famous work of Gell-Mann and Brueckner.[1] For instance, the terms of order r_s have been treated by DuBois, Carr, and Maradudin and by Kojima and Isihara.[2] The second-order exchange energy has been evaluated by Onsager, Mittag, and Stephen[3] rigorously. Such a precise evaluation is important because the second-order exchange energy contributes to the correlation energy which is small.

It is the purpose of the present paper to investigate the case of a two-dimensional electron gas. We have found an entirely new and promising method for the rigorous evaluation of this quantity. The ring and other diagrams have been treated by Isihara and Toyoda.[4] They also treated the second-order exchange energy by a Monte Carlo method.

We have noticed that two-dimensional electron fluids in metal-oxide-semiconductor (MOS) interfaces were attracting much attention recently for their wide density variations and prominent many-body effects.[5] As shown by Isihara and Toyoda[4] the ring diagram contribution to the correlation energy of the two-dimensional electron fluids does not have a logarithmic term without a factor r_s, i.e., $\ln r_s$, as in the three-dimensional case. Therefore, a careful evaluation of the second-order exchange contribution is of particular interest for the two-dimensional case, since it is important in the small-r_s limit.

In comparison with the three-dimensional case, the evaluation of the exchange integrals is harder for the two-dimensional case mainly because of the angle integrals. Nevertheless, in what follows in the present paper we shall report a simple but powerful method for the exact evaluation. Although it is beyond the scope of the present paper to consider some other cases, we believe that essentially the same method is applicable to the three-dimensional case and also to higher-order exchange integrals.

The second-order exchange graphs are classified into two groups, regular and anomalous. The latter has been rigorously treated by Isihara and Toyoda. Therefore, we shall work only on the regular exchange graphs. The theory of Onsager, Mittag, and Stephen was also on these graphs.

II. THEORY

The contribution from the regular second-order exchange graphs to the logarithm of the grand partition function is given by

$$\ln\Xi = -\frac{\beta A}{(2\pi)^6}\int u(q)\Lambda(q)\,d\vec{q}\ , \tag{1}$$

where $\beta = 1/kT$, $u(q)$ is the Coulomb potential, A is the surface area, and [with $f(p)$ for the Fermi distribution]

$$\Lambda(q) = \int\int d\vec{p}\,d\vec{k}\,\frac{u(\vec{p}+\vec{k}+\vec{q})}{2[q^2+\vec{q}\cdot(\vec{p}+\vec{k})]}f(\vec{p})f(\vec{k})[1-f(\vec{p}+\vec{q})][1-f(\vec{k}+\vec{q})]\ . \tag{2}$$

The main source of difficulty in evaluating the four-dimensional integral in Eq. (2) is that four Fermi circles define the integration domain. In order to overcome this difficulty, let us try to separate the integrand into two parts, each depending only on one of the variables p and k. As shown in Appendix A, we first note

$$\Lambda(q) = \frac{1}{2\beta}\sum_j\int\int d\vec{p}\,d\vec{k}\,u(\vec{p}-\vec{k})\left(\frac{f(\vec{p}+\vec{q})-f(\vec{p})}{2\pi ij/\beta+(q^2+2\vec{p}\cdot\vec{q})}\right)\left(\frac{f(\vec{k}+\vec{q})-f(\vec{k})}{2\pi ij/\beta+(q^2+2\vec{k}\cdot\vec{q})}\right)\ . \tag{3}$$

In Eq. (3), $\vec{k}$ and $\vec{p}$ are still coupled through the potential $u(\vec{p}-\vec{k})$. A complete separation can be made bring-

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ing back this potential into coordinate space:

$$u(\vec{p}-\vec{k})=\int \phi(r)e^{i(\vec{p}-\vec{k})\cdot\vec{r}}d\vec{r} \ . \tag{4}$$

Combining Eqs. (3) and (4) we find

$$\Lambda(q)=\frac{1}{2\beta}\sum_j\int d\vec{r}\phi(r)\lambda_j(\vec{q},\vec{r})\lambda_j(\vec{q},-\vec{r}) \ , \tag{5}$$

where

$$\lambda_j(\vec{q},\vec{r})=\int\frac{f(\vec{p}+\vec{q})-f(\vec{p})}{2\pi ij/\beta+q^2+2\vec{p}\cdot\vec{q}}e^{i\vec{p}\cdot\vec{r}}d\vec{p} \ . \tag{6}$$

In Eq. (6) we notice that apart from a factor $1/(2\pi)^2$, $\lambda_j(\vec{q},\vec{r})$ are essentially the position dependent quantum eigenvalues first introduced by Isihara in the study of the pair distribution function of the electron system.[6]

Note in Eq. (5) that the form is general and does not depend on dimensionality. In the zero temperature limit, we can use a continuous variable

$$\nu=2\pi j/\beta \ . \tag{7}$$

In the limit, the Fermi circle is sharp. For simplicity, let us choose $p_F=1$. Since

$$\lambda_{-\nu}(\vec{q},-\vec{r})=e^{i\vec{q}\cdot\vec{r}}\lambda_n(q,r) \tag{8}$$

the product $\lambda_\nu(\vec{q},\vec{r})\lambda_\nu(\vec{q},-\vec{r})$ is invariant under the change $\nu\rightarrow-\nu$. We can then consider only the case $\nu>0$ and introduce a factor of 2.

Hence, we introduce a Laplace integral for positive ν:

$$\frac{1}{\nu i+q^2+2\vec{p}\cdot\vec{q}}=-i\int_0^\infty e^{-\nu t}\exp[it(q^2+2\vec{p}\cdot\vec{q})]\,dt \ . \tag{9}$$

Furthermore, we note

$$\lambda_\nu(\vec{q},\vec{r})=\int d\vec{p}e^{i\vec{p}\cdot\vec{r}}[f(\vec{p}+\vec{q})-f(p)]\int_0^\infty e^{-\nu t}\exp[it(q^2+2\vec{p}\cdot\vec{q})]\,dt \ . \tag{10}$$

Performing the p integration we get

$$\lambda_\nu(\vec{q},\vec{r})=-4\pi e^{-i\vec{q}\cdot\vec{r}/2}\int_0^\infty e^{-\nu t}\frac{J_1(|\vec{r}+2\vec{q}t|)}{|\vec{r}+2\vec{q}t|}\sin[\tfrac{1}{2}\vec{q}\cdot(\vec{r}+2\vec{q}t)]\,dt \ , \tag{11}$$

where J_1 is the Bessel function.

Introducing Eq. (11) into Eq. (5) and performing the ν integration we find

$$\Lambda(q)=4(2\pi)e^2\int_0^\infty\int_0^\infty\frac{dtdx}{t+x}\int\frac{d\vec{r}}{r}\frac{J_1(|\vec{r}+2\vec{q}t|)}{|\vec{r}+2\vec{q}t|}\sin[\tfrac{1}{2}\vec{q}\cdot(\vec{r}+2\vec{q}t)]\times\frac{J_1(|-\vec{r}+2\vec{q}x|)}{|-\vec{r}+2\vec{q}x|}\sin[\tfrac{1}{2}\vec{q}\cdot(-\vec{r}+2\vec{q}x)] \ . \tag{12}$$

The next step is to perform the q integration as required in Eq. (1). We first change the variables in Eq. (12) such that

$$t\rightarrow t/q, \quad x\rightarrow x/q$$

to find

$$\Lambda(q)=\frac{4(2\pi)}{q}e^2\int\frac{d\vec{r}}{r}\int\int\frac{dxdt}{t+x}\frac{J_1(|\vec{r}+2\hat{u}t|)}{|\vec{r}+2\hat{u}t|}\frac{J_1(|-\vec{r}+2\hat{u}x|)}{|-\vec{r}+2\hat{u}x|}\sin\tfrac{1}{2}\hat{u}q\cdot(\vec{r}+2\hat{u}t)\sin\tfrac{1}{2}\hat{u}q\cdot(-\vec{r}+2\hat{u}x) \ , \tag{13}$$

where $\hat{u}$ is a unit vector. Multiplying this expression by $u(q)$ and integrating over q, we arrive at

$$\int u(q)\Lambda(q)d\vec{q}=2(2\pi)^3e^4\int\frac{d\vec{r}}{r}\int\int\frac{dxdt}{(t+x)}\frac{J_1(|\vec{r}+2\hat{u}t|)}{|\vec{r}+2\hat{u}t|}\frac{J_1(|-\vec{r}+2\hat{u}t|)}{|-\vec{r}+2\hat{u}t|}\ln\left|\frac{2(t+x)}{\hat{u}\cdot[2\vec{r}+\hat{u}(t-x)]}\right| \ , \tag{14}$$

where we have used an integral

$$\int_0^\infty \frac{\sin ax \sin bx}{x}\, dx = \frac{1}{2} \ln\left|\frac{a+b}{a-b}\right| \quad . \tag{15}$$

Equation (14) can be simplified if we change variables such that

$$\vec{r} \rightarrow (t+x)\vec{r} + \hat{u}(x-t) \quad .$$

We obtain

$$I = \int u(q)\Lambda(q)d\vec{q} = 2(2\pi)^3 e^4 \int\int \frac{dxdt}{(x+t)} \int \frac{d\vec{r}}{|(t+x)\vec{r}+\hat{u}(x-t)|} \times \frac{J_1[(x+t)|\vec{r}+\hat{u}|]}{|\vec{r}+\hat{u}|} \frac{J_1[(x+t)|\vec{r}-\hat{u}|]}{|\vec{r}-\hat{u}|} \ln\left|\frac{1}{\vec{r}\cdot\hat{u}}\right| \quad . \tag{16}$$

A decoupling of the integration variables in this expression can be achieved if we change the variables as follows:

$$x = \frac{1}{2}(1+\xi)y, \quad t = \frac{1}{2}(1-\xi)y \quad , \tag{17}$$

where

$$0 < y < \infty, \quad -1 < \xi < 1 \quad , \quad dxdt = \frac{1}{2} y d\xi dy \quad . \tag{18}$$

We obtain

$$I = (2\pi)^3 e^4 \int d\vec{r} \left(\int_{-1}^{1} \frac{d\xi}{|\vec{r}+\xi\hat{u}|}\right) \ln\left|\frac{1}{\vec{r}\cdot\hat{u}}\right| \int_0^\infty \frac{dy}{y} \frac{J_1(y|\vec{r}+\hat{u}|)}{|\vec{r}+\hat{u}|} \frac{J_1(y|\vec{r}-\hat{u}|)}{|\vec{r}-\hat{u}|} \quad . \tag{19}$$

We can make use of the formulas

$$\int_0^\infty \frac{dy}{y} J_1(ay)J_1(by) = \frac{1}{2}\begin{cases} a/b, & 0 < a < b \\ b/a, & a > b > 0 \end{cases} , \tag{20}$$

$$\int_{-1}^{1} \frac{d\xi}{|\vec{r}+\xi\hat{u}|} = \ln\left(\frac{|\vec{r}+\hat{u}|+1+\vec{r}\cdot\hat{u}}{|\vec{r}-\hat{u}|-1+\vec{r}\cdot\hat{u}}\right) \quad . \tag{21}$$

Equation (19) becomes

$$I = -2(2\pi)^3 e^4 \int_0^\infty \int_0^\infty \frac{dxdy}{(x+1)^2+y^2} \ln\left(\frac{1+x[(1+x)^2+y^2]^{1/2}}{x-1+[(1-x)^2+y^2]^{1/2}}\right) \ln x \quad , \tag{22}$$

where we have used $\vec{r} = (x,y)$ and $\hat{u} = (1,0)$.

The double integral of Eq. (22) is difficult to obtain. In order to simplify it, we use

$$y \rightarrow (1+x)y, \quad z = \frac{x-1}{x+1} \quad , \tag{23}$$

as new variables. We then find

$$I = -2(2\pi)^3 e^4 \int_{-1}^{1} \frac{dz}{1-z} \ln\left(\frac{1+z}{1-z}\right) F(z) \quad , \tag{24}$$

where

$$F(z) = \int_0^\infty \ln\left(\frac{1+(1+y^2)^{1/2}}{z+(z^2+y^2)^{1/2}}\right) \frac{dy}{1+y^2} \quad . \tag{25}$$

In Appendix B, the following properties are found

$$F(-z) = -F(z) + 2F(0) \quad , \qquad F(0) = 2G = 1.831\,931\,188 \quad , \tag{26}$$

where G is Catalan's constant. Using these results we arrive at

$$I=-2(2\pi)^3e^4\left[\int_0^1 \frac{2dz}{1-z^2}\ln\left|\frac{1-z}{1+z}\right|+2F(0)c\right] , \tag{27}$$

where

$$c=\int_0^1 \frac{dz}{1+z}\ln\left|\frac{1-z}{1+z}\right|=-\frac{\pi^2}{12} . \tag{28}$$

In Eq. (27) we integrate by parts to obtain

$$I=-2(2\pi)^3e^4\left[-\frac{1}{2}\int_0^1\left(\ln\frac{1+z}{1-z}\right)^2F'(z)dz+2F(0)c\right] , \tag{29}$$

where

$$F'(z)=-\frac{1}{2(1-z^2)^{1/2}}\ln\left|\frac{1+(1-z^2)^{1/2}}{1-(1-z^2)^{1/2}}\right| . \tag{30}$$

The numerical value of the integral in Eq. (29) is given in Appendix C. We have found

$$\begin{aligned}\gamma&=\tfrac{1}{8}\int_0^1\frac{dz}{(1-z^2)^{1/2}}\left(\ln\left|\frac{1+z}{1-z}\right|\right)^2\ln\left|\frac{1+(1-z^2)^{1/2}}{1-(1-z^2)^{1/2}}\right|\\&=1-(1-\tfrac{1}{3})1/2^3+(1-\tfrac{1}{3}+\tfrac{1}{5})1/3^3-(1-\tfrac{1}{3}+\tfrac{1}{5}-\tfrac{1}{7})1/4^3+\cdots=0.942\ 372\ 18,\ \ldots .\end{aligned} \tag{31}$$

Therefore

$$I=-2(2\pi)^3e^4(2\gamma-\tfrac{1}{3}\pi^2G) . \tag{32}$$

Our final result is

$$\begin{aligned}\ln\Xi&=-\beta\frac{p_F^2e^4A}{32\pi^4}[8\pi(\tfrac{1}{3}\pi^2G-2\gamma)]\\&=-\beta\frac{p_F^2e^4A}{32\pi^4}(28.366\ 361) .\end{aligned} \tag{33}$$

This represents the rigorous second-order regular exchange contribution to the grand partition function.

This result should be compared with the Monte Carlo result of Isihara and Toyoda. The numerical factor obtained by them was 27.3 ± 1.3. Therefore, their result agrees with the above rigorous result.

The second-order exchange energy is then given by

$$\epsilon=28.36631/4\pi^3=0.2287 \text{ Ry} .$$

This contrasts to the Monte Carlo value of 0.220.

III. CONCLUDING REMARKS

We have evaluated exactly the second-order exchange energy for the electrons in two dimensions. The interaction potential which has been used is Coulombic, and therefore the system is quasi-two dimensional. However, we have not considered a thickness effect. A finite thickness of the inversion and accumulation layers certainly affect the form of the interaction potential.[7] At the expense of using the idealized model, we have succeeded to obtain the rigorous result. We remark that the integral in Eq. (31) can be represented by known functions. Similar integrals appear in the three-dimensional case treated by Onsager *et al.*[3]

For the present model, the first-order exchange energy varies as $-1.2/r_s$ Ry. Therefore, the r_s of order 3 or 4, the second-order exchange energy becomes comparable. On the other hand, the second-order ring contribution is characterized by a factor $1.93/8\pi^2\cong0.0244$ [Eq. (2.21) of Isihara and Toyoda, Ref. 4] in contrast to a factor $28.366/32\pi^4=0.0091$ of Eq. (33). Therefore, again the second-order exchange contribution is not negligible. For the three-dimensional case, Onsager *et al.* found that the second-order exchange energy is 0.048 36. The two-dimensional energy 0.2287 which we have found is considerably larger, indicating larger correlations in two dimensions.

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APPENDIX A

Let us start with the real quantity

$$\sum_j\left[\frac{f(\vec{p}+\vec{q})-f(\vec{p})}{2\pi ij/\beta+(q^2+2\vec{p}\cdot\vec{q})}\right]\left[\frac{f(\vec{k}+\vec{q})-f(\vec{k})}{-2\pi ij/\beta+(q^2+2\vec{k}\cdot\vec{q})}\right] . \tag{A1}$$

Decomposing the denominator of the above quantity in partial fractions, we find

$$\sum_j \frac{f(\vec{k}+\vec{q})-f(\vec{k})}{2[q^2+\vec{q}\cdot(\vec{p}+\vec{k})]}\,\frac{f(\vec{p}+\vec{q})-f(\vec{p})}{2\pi ij/\beta+(q^2+2\vec{p}\cdot\vec{q})}+(\,\cdots\,)\ , \tag{A2}$$

where $(\,\cdots\,)$ denotes the contribution obtained by exchanging $\vec{p}$ with $\vec{q}$ and vice versa in the first term of the above equation.

By means of the formula

$$\coth x=\sum_j \frac{1}{(\pi ij+x)} \tag{A3}$$

the discrete sum in Eq. (A2) can be found as

$$\sum_j \frac{1}{2\pi ij/\beta+(q^2+2\vec{p}\cdot\vec{q})}=\tfrac{1}{2}\beta\coth[\tfrac{1}{2}\beta(q^2+2\vec{p}\cdot\vec{q})]\ . \tag{A4}$$

Putting Eq. (A4) back in Eq. (A2) and making use of the identity

$$[f(\vec{p}+\vec{q})-f(\vec{p})]\coth[\tfrac{1}{2}\beta(q^2+2\vec{p}\cdot\vec{q})]=-\{f(\vec{p})[1-f(\vec{p}+\vec{q})]+f(\vec{p}+\vec{q})[1-f(\vec{p})]\} \tag{A5}$$

we find

$$\sum_j \frac{f(\vec{p}+\vec{q})-f(\vec{p})}{2\pi ij/\beta+(q^2+2\vec{p}\cdot\vec{q})}\,\frac{f(\vec{k}+\vec{q})-f(\vec{k})}{-2\pi ij/\beta+(q^2+2\vec{k}\cdot\vec{q})}$$

$$=-\tfrac{1}{2}\beta\frac{[f(\vec{k}+\vec{q})-f(\vec{k})]}{2[q^2+\vec{q}\cdot(\vec{p}+\vec{k})]}\{f(\vec{p})[1-f(\vec{p}+\vec{q})]+f(\vec{p}+\vec{q})[1-f(\vec{p})]\}+(\,\cdots\,)\ . \tag{A6}$$

By considering the contribution $(\,\cdots\,)$ explicitly and adding it to the first term in the right-hand side of the above equation, we get

$$\frac{1}{\beta}\sum \frac{f(\vec{p}+\vec{q})-f(\vec{p})}{2\pi ij/\beta+(q^2+2\vec{p}\cdot\vec{q})}\,\frac{f(\vec{k}+\vec{q})-f(\vec{k})}{-2\pi ij/\beta+(q^2+2\vec{k}\cdot\vec{q})}$$

$$=\frac{f(\vec{k})f(\vec{p})[1-f(\vec{k}+\vec{q})][1-f(\vec{p}+\vec{q})]-f(\vec{k}+\vec{q})f(\vec{p}+\vec{q})[1-f(\vec{k})][1-f(\vec{p})]}{2[q^2+\vec{q}\cdot(\vec{p}+\vec{k})]}\ . \tag{A7}$$

Finally, multiplying both members of the above equation by $u(\vec{p}+\vec{k}+\vec{q})$ and integrating with respect to $\vec{k}$ and $\vec{p}$, noticing that

$$-\frac{u(\vec{p}+\vec{k}+\vec{q})}{q^2+\vec{q}\cdot(\vec{p}+\vec{k})}f(\vec{k}+\vec{q})f(\vec{p}+\vec{q})[1-f(\vec{k})][1-f(\vec{p})]\rightarrow\frac{u(\vec{p}+\vec{k}+\vec{q})}{q^2+\vec{q}(\vec{p}\cdot\vec{k})}f(\vec{p})f(\vec{k})$$

$$\times[1-f(\vec{k}+\vec{q})][1-f(\vec{p}+\vec{q})] \tag{A8}$$

under the change of variables

$$\vec{p}\rightarrow-(\vec{p}+\vec{q})\ ,\qquad \vec{k}\rightarrow-(\vec{k}+\vec{q})\ , \tag{A9}$$

we arrive at

$$\sum_j \frac{1}{2\beta}\int d\vec{p}\,d\vec{k}\,u(\vec{p}+\vec{k}+\vec{q})\frac{f(\vec{p}+\vec{q})-f(\vec{p})}{2\pi ij/\beta+(q^2+2\vec{p}\cdot\vec{q})}\,\frac{f(\vec{k}+\vec{q})-f(\vec{k})}{-2\pi ij/\beta+(q^2+2\vec{k}\cdot\vec{q})}$$

$$=\int d\vec{p}\,d\vec{k}\frac{u(\vec{p}+\vec{k}+\vec{q})}{2[q^2+\vec{q}\cdot(\vec{p}+\vec{k})]}f(\vec{k})f(\vec{p})[1-f(\vec{k}+\vec{q})][1-f(\vec{p}+\vec{q})]\ . \tag{A10}$$

The slightly modified version of Eq. (A10) given in Eq. (3) is easily obtained by the change of variable $k\rightarrow-(\vec{k}+\vec{q})$ in the left-hand side of the above identity.

APPENDIX B

$$F(-z)=\int_0^\infty \ln\left[\left(\frac{1+(1+y^2)^{1/2}}{y^2}\right)[(z^2+y^2)^{1/2}+z]\right]\frac{dy}{1+y^2}=\int_0^\infty \frac{dy}{1+y^2}\left\{\ln\left(\frac{z+(y^2+z^2)^{1/2}}{1+(1+y^2)^{1/2}}\right)+\ln\left[\left(\frac{(1+y^2)^{1/2}+1}{y}\right)^2\right]\right\}$$

$$=-F(+z)+2F(0)\ ,$$

$$F'(z)=-\int_0^\infty \frac{dy}{1+z^2\sinh^2 y}=-\frac{1}{2(1-z^2)^{1/2}}\ln\left(\frac{1+(1-z^2)^{1/2}}{1-(1-z^2)^{1/2}}\right)\ .$$

APPENDIX C

$$\gamma=\tfrac{1}{8}\int_0^1 \frac{dz}{(1-z^2)^{1/2}}\left[\ln\left(\frac{1+z}{1-z}\right)\right]^2\ln\left(\frac{1+(1-z^2)^{1/2}}{1-(1-z^2)^{1/2}}\right)\ . \tag{C1}$$

Making the change of variable

$$z=\frac{x-1}{x+1}\ , \tag{C2}$$

we find

$$\gamma=2\int_0^1 \frac{dx}{1+x^2}(\ln x)^2\ln\left(\frac{1+x}{1-x}\right)\ . \tag{C3}$$

Since

$$\frac{1}{1+x^2}\ln\left(\frac{1+x}{1-x}\right)=2x[1+(\tfrac{1}{3}-1)x^2+(\tfrac{1}{5}-\tfrac{1}{3}+1)x^4+\cdots] \tag{C4}$$

and

$$\int_0^1 (\ln x)^2 x^{2n+1}=\frac{2}{(2n+2)3}\ ,$$

we find

$$\gamma=1-\frac{1}{2^3}(1-\tfrac{1}{3})+\frac{1}{3^3}(1-\tfrac{1}{3}+\tfrac{1}{5})-\frac{1}{4^3}(1-\tfrac{1}{3}+\tfrac{1}{5}-\tfrac{1}{7})+\cdots=0.942\,372\,18\ .$$

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