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CORRELATION ENERGY OF HIGH-DENSITY ELECTRON GAS IN NARROW-GAP MULTIVALLEY SEMICONDUCTORS

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We calculate the correlation energy of high-density electron gas in narrow-gap multivalley semiconductors in the random-phase approximation. An analytical density dependence of the correlation energy, exact in a small parameter, is obtained in the model of strongly anisotropic semiconductor structures.

We consider an electron gas in narrow-gap multivalley semiconductors with the Dirac dependence of energy E on quasi-momentum k [1]

$$E(p) = \sqrt{k^2 s^2 + \Delta^2}, \tag{1}$$

where s is Kane's interband matrix element (the quasi-velocity of light) and Δ the halfwidth of the band gap. There are ν similar electronic and hole valleys in these semiconductors. and we therewith assume that $\nu >> 1$.

The approximation employed for strongly anisotropic wide-gap semiconductor structures (e.g.. see [2]) is applicable for calculating the correlation energy of the electron gas for a sufficiently high electron concentration n. Since $s << c$, where c is the velocity of light. we can neglect the Coulomb interaction retardation [3] and set $V(k) = 4\pi e^2/\epsilon k^2$, where ϵ is the permittivity now taken to be constant for brevity. Consistent inclusion of frequency dielectric dispersion was performed in [4, 5] and will be reproduced in the final formulas.

Under the specified assumptions, the expression for the correlation energy per electron is of the form ($\hbar = 1$) [2]

$$E_{corr} = \frac{1}{2n} \int \frac{d^3\vec{q}dq_4}{(2\pi)^4} \left\{ \ln(1 - \nu V(\tilde{q})\Pi_{44}(q)) + \nu V(\tilde{q})\Pi_{44}(q) \right\}, \tag{2}$$

where $q = (\vec{q}, q_4)$ and $\tilde{q} = |\vec{q}|$.

The polarization operator in (2) calculated in the lowest order in interaction takes into account the relationship between the correlation energy and the band gap width 2Δ [6]:

$$\Pi_{\mu\nu}(q) = is \int Sp\gamma_\mu G(p)\gamma_\nu G(p-q)(2\pi)^{-4} d^3\vec{p}dp_0, \tag{3}$$

where γ_μ are Dirac matrices.

The Green function $G(p)$ is of the form [6 - 8]

$$G(p) = \frac{1}{i}\frac{\Delta - is\hat{p}}{s^2p^2 + \Delta^2 - i0} - 2\pi\delta(s^2p^2 + \Delta^2)(\Delta - is\hat{p})N_p, \tag{4}$$

where $p = (\vec{p}, ip_0)$, $\hat{p} = p_i\gamma_i$, $p_4 = ip_0$, $N_p = \theta(\tilde{p} - p_F)\theta(p_0)$, $p_F = (3\pi^2 n/\nu)^{1/3}$ is the Fermi momentum, and $\theta(p_0) = \begin{cases} 1, & p_0 > 0 \\ 0, & p_0 \le 0. \end{cases}$

Here, the pseudoeuclidean metric with the fourth imaginary component is used. As is clear from (3) and (4), the polarization operator is of the form $\Pi_{\mu\nu}(q) = \Pi^0_{\mu\nu}(q) + \Pi^1_{\mu\nu}(q)$, where $\Pi^0_{\mu\nu}(q)$ is the vacuum polarization operator and $\Pi^1_{\mu\nu}(q)$ the part of the polarization operator dependent on the electron gas concentration.

The vacuum polarization operator contributes to a renormalization of the quantities ϵ, Δ, and s and the dispersion relation (1) [9]. Subsequently, we omit $\Pi^0_{\mu\nu}(q)$ and treat these quantities as renormalized (1). We also assume that the renormalized dispersion relation is of the Dirac form (1).

The polarization operator component of interest is

$$\Pi_{44}(q) = 16\int \frac{d^3\tilde{p}}{(2\pi)^3}\frac{\theta(\tilde{p} - p_F)}{2E(p)}\frac{(\tilde{q}\tilde{p})^2 - \tilde{q}^2\frac{E^2(p)}{s^2}}{(q^2)^2 - 4(pq)^2} - 16\pi^2 si\int \frac{d^4p}{(2\pi)^4}N_pN_{p-q}\delta(s^2p^2 + \Delta^2)\times$$
$$\times\delta(s^2(p-q)^2 + \Delta^2)\{2E^2(p) - 2E(p)q_0 s - pqs^2\}. \tag{5}$$

The first term in (5) makes the main contribution. It is easily seen that in the nonrelativistic case (i.e., for $\Delta >> sp_F$) we obtain, in the limiting case of interest $\tilde{q} >> p_F$, the known expression [2]

$$\nu\Pi_{44}(q)V(\tilde{q}) = -\frac{4\pi e^2 n}{\epsilon m}\frac{1}{\left(\frac{\tilde{q}^2}{2m}\right)^2 + q_4^2}, \tag{6}$$

($m = \Delta/s^2$ is the effective electron mass), which results in the characteristic density dependence of the correlation energy $E_{corr} \sim -n^{1/4}$ [2]. In the case of a narrow-gap multivalley semiconductor, i.e., in the limit of $p_F s >> \Delta$, considering that the main contribution to the correlation energy (2) is made by $\tilde{q} >> p_F$, from (5) we obtain that

$$\nu\Pi_{44}(q)V(\tilde{q}) = -\frac{q'^4}{q^4},\quad q' = [8\pi(3\pi^2)^{1/3}n^{4/3}\alpha^*/\nu^{1/3}]^{1/4} = \left(\frac{8}{3\pi}\right)^{1/4} p_F(\alpha^*\nu)^{1/4},$$

where α^* is the semiconductor analog of the fine structure constant ($\alpha^* = e^2/\epsilon s$). Notice that, by contrast to quantum electrodynamics where the fine structure constant $\alpha = e^2/c = 1/137$, it may not be very small for narrow-gap semiconductors [3].

Replacing the integration variable q by $x = q/q'$, we obtain for the correlation energy

$$E_{corr} = \frac{4(3\pi^2)^{1/3} n^{1/3} \alpha^*}{3\pi\nu^{1/3}} \int \frac{dx^4}{(2\pi)^4} \left\{ \ln\left(1 + \frac{1}{x^4}\right) - \frac{1}{x^4} \right\} \theta\left(x - \left[\frac{3\pi}{8\alpha^*\nu}\right]^{1/4}\right). \quad (7)$$

The integral (7) is easily calculated to give

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

where

$$E_x = me^4/\epsilon^2\hbar^2 \text{ and } a_x = \hbar^2\epsilon/me^2 \quad (9)$$

are the binding energy and the Bohr radius of the donor. In the opposite (nonrelativistic) case, ($\Delta >> sp_F$), from (2), with (6), we obtain

$$E_{corr} = -A E_x (n a_x^3)^{1/4}, \quad (10)$$

where $A = 16\pi^{3/4}/5\left[\Gamma\left(\frac{1}{4}\right)\right]^2 = 0.57$.

Now consider the effect of permittivity dispersion. It is well known that the permittivity in polar semiconductors, and in narrow-gap multivalley semiconductors of the group IV-VI in particular, has a strong frequency dispersion [4, 5], $\epsilon(\omega) = \epsilon_\infty \epsilon_0 (\omega_l^2 - \omega^2)/(\epsilon_\infty \omega_l^2 - \epsilon_0 \omega^2)$, where ω_l is the frequency of a longitudinal optical phonon, while ϵ_0 and ϵ_∞ are the static (for $\omega \to 0$) and high-frequency permittivity values (commonly, with $\epsilon_0/\epsilon_\infty >> 1$).

We should replace ϵ by ϵ_∞ in (8) and (9) because the frequencies much greater than ω_l make the main contribution to the correlation energy. Since the binding energy of the donor $E_x << \hbar\omega_l$, E_x, and the Bohr radius a_x (9) are determined by using ϵ_0, namely, $a_{x0} = \hbar^2\epsilon_0/me^2$ and $E_{x0} = me^4/\epsilon_0^2\hbar^2$. Hence, instead of (8) and (10), we obtain ($\alpha_\infty = e^2/\epsilon_\infty \hbar s$)

$$E_{corr} = -E_{x0}\frac{\epsilon_0}{\epsilon_\infty}\left(\frac{n a_{x0}^3}{\nu}\right)^{1/3} \frac{1}{8\pi^{7/3}3^{2/3}} \ln\left(\frac{8\alpha_\infty \nu}{3\pi}\right), \quad \frac{1}{\alpha_\infty} << \nu, \quad \Delta << sp_F.$$

$$E_{corr} = -A E_{x0}\left(\frac{n a_{x0}^3}{\nu}\right)^{1/4}\left(\frac{\epsilon_0}{\epsilon_\infty}\right)^{5/4}, \quad \nu >> 1, \quad \Delta >> sp_F.$$

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