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Exchange energy of a quasi-2D electron gas in a V-shaped potential

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Abstract. The Hartree–Fock formulae are evaluated for a model consisting of an uncompensated electron gas in an infinite V-shaped potential well. This contains a diverging electrostatic term. The elimination of this term is discussed on physical grounds, as is the relevance of such an extreme model. Similarities with and differences from the case of an infinite square well are discussed. The exchange energy is found to be always unimportant.

1. Introduction

In a homogeneous electron gas embedded in a uniform background of positive charge—the standard *jellium* model—local charge neutrality entails a cancellation of the electrostatic energy terms and then in the Hartree approximation the energy of the electron gas is purely kinetic. In mesoscopic semiconductor systems one encounters the problem of a confined quasi-2D electron gas which may present an entirely different situation, depending on how the electron gas has been produced. Consider the case of quantum wells. Different experimental techniques can be used to populate quantum wells (Jusserand *et al* 1989), among which the so called *modulation doping* is widely employed. This is illustrated in figure 1 (upper half). In this case the electron gas populating the well is not locally compensated by the positive charges of the ionized donors and thus we expect the Hartree energy to contain a significant electrostatic contribution. Various experimental techniques are used to probe the many-body interactions of a confined electron gas (Jusserand *et al* 1989, Delalande *et al* 1987, Pinczuk *et al* 1989, Levenson *et al* 1988). The lower part of figure 1 illustrates a similar system called δ -doping (Ploog 1987). All these cases have two basic features in common, namely: (i) while the system overall is electrically neutral, there is no local charge neutrality anywhere in the domain in which the electron gas is confined; (ii) the quasi-2D electron gas may occupy different subbands—shown as parabolae in figure 1—due to the quantization of the 1D motion.

Typical confinement distances are often in the range 100–300 Å and typical areal densities in the range 10^{10} – 10^{12} electrons cm^{-2} . Under these circumstances it is reasonable to enquire about many-body interactions, especially exchange, as one may expect these to be sensitive to the confinement which tends to prevent the electrons from keeping apart as freely as they can do in a 3D electron gas. Moreover, one may expect some significant consequences to follow when there are electrons populating

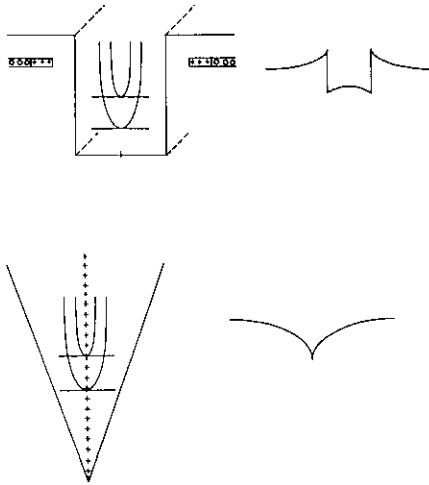


Figure 1. Upper half: modulation-doped quantum well. The barrier is doped with donors up to a distance (spacer layer) of the well. Positively ionized donors stay fixed in the barrier while the corresponding electrons *fall* into the well and constitute a quasi-2D electron gas with free motion parallel to the interfaces and quantized 1D motion perpendicular to these. Lower half: δ -doping system. A sheet of donors becomes ionized and the corresponding electrons become mobile in the 2D plane parallel to the impurity sheet while staying confined in the quantized 1D motion perpendicular to it. The corresponding self-consistent potential wells have the qualitative shape shown on the right.

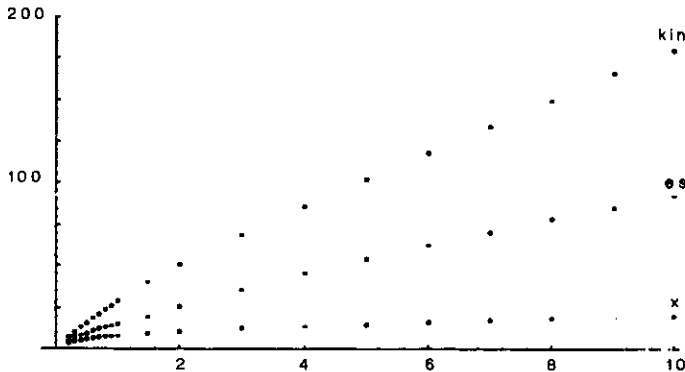


Figure 2. Absolute values of the kinetic, electrostatic and exchange energies per particle (in meV) versus N_s (in units of 10^{12} cm^{-2}) for the V-shaped well.

different subbands: if the electronic wavefunctions are orthogonal with respect to the coordinate of the 1D motion, then this allows for a greater overlap with respect to the other two in-plane coordinates, which tends to allow for a larger exchange interaction. Thus one may expect some differences between intra- and inter-subband terms.

A full self-consistent calculation can be rather elaborate or in any case numerically costly, but, at least up to exchange interactions, one can obtain a physical picture of the problem by adequate modelling of the confined electron gas and by then

evaluating explicitly the Hartree–Fock energy terms, which can be done directly and, for some models, can be formulated analytically down to the final stage of numerical evaluation. It is instructive to study such a model, which provides an insight into an interesting and otherwise complicated aspect of the physics of a confined electron gas.

The simplest way to model a quantum well is to consider a rectangular well with infinite potential barriers. For a given real well with finite barriers and a given ground-state energy E_0 —for the 1D motion—one can take an infinite square well a little wider, adjusting its width so as to reproduce the same ground level E_0 , and take this as an approximation to the real well. The electronic wavefunctions are then very simple and one can readily evaluate the Hartree–Fock terms, as was done by Glasser *et al* (1991). In the same spirit one can try to model the self-consistent well of the δ -doping case—bottom half of figure 1—by considering a somewhat wider V-shaped well with a linear potential growing to infinity. The electronic wavefunctions are then also known, as they are simply Airy functions and one can then proceed in the same manner.

The purpose of this paper is to discuss the V-shaped potential, herewith denoted V, and to compare it with the situation in the case of the square infinite well, henceforth denoted S. Section 2 sets out the problem in a general way and summarizes the main results for case S, while case V is discussed in section 3, where both cases are also compared.

2. General formulation and results for the infinite square well

The problem in general is defined as follows. We start from a given total population of N_s electrons cm^{-2} which are confined in 1D and have free motion in 2D with position vector ρ and wavevector κ . The electronic wavefunctions are of the form

$$\psi_{\nu\kappa}(r) = (1/\sqrt{A})e^{i\kappa\cdot\rho}\varphi_\nu(z) \quad (1)$$

where A is a normalization area and ν is the quantum number—subband index—associated with the quantization of the motion in 1D. The eigenvalues are

$$E_\nu(\kappa) = E_\nu(\kappa) = E_\nu + (\hbar^2/2m)\kappa^2 \quad (2)$$

and m can be regarded as an effective mass (which we comment on below). We take N_s as the fundamental parameter and study the kinetic, electrostatic and exchange energy of this electron gas, which we assume to be degenerate. In practice one can see from general statistical considerations (Arora 1982, Toda *et al* 1983) that in typical mesoscopic semiconductor systems the quasi-2D electron gas is degenerate up to $T = 77$ K and sometimes even more. It is important in the analysis to follow to keep track of all appropriate normalization factors and it may be in order to recall the general rule (Kittel 1963) that a sum over the spectrum means

$$\sum_\nu \sum_\kappa \rightarrow 2A \sum_\nu \int \frac{d^2\kappa}{(2\pi)^2}. \quad (3)$$

Thus, for instance, the total kinetic energy is

$$E_{\text{kin}} = 2A \sum_\nu \int \frac{d^2\kappa}{(2\pi)^2} E_\nu(\kappa) f_\nu(\kappa) \quad (4)$$

where f_ν —the degenerate Fermi–Dirac distribution function for each subband ν —cuts the 2D integration over κ when $E_\nu(\kappa)$ equals the Fermi energy E_F . This is determined by N_s in the following manner. The particle density is

$$n(z) = 2 \sum_\nu \int \frac{d^2\kappa}{(2\pi)^2} |\varphi_\nu(z)|^2 f_\nu(\kappa) \quad (5)$$

which contains E_F . The integral of $n(z)$ over z must equal the given areal density N_s and this determines E_F . Note the correct dimensions of (5) and (4) and note, in particular, the factor A in (4) which comes from (3) and guarantees the correct dimensions. We shall be interested in energies *per particle*. Since the number of particles in the normalization area is AN_s (a dimensionless number) the kinetic energy per particle is

$$\frac{2}{N_s} \sum_\nu \int \frac{d^2\kappa}{(2\pi)^2} E_\nu(\kappa) f_\nu(\kappa). \quad (6)$$

This pattern will hold for the other energies to be presently studied, but before proceeding a comment is required on the formula (5). If m is an effective mass different from the free electron mass m_0 , then $\psi_{\nu\kappa}(\mathbf{r})$ is *not a true electronic wavefunction* because it contains $\varphi_\nu(z)$ which is an *envelope function* and one must enquire whether it is correct to write down a formula for a physical quantity like (5) in terms of envelope functions. In this case, as in the rest of the formulae to be evaluated in this paper, it turns out that this can be justified (García-Moliner and Velasco 1992), though this cannot be taken as a general rule valid for any physical quantity. After this note of caution we shall proceed with the rest of the formulae in terms of wavefunctions $\psi_{\nu\kappa}(\mathbf{r})$ involving $\varphi_\nu(z)$ and we shall use (3) as explained. The introduction of a normalization area—which in the end we take in the limit $A \rightarrow \infty$ —can easily be avoided by normalizing the 2D plane waves in the δ function sense, in which case the amplitude factor is simply $(2\pi)^{-1/2}$ and there is no need for A to appear and then disappear in a formula like (6). However, the explicit introduction of a normalization area is very convenient in making visible an interesting point concerning the electrostatic energy:

$$E_{\text{es}} = \frac{4e^2}{\epsilon} \frac{1}{2} \sum_{\nu\nu'} \iint \frac{d^2\kappa}{(2\pi)^2} \frac{d^2\kappa'}{(2\pi)^2} \iint d^3\mathbf{r} d^3\mathbf{r}' \frac{|\psi_{\nu\kappa}(\mathbf{r})|^2 |\psi_{\nu'\kappa'}(\mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|}. \quad (7)$$

The factor 4 accounts for spin degeneracy, the factor $\frac{1}{2}$ ensures that we do not count each charge twice. We can conveniently rewrite this as an energy per particle in the form

$$\begin{aligned} \frac{E_{\text{es}}}{\text{Part}} &= \frac{e^2}{8\pi^4 \epsilon N_s} \sum_{\nu\nu'} \iint d^2\kappa d^2\kappa' f_\nu(\kappa) f_{\nu'}(\kappa') \\ &\quad \times \iint dz dz' |\varphi_\nu(z)|^2 |\varphi_{\nu'}(z')|^2 \frac{I(z - z')}{A} \end{aligned} \quad (8)$$

where

$$I(z - z') = \iint d^2\rho d^2\rho' 1/\sqrt{|\rho - \rho'|^2 + (z - z')^2}. \quad (9)$$

Put $A = \pi R^2$, so the limit $A \rightarrow \infty$ is also the limit $R \rightarrow \infty$. Then

$$\frac{I(z - z')}{A} = 2\pi R - 2\pi|z - z'|. \tag{10}$$

Now, in the limit $R \rightarrow \infty$ the first term on the RHS diverges. What does this mean? We have naïvely calculated the electrostatic energy of a system which is not electrically neutral. In the actual system the confined electron gas is locally uncompensated, but the entire system is altogether electrically neutral on account of the positive charges created when the donors are ionized and these charges enter explicitly the self-consistent calculation. We can model the confined electron gas by confining it with some model infinite barriers and this provides an *ad hoc* way of preventing the charged electron gas from blowing up, but we cannot ignore charge neutrality without obtaining a divergent term. This term is actually to be cancelled by the interaction with the positive charges, so the energy we really want to calculate is simply the finite term

$$\begin{aligned} \frac{E_{es}}{\text{Part}} = & -\frac{e^2}{4\pi^3\epsilon N_s} \sum_{\nu\nu'} \int \int d^2\kappa d^2\kappa' f_{\nu}(\kappa) f_{\nu'}(\kappa') \\ & \times \int \int dz dz' |\varphi_{\nu}(z)|^2 |\varphi_{\nu'}(z')|^2 |z - z'|. \end{aligned} \tag{11}$$

This was evaluated by Glasser *et al* (1991) by using an apparently quite different formula. It is very instructive to see the relationship between the two approaches.

We define for each subband ν the maximum value of $\kappa = \kappa_{F\nu}$ at which $E_{\nu}(\kappa_{F\nu})$ equals E_F . Then

$$\frac{E_{es}}{\text{Part}} = -\frac{e^2}{4\pi\epsilon N_s} \sum_{\nu\nu'} \kappa_{F\nu}^2 \kappa_{F\nu'}^2 \int \int dz dz' |\varphi_{\nu}(z)|^2 |\varphi_{\nu'}(z')|^2 |z - z'| \tag{12}$$

which, on account of (5), is

$$\frac{E_{es}}{\text{Part}} = -\frac{\pi e^2}{\epsilon N_s} \int dz n(z) \int dz' n(z') |z - z'|. \tag{13}$$

Now, the electrostatic *potential energy* drop multiplied by the electronic charge $-e$ satisfies the Poisson equation

$$d^2 V_{es}(z)/dz^2 = -(4\pi/\epsilon)e^2 n(z) \tag{14}$$

for which

$$V_{es}(z) = -\frac{2\pi e^2}{\epsilon} \int dz' n(z') |z - z'| \tag{15}$$

is the solution growing linearly according to

$$V_{es}(z) = -2\pi eQ|z|/\epsilon \quad Q = e \int dz' n(z') \tag{16}$$

for z asymptotically far away. Indeed, an electronic charge at a distance sufficiently large that $|z| \gg |z'|$ sees just the field created by a 2D sheet of charge density Q located at the origin. This is the meaning of (16). Then, returning to (13), we see that this is

$$\frac{E_{es}}{\text{Part}} = \frac{1}{2} \int dz n(z) V_{es}(z). \tag{17}$$

Thus, on neglecting—for the reason explained above—the divergent term of (7) we are left with just the electrostatic self-energy of the electronic charge distribution in its own electrostatic field, as one might have expected on intuitive grounds. This was the formula used by Glasser *et al* (1991).

The last term to study is the exchange energy.

$$\begin{aligned} \frac{E_x}{\text{Part}} = & -\frac{e^2}{8\epsilon\pi^4 A N_s} \sum_{\nu\nu'} \int \int d^2\kappa d^2\kappa' f_\nu(\kappa) f_{\nu'}(\kappa') \int \int \frac{d^3r d^3r'}{|r-r'|} \\ & \times e^{i(\kappa-\kappa')\cdot(\rho-\rho')} \varphi_\nu(z) \varphi_{\nu'}(z') \varphi_{\nu'}(z) \varphi_\nu(z'). \end{aligned} \tag{18}$$

Note the presence of a factor A in the denominator. But on performing the 2D integration over ρ and ρ' contained in the integration over r and r' we obtain, putting $q = \kappa - \kappa'$

$$\int \int \frac{d^2\rho d^2\rho'}{\sqrt{|\rho-\rho'|^2 + (z-z')^2}} e^{iq\cdot(\rho-\rho')} = \frac{2\pi A}{q} e^{-q|z-z'|}. \tag{19}$$

This contains a factor A which cancels that in the denominator, whence the finite result

$$\begin{aligned} \frac{E_x}{\text{Part}} = & -\frac{e^2}{4\pi\epsilon\pi^3 N_s} \sum_{\nu\nu'} \int \int \frac{d^2\kappa d^2q}{q} f_\nu(\kappa) f_{\nu'}(\kappa') \int \int dz dz' \\ & \times e^{-q|z-z'|} \varphi_\nu(z) \varphi_{\nu'}(z') \varphi_{\nu'}(z) \varphi_\nu(z'). \end{aligned} \tag{20}$$

The explicit evaluation of these energy terms depends on the eigenfunctions. For the S case these are simply

$$\varphi_\nu(z) = \sqrt{2/L} \sin(\nu\pi z/L) \tag{21}$$

where L is the width of the infinite square well, which is also the confinement length for the quasi-2D electron gas. We now summarize the main results found for this case (Glasser *et al* 1991). These depend on how many subbands are occupied and it suffices to consider just two subbands in order to see the parameters which characterize the system. For the first subband κ_{F1} is related to the areal density N_s by

$$\kappa_{F1} = \sqrt{2\pi N_s} \tag{22}$$

and hence we define

$$\alpha = 2\kappa_F L. \tag{23}$$

This is the essential dimensionless parameter which combines the values of N_s and L and characterizes each system. It is easily seen, for instance, that the threshold for the onset of the population of a second subband is not given by some value of N_s alone, but by the threshold value $\alpha_{th} = 2\pi\sqrt{3}$. Also, the ratio

$$\kappa_{F2}/\kappa_{F1} = \gamma = \sqrt{1 - 12\pi^2/\alpha^2} \tag{24}$$

depends on α . Then the results for the S case can be expressed in terms of the effective-mass ratio $\mu = m/m_0$ and of the Bohr radius $a_0 = \hbar^2/m_0e^2$. In the calculation of Glasser *et al* (1991) the origin of energies was taken to be the ground state E_0 of the lowest subband $\nu = 0$. The main results thus obtained (up to two populated subbands) were as follows.

Kinetic energy:

$$\left(\frac{E_{kin}}{Part}\right)_S = (\alpha^2 E_F / 16\pi L^2 N_s) \eta_{kin} \quad \eta_{kin} = 1 + \gamma^2(\gamma^2 + 24\pi^2/\alpha^2)\theta(\alpha - \alpha_{th}). \tag{25}$$

Electrostatic energy:

$$\left(\frac{E_{es}}{Part}\right)_S = -(\alpha^2 E_F / 16\pi L^2 N_s) \eta_{es}$$

$$\eta_{es} = 0.413(\mu/\epsilon)(L/a_0) [1 + \gamma^2 (1.460\gamma^2 + 2.613) \theta(\alpha - \alpha_{th})]. \tag{26}$$

Exchange energy:

$$\left(\frac{E_x}{Part}\right)_S = (E_F / 16\pi L^2 N_s)(\mu/\epsilon)(L/a_0) \eta_x \tag{27}$$

and η_x —a dimensionless number—is a function of α only which can be readily evaluated from (20) and (21). Numerical values of η_x are given in the paper of Glasser *et al* (1991).

The point is that the kinetic and electrostatic energies have opposite signs. Then the Hartree energy is

$$\left(\frac{E_H}{Part}\right)_A = (\alpha^2 E_F / 16\pi^2 L^2 N_s)(\eta_{kin} - \eta_{es}). \tag{28}$$

This is only an approximate model, but it does show that, depending on circumstances, we may expect a tendency to cancellation of the two terms in E_H . Note that

$$L_c = \epsilon a_0 / 0.413\mu \tag{29}$$

has dimensions of length and the cancellation of η_{kin} and η_{es} takes place for

$$(L/L_c) = [1 + \gamma^2(\gamma^2 + 24\pi^2/\alpha^2)\theta(\alpha - \alpha_{th})] / [1 + \gamma^2(1.460\gamma^2 + 2.613)\theta(\alpha - \alpha_{th})] \tag{30}$$

while the exchange energy increases monotonically with increasing population. Thus there is a tendency to enhancement of the importance of the exchange energy relative to the Hartree energy. For low populations—only one occupied subband—the cancellation of η_{kin} and η_{es} occurs in this model when L equals the critical length L_c . For a material like GaAs this is about 239 Å, which is in the range of typical experimental values.

With all the limitations of a crude model, this analysis focuses on the key parameters which determine the physical situation. This is mostly the combination of L and N_s embodied in α and partly also L alone. Furthermore, in practical calculations the carriers are sometimes assumed to be all in the lowest subband and even in the ground state $\kappa = 0$, on the grounds that this does not change the main statistical result like the relationship between κ_F and N_s . However, it may affect the actual evaluation of the energy terms. This issue can also easily be studied within this model and one can see that this approximation may be significantly unjustified in some situations (Glasser *et al* 1991).

3. The V-shaped potential

It is now interesting to make a similar analysis for the V case. We consider a 1D Schrödinger equation of the form

$$-(\hbar^2/2m)\varphi''(z) + (eFz - E)\varphi(z) = 0. \quad (31)$$

The linear potential is supposed to model the field created by a sheet of N_s donors cm^{-2} (figure 1, bottom right), so $F = 2\pi N_s/\epsilon$. This bears the same relation to the real system as the infinite square well does to the well of figure 1, top right. As in that case, F could be interpreted as an equivalent value, somewhat *smaller* than the actual F , so as to make the infinite V-shaped well a little wider. Note that N_s is also the areal concentration of 2D free electrons in the well. The analysis runs in the same way and we expect it to produce similar results but in terms of suitable parameters which ought to be different. The identification of these parameters can be guessed on intuitive grounds. Firstly, by inspection of (29) we expect the combination

$$\ell = \epsilon a_0/\mu \quad (32)$$

to represent some characteristic length of the host material. The precise numerical factor appearing in (29) is a result of the rectangular geometry and there is no reason why this should have any relevance in the V case, but ℓ pertains to the background material, and we expect it to be a significant parameter. Secondly, it is well known (Abramowitz and Stegun 1966) that (31) is transformed into the Airy differential equation by a change of variable

$$\xi = (z - \beta)/\lambda \quad \beta = E/eF \quad \lambda = (\hbar^2/2m\epsilon F)^{1/3} \quad (33)$$

whereupon the wavefunction $\varphi(z)$ becomes a function $\Phi(\xi)$ which satisfies the Airy equation

$$\Phi''(\xi) - \xi\Phi(\xi) = 0. \quad (34)$$

This introduces another parameter λ with dimensions of length, which is obviously related to the effective width of the well and we may expect this to be the analogue of L in the S case, so we now define

$$\alpha = 2\kappa_F \lambda \tag{35}$$

and expect this dimensionless parameter to characterize the situation as the α defined in (23) does for the S case.

Each eigenstate corresponds to a quantized value E_ν of E , whence β_ν and ξ_ν . On the other hand all quantized state amplitudes must vanish at infinity and this rules out the Bi function, and thus leaving us with solutions of the form

$$\Phi(\xi) = CAi(\xi). \tag{36}$$

Put

$$\zeta_\nu = \xi_\nu(z = 0) = -\beta_\nu/\lambda. \tag{37}$$

Then

$$\varphi'(\zeta_\nu) = 0 \text{ (even states)} \quad \varphi(\zeta_\nu) = 0 \text{ (odd states)}. \tag{38}$$

This yields the eigenvalues, for which from the book of Abramowitz and Stegun (1966) one can obtain analytical approximations which are actually rather accurate in practice:

$$\begin{aligned} E_\nu &\simeq \lambda e F(\frac{3}{8}\pi)(4\nu - 3)^{2/3} [1 + \frac{7}{48}(4\nu - 3)^{-2}] - E_r \\ E_\nu &\simeq \lambda e F(\frac{3}{8}\pi)(4\nu - 1)^{2/3} \{1 + \frac{5}{48}[(\frac{3}{8}\pi)(4\nu - 1)^{-2}]\} - E_r \end{aligned} \tag{39}$$

where

$$E_r = a^{1/3} [1 + \frac{7}{432}]. \tag{40}$$

This sets the reference level to give $E_0 = 0$, consistently with the convention set out in section 2.

From the normalization condition

$$2 \int_0^\infty \varphi^2(\xi) dz = 2\lambda C^2 \int_{-\zeta}^\infty Ai^2(\xi) d\xi = 1 \tag{41}$$

we find the normalized eigenfunctions

$$\begin{aligned} \Phi_\nu &= (1/2\lambda)^{1/2} B_\nu^{1/2} Ai(\xi_\nu) \\ B_\nu &= \begin{cases} [-\zeta_\nu Ai^2(\zeta_\nu)]^{-1} & (\nu \text{ even}) \\ [Ai'(\zeta_\nu)]^{-2} & (\nu \text{ odd}). \end{cases} \end{aligned} \tag{42}$$

The various energy terms can now be obtained by following the same general pattern. Before proceeding we note that the results (25)–(27) given by Glasser *et al* (1991) contain a factor $\alpha^2/16\pi L^2 N_s$. It is easily seen by using the definition (23)

and the general statistical formula (22) that this factor is simply equal to $\frac{1}{2}$. Then, remembering the definitions (29) and (32), the main results (25)–(27) for the S case, when only one subband is occupied, can be written as

$$\begin{aligned} \left(\frac{E_{\text{kin}}}{\text{Part}}\right)_S &= \frac{1}{2} E_F \\ \left(\frac{E_{\text{es}}}{\text{Part}}\right)_S &= -\frac{1}{2} E_F \times 0.429 L/\ell \\ \left(\frac{E_x}{\text{Part}}\right)_S &= \frac{1}{2} E_F \times 0.429(L/\ell) \alpha \eta_x. \end{aligned} \quad (43)$$

In order to compare the two cases (S and V) it suffices to look at the situation when only one subband is occupied. A direct numerical comparison is difficult and might not be clear. For the S case there are the two independent input parameters N_s and L , the latter determining the electron wavefunction confinement. For the V case there is only one input parameter (N_s) which determines the value of λ . This plays a role which is formally analogous to that of L , but the resulting wavefunction confinement bears no relation to the one due to any given value of L in the S case. Thus only a qualitative comparison of the main trends and key features of the results is fully realizable. The main results obtained in the present analysis under these conditions are as follows.

For the kinetic energy

$$\left(\frac{E_{\text{kin}}}{\text{Part}}\right)_V = \frac{1}{2} E_F \quad (44)$$

just as in the S case. Indeed, with the energy reference level taken at E_0 and only one occupied subband the only kinetic energy we are counting is that of the in-plane motion. With a parabolic dispersion law the mean kinetic energy in 2D for a degenerate electron gas is precisely $E_F/2$ and this does not depend at all on the shape of the confining well in 1D.

For the electrostatic energy we obtain

$$\left(\frac{E_{\text{es}}}{\text{Part}}\right)_V = \frac{1}{2} E_F \left[\frac{1.500}{\text{Ai}^2(\zeta_0)} \int_{-\zeta_0}^{\infty} \text{Ai}^2(\xi) d\xi \right] \frac{\lambda}{\ell} \quad (45)$$

and for the exchange energy

$$\left(\frac{E_x}{\text{Part}}\right)_V = \frac{1}{2} E_F \times 0.318(\lambda/\ell) \alpha (\eta_x)_V \quad (46)$$

where $(\eta_x)_V$ is a dimensionless number which can be calculated from (20) by means of the wavefunctions (42), much as the η_x appearing in the S case (27) is calculated from (20) but with the wavefunctions (21).

These results can be compared with those for the S case given in (43). The formulae have the same structure and corroborate that, as expected on intuitive grounds, λ is indeed a kind of confining length playing the role analogous to the

width L of the square well. Like L , λ is also a parameter determined by the composition of the sample, as F is determined by the areal density N_s .

However, while the formulae have the same structure the physical situation actually differs significantly for each case. Figure 2 shows the absolute values of the mean energies (kinetic, electrostatic and exchange) as functions of N_s . The onset for the population of a second subband is at a value N_0 of $N_s = 1.47 \times 10^{12}$ electrons cm^{-2} . No matter how much N_s increases only two subbands are populated. This is because the effective confining length

$$\lambda = (\epsilon \hbar^2 / 4\pi m e N_s)^{1/2} \quad (47)$$

decreases as N_s increases and, although E_F also increases, the higher level E_3 increases faster so as to stay above E_F . The kinetic energy increases at first linearly with N_s , as is obvious from (43) and from the fact that E_F is proportional to N_s (22). On going beyond the threshold N_0 some of the electrons populate states where κ starts from zero again, and the rate of increase of $(E_{\text{kin}}/\text{Part})$ is somewhat reduced, but continues to increase. The electrostatic energy has a lower rate of increase everywhere. This is easily understood for the low N_s range from (45). As N_s increases, λ decreases, although this decrease is compensated for by the factor preceding (λ/ℓ) which altogether determines an increase in magnitude of $(E_{\text{es}}/\text{Part})$ with increasing N_s , but at much reduced rate. The same trend is maintained for all N_s . The result is that the two energies differ in magnitude by an increasing amount, while (E_x/Part) turns out to increase so slowly that it practically levels off. Altogether the ratio $E_x/(E_{\text{kin}} + E_{\text{es}})$ decreases with increasing N_s , so we expect the Hartree approximation to be quite appropriate in this case.

These results cannot, of course, be taken literally, since the infinite V-shaped well is merely a crude model. The main difference with a real self-consistent potential well is that in the latter the electrostatic potential levels off, the higher excited states form a sequence with an accumulation point, as in the hydrogenic sequence, and in fact three and almost four subbands are often populated in actual experimental samples. However, the strong tendency exhibited by this simple model does suggest that we should expect the Hartree approximation to work well for δ -doping systems, as indeed seems to be the case in practice under typical experimental conditions (Koenraad *et al* 1990). On the other hand it is very instructive to compare the S and V cases, to identify the key parameters which play equivalent roles and to see the similarities and the differences between the two cases.

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References

- Abramowitz M and Stegun I A (ed) 1966 *Handbook of Mathematical Functions (Applied Mathematics Series 55)* (Washington, DC: National Bureau of Standards)

Arora V K 1982 *Phys. Rev. B* **26** 2247

Delalande C, Bastard G, Orgonasi J, Brum J A, Lin H W and Voos M 1987 *Phys. Rev. Lett.* **23** 2690

García-Moliner F and Velasco V R 1992 *Theory of Single and Multiple Interfaces* (Singapore: World Scientific)

Glasser M L, García-Moliner F and Velasco V R 1991 *Plasma Sources* **43** 512

Jusserand B, Brum J A, Gardin D, Liu H W, Weimann G and Schlapp W 1989 *Phys. Rev. B* **40** 4220

Kittel C 1963 *Quantum Theory of Solids* (New York: Wiley)

Koenraad P *et al* (unpublished work) Reference 17 of Ioratti L 1990 *Phys. Rev. B* **41** 8340

Levenson J A, Abram I, Raj R, Dolique G, Oudar J L and Alexandre F 1988 *Phys. Rev. B* **38** 1443

Pinczuk A, Smitt-Rink S, Danan G, Valladares J P, Pfeiffer L N and West K W 1989 *Phys. Rev. Lett.* **63** 1633

Ploog K 1987 *J. Crystal Growth* **81** 304

Toda M, Kubo R and Saito N 1983 *Statistical Physics I* (*Springer Series in Solid State Sciences*) (Heidelberg: Springer)