

THE CORRELATION ENERGY OF THE ELECTRON GAS IN LAYERED NARROW-GAP SEMICONDUCTORS

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The correlation energy of a high-density electron gas in layered narrow-gap semiconductors was calculated to the random-phase approximation.

Let us consider a layered semiconductor composed of alternating layers of semiconductors I and II. We take the permittivities of both layers as identical and equal to ϵ . In what follows (as in [1]), we take into account the dispersion of ϵ . We consider semiconductor I as a wide-gap one with the energy gap $2\Delta_I$ so wide that the separation κ of size-quantization levels in the superlattice, which is due to a nonperiodicity of the wave vector in the layer plane, is small compared to the energy gap $2\Delta_{II}$ of the second semiconductor and to the energy difference σ between the first excited and the ground states. The energy separation between the ground and the first excited states of size quantization is assumed to be so large in the layer II that

$$\sigma \gg \Delta_{II}. \quad (1)$$

The electron gas can exist then at the lowest energy level so that the corresponding relativistic two-dimensional dispersion relation is given by $E(p) = \sqrt{\Delta_{II}^2 + p^2 s^2}$, where p is the two-dimensional momentum in the direction parallel to the layers and s is Kane's interband matrix element (the quasi-speed of light).

We assume that

$$\sigma \gg E(p_F) \gg \kappa, \quad (2)$$

where p_F is the Fermi momentum.

The superlattice period c is assumed to be so small that

$$\beta = p_F c \ll 1. \quad (3)$$

Henceforth, we set $\hbar = 1$ for simplicity.

In view of (3), the thickness $l < c$ of layer II satisfies the condition

$$p_F l \ll 1.$$

Any type of systems considered in [2], [3] may serve as structure II.

With conditions (1), (2), and (4) fulfilled, the correlation energy per electron is given (see Appendix)

$$E_{corr} = \frac{1}{2\rho} \int \frac{d^2 \vec{q} d\omega}{(2\pi)^3} \int_0^{2\pi} \frac{d\omega}{2\pi} \{ \ln(1 - v\bar{V}(\vec{q}, \omega)\Pi_{44}(q)) + v\bar{V}(\vec{q}, \omega)\Pi_{44}(q) \}, \quad (5)$$

where $\rho = p_F^2 v / 2\pi$ is the two-dimensional density of the electron gas in a layer; v is the number of valleys (for generality, we consider a many-valley semiconductor); $q = (\vec{q}, \omega)$ is three-dimensional Euclidean vector; $\vec{q} = |\vec{q}|$, $\bar{V}(\vec{q}, \omega)$ is the Fourier transform of the Coulon potential $V(\vec{r}) = e^2/\epsilon r$ and is given by

$$\bar{V}(\vec{q}, \omega) = \int \int dx dy e^{iq_x x + iq_y y} \sum_{m=-\infty}^{m=+\infty} e^{i\omega m} V(x, y, cm) = \frac{2\pi e^2}{c\vec{q}} \frac{\sinh(\vec{q}c)}{\cosh(\vec{q}c) - \cos(\omega)}; \quad (6)$$

and $\Pi_{44}(q)$ is the polarization operator for two-dimensional electron gas, which is formally obtained by discarding the third component of the three-dimensional polarization operator [1],

$$\Pi_{44}(q) = 16 \int \frac{d^2 \vec{p}}{(2\pi)^2} \frac{\theta(\vec{p} - p_F)}{2E(\vec{p})} \frac{(\vec{q}\vec{p})^2 - \vec{q}^2 E(\vec{p})^2}{(q^2)^2 - 4(\vec{p}\vec{q} - iE(\vec{p})\omega)^2}, \quad (7)$$

where $\vec{p} = |\vec{p}|$.

We consider an ultrarelativistic case when $sp_F \gg \Delta_{II}$. Then, integrating with respect to ω and introducing a new integration variable y , we can transform integral (5) to the form convenient for analysis:

$$E_{corr} = -\frac{p_F^3}{2\rho} \int_0^{+\infty} r^2 dr \int_0^\pi \frac{\sin\theta d\theta}{2\pi^2} \int_0^{D(r,\theta)} dy \left(1 - \frac{1}{\sqrt{1 + y^2 + 2y\coth(r\beta\sin\theta)}} \right), \quad (8)$$

where

$$D(r, \theta) = -\frac{2\pi e^2}{r} \tilde{\Pi}_{44}(r, \theta) = \begin{cases} e^2 \sin\theta / 12r^3, & \text{for } r \gg 1 \\ (e^2/8r)(1 - |\cos\theta|), & \text{for } r \ll 1; \end{cases} \quad (9)$$

and $\tilde{\Pi}_{44}(r, \theta)$ is the polarization operator which was rendered dimensionless by dividing by sp_F ; it depends on the variable $r = \sqrt{\omega^2 + s^2 \vec{q}^2} / sp_F$ and on the angle θ defined by the equation $\sin\theta = s\vec{q} / \sqrt{s^2 \vec{q}^2 + \omega^2}$.

It is evident from (8) and (9) that the major contribution to the correlation energy is provided by such r that $1 \ll r \ll 1/\beta$, i.e., when the radicand in (8) is much larger than unity. This contribution exceeds the one provided by $r < 1$ by a factor of $\ln\beta^{-1}$.

Therefore, setting unity as the lower limit of integration with respect to r , using an asymptotic expression for $D(r, \theta)$ in the case of $r \gg 1$, and assuming that $\coth(r\beta\sin\theta) \approx 1/(r\beta\sin\theta)$, we obtain the following formula for correlation energy:

$$E_{corr} = -\frac{e^2}{48\epsilon} \left(\frac{2\pi\rho}{v}\right)^{1/2} \ln \frac{\alpha v}{\beta} \quad (10)$$

under the conditions $p_F a_x \gg \alpha^{-1} > 1$ and $\alpha v \gg \beta = p_F c$ with $\alpha = e^2/\epsilon s$.

This correlation energy exceeds the contribution of the exchange energy by the factor $\ln(\alpha v/\beta)$.

In the nonrelativistic case, formula (5) yields the following expression for the correlation energy of the quasi-two-dimensional electron gas in the layered system under consideration [4 - 6]:

$$E_{corr} = -A E_x (n a_x^3)^{1/4}, \quad (11)$$

where $E_x = 2m\epsilon^4/\epsilon\hbar^2$, $A = 2^{31/4}\pi^{9/4}/5 \left[\Gamma\left(\frac{1}{4}\right)\right]^4 = 3.27$, $m = \Delta_{II}/s^2$, $a_x = \epsilon/2me^2$, and $n = \rho/c$ is the total electron density.

Taking into account, as in [1] (see also [7], [8]), the frequency dispersion, we realize that ϵ should stand for the high-frequency permittivity in formulas (10) and (11).

Thus, it is clear that finiteness of the energy gap and the Dirac dispersion relation affect the trend of the density dependence of correlation energy.

Let us now compare the conditions for applicability of the approximations (pronounced confinement of the system, ultrarelativistic dispersion relation, and strong anisotropy of the system) employed in the calculations of correlation energy in the quasi-two-dimensional and three-dimensional cases.

In the three-dimensional case, $\alpha/v^{1/3}$, $1/v^{4/3}$, and $1/v^{1/3}$ are the characteristic parameters for the quantity r_s (average dimensionless distance between particles). With $\alpha v \ll 1$, the formula

$$E_{corr} = -A E_x (n a_x^3)^{1/4} \quad (12)$$

is valid for $1/v^{4/3} \ll r_s \ll 1/v^{1/3}$ in the nonrelativistic case. With $\alpha v \gg 1$, the formula

$$E_{corr} = -E_x \left(\frac{n a_x^3}{v}\right)^{1/3} \frac{1}{8\pi^{7/3} 3^{2/3}} \ln(\alpha v)$$

is applicable to the relativistic case if $r_s \ll \alpha/v^{1/3}$, whereas formula (12) holds in the nonrelativistic case if $\alpha/v^{1/3} \ll r_s \ll 1/v^{1/3}$.

The quantities $c/\alpha v^{3/2} a_x$, $\alpha/v^{1/2}$, $(c/a_x)^{1/2} v^{-1}$, and $1/v^{1/2}$ are characteristic parameters for a layered semiconductor. Formula (11) is valid in the nonrelativistic case if $\alpha/v^{1/2} \ll r_s$ and $(c/a_x)^{1/2} v^{-1} \ll r_s \ll 1/v^{1/2}$. Formula (10) is applicable to the relativistic case if $c/\alpha v^{3/2} a_x \ll r_s \ll \alpha/v^{1/2}$. It is evident that the imposed conditions are less severe in the

relativistic quasi-two-dimensional case than they are in the three-dimensional relativistic case.

We note also the general trends common to the quasi-two-dimensional and three-dimensional cases. While the correlation energy is proportional to $n^{1/4}$ in the nonrelativistic case, it is proportional to $n^{1/d}$ in the relativistic case (d is dimensionality of the space where the electron motion is unbounded). The appearance of a logarithm, which plays the role of large parameter, in the expression for correlation energy is also typical of the latter case. This suggests that a similar behavior for the correlation energy of electron systems would be observed in all the cases outlined above.

APPENDIX

We consider the nonrelativistic case for simplicity. Then, proceeding from conventional diagram technique, we infer that a Fourier transform is possible along the x and y coordinates in the layer. In this case, if conditions (1) and (2) are met (i.e., the effect of excited states is ignored), the Green function has the form

$$G(p, z, z', \omega) = \sum_m \frac{\chi_m(z)\chi_m^*(z')}{\omega - E(p) - i\delta \text{sgn}(\omega - E(p))},$$

where $\chi_m(z)$ is the wave function of the ground state in the well with the coordinate cm .

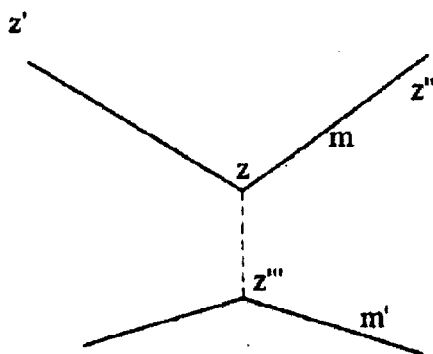


Fig. 1.

Let us consider the vertex shown in Fig. 1. Provided condition (4) is met, the integral with respect to z is of the form:

$$\int dz \sum_m \sum_n \chi_m(z)\chi_m^*(z')\chi_n(z'')\chi_n^*(z)\tilde{V}(z - z''') = \sum_m \chi_m(z''')\chi_m^*(z')\tilde{V}(cm - z'''),$$

where $\tilde{V}(z) = \iint dx dy e^{iq_x x + iq_y y} V(\vec{r}) = 2\pi e^2 e^{-\bar{q}|z|} / \epsilon \bar{q}$.

Thus, if we consider a loop of Green functions, all the Green functions in this loop will have the same index m . All the potentials originating from this loop will also have one index

equal to m , and the summation will be taken over m . In this context, the quantity m resembles a coordinate (however, it is discrete, rather than continuous). Applying the Fourier transform for this coordinate, we observe that the rules of the diagram technique remain unchanged for the new momentum. Thus, the two-dimensional Green functions, and, consequently, the polarization operator (7) and the Fourier transform of the potential according to (6) should be used in the resulting diagram technique. Using the above-mentioned rules of diagram technique, we obtain formula (5) for correlation energy.

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