Novel properties of the Kohn-Sham exchange potential for open systems: application to the two-dimensional electron gas

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Abstract. – The properties of the Kohn-Sham (KS) exchange potential for open systems in thermodynamical equilibrium, where the number of particles is non-conserved, are analyzed with the Optimized Effective Potential (OEP) method of Density Functional Theory (DFT) at zero temperature. The quasi two-dimensional electron gas (2DEG) is used as an illustrative example. The main findings are that the KS exchange potential builds a significant barrier-like structure under slight population of the second subband, and that both the asymptotic value of the KS exchange potential and the inter-subband energy jump discontinuously at the one-subband (1S) → two-subband (2S) transition. The results obtained in this system offer new insights on open problems of semiconductors, such as the band-gap underestimation and the band-gap renormalization by photo-excited carriers.

Density Functional Theory (DFT) has become a most used computational tool in the study of strongly inhomogeneous interacting systems such as atoms, molecules, clusters, and solids. [1] A crucial step for any DFT calculation is the approximation used to evaluate the exchange-correlation (xc) contribution \( E_{xc} \equiv E_x + E_c \) to the total energy. Traditionally, \( E_{xc} \) has been evaluated by using density-dependent xc-functionals, either of local (LDA) or semi-local (GGA, meta-GGA,...) character. [2] In the last few years, however, considerable interest has arisen around orbital-dependent xc functionals, which are implicit functionals of the density and whose implementation in the KS scheme is known as the OEP method. [3] If the Hartree-Fock expression for the exchange energy functional is used, and \( E_c \) is neglected, the OEP method is equivalent to the exact x-only implementation of KS theory. [4] Several advantages are associated to the use of exact x-only DFT calculations for (closed) systems with a fixed number of particles: cancellation of the spurious Hartree self-interaction energy, [5] correct high-density limit, [2] great improvement in the KS eigenvalue spectrum, [6] semiconductor band structure and excitations, [7] and nonlinear optical properties. [8] It is the aim of this work to report on further novel features of the OEP scheme for open configurations where the system under study is in thermodynamical equilibrium with a reservoir and can exchange

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particles with it, using a quasi-two-dimensional electron gas at zero temperature to illustrate our results. We compare usual approximations against our exact (OEP) x-only results.

The present theory can be applied to any system with translational symmetry in a plane. For instance, a semiconductor modulation-doped quantum well (QW) grown epitaxially as shown in the inset of Fig. 1. In these systems, it is possible to confine an electron gas by changing the semiconductor in the growth direction \( z \). If the larger gap semiconductor is doped with donors, it provides electrons to the trap formed by the smaller gap semiconductor, until the charge-transfer field equilibrates the common chemical potential \( \mu \) in the QW and a doped region acting as particle reservoir. The charge transferred from the reservoir to the QW can be tuned by an external electric field. Assuming translational symmetry of the 2DEG in the \( x-y \) plane (area \( A \)), and proposing accordingly a solution of the type \( \phi_{\mathbf{k}\mathbf\sigma}(\mathbf{r}, z) = \exp(i \mathbf{k} \cdot \mathbf{r}) \xi_{\mathbf{k}\sigma}(z) / \sqrt{A} \), the ground-state electron density can be obtained by solving a set of effective one-dimensional Kohn-Sham equations of the form

\[
\hat{h}_{K-S}^{\mathbf{k}\sigma}(z) \xi_{\mathbf{k}\sigma}^\sigma(z) = \left[ -\frac{\partial^2}{2\partial z^2} + V_{K-S}^{\mathbf{k}\sigma}(z) - \varepsilon_{\mathbf{k}\sigma}^\sigma \right] \xi_{\mathbf{k}\sigma}^\sigma(z) = 0, \tag{1}
\]

where effective atomic units have been used. \( \xi_{\mathbf{k}\sigma}^\sigma(z) \) is the eigenfunction for electrons in subband \( i (= 0, 1, \ldots) \), spin \( \sigma (= \uparrow, \downarrow) \), and eigenvalue \( \varepsilon_{\mathbf{k}\sigma}^\sigma \). The local (multiplicative) Kohn-Sham potential \( V_{K-S}^{\mathbf{k}\sigma}(z) \) is the sum of several terms: \( V_{K-S}^{\mathbf{k}\sigma}(z) = V_{\text{ext}}(z) + V_{\text{H}}(z) + V_{\text{xc}}^{\mathbf{k}\sigma}(z) \). \( V_{\text{ext}}(z) \) is given by the sum of the epitaxial potential plus an external electric field. \( V_{\text{H}}(z) \) is the Hartree potential. Within DFT, \( V_{\text{xc}}^{\mathbf{k}\sigma}(z) = \delta E_{\text{xc}} / \delta n_{\mathbf{k}\sigma}(z) \). In an open system, \( E_{\text{xc}} = E_{\text{xc}}[\{\xi_{\mathbf{k}\sigma}^\sigma(z)\}, \{\varepsilon_{\mathbf{k}\sigma}^\sigma(z)\}] \) is a functional of the set of \( \varepsilon_{\mathbf{k}\sigma}^\sigma \)'s and \( \xi_{\mathbf{k}\sigma}^\sigma \)'s. The zero-temperature 3D electron density is

\[
n_{\mathbf{k}\sigma}(z) = \sum_{\xi_{\mathbf{k}\sigma}^\sigma < \mu} (k_{\mathbf{k}p})^2 |\xi_{\mathbf{k}\sigma}^\sigma(z)|^2 / 4\pi, \tag{2}
\]

with \( k_{\mathbf{k}p} = \sqrt{2(\mu - \varepsilon_{\mathbf{k}\sigma}^\sigma)} \). After some lengthy but standard manipulations of the OEP scheme, \( [3, 9] \) the calculation of \( V_{\text{xc}}^{\mathbf{k}\sigma}(z) \) for an open system can be summarized in the following set of equations:

\[
\sum_{i} \text{occ.} \text{s} S_{i\sigma}(z) = 0, \tag{2}
\]

\[
S_{i\sigma}(z) = (k_{\mathbf{k}p})^2 \psi_{\mathbf{k}\sigma}^\sigma(z)^* \varepsilon_{\mathbf{k}\sigma}^\sigma - C_{\mathbf{k}\sigma}^{\mathbf{k}\sigma}(z) |\xi_{\mathbf{k}\sigma}^\sigma(z)|^2 + c.c., \tag{3}
\]

\[
\psi_{\mathbf{k}\sigma}^\sigma(z) = \sum_{i \neq i'} \frac{\xi_{\mathbf{k}\sigma}^\sigma(z')}{\varepsilon_{\mathbf{k}\sigma}^\sigma(z') - \varepsilon_{\mathbf{k}\sigma}^\sigma(z)} \int dz' \xi_{\mathbf{k}\sigma}^\sigma(z')^* \Delta V_{\text{xc}}^{\mathbf{k}\sigma}(z') \xi_{\mathbf{k}\sigma}^\sigma(z'). \tag{4}
\]

The sum in Eq. (2) runs over the occupied subbands, \( C_{\mathbf{k}\sigma}^{\mathbf{k}\sigma}(z) = V_{\text{xc}}^{\mathbf{k}\sigma}(z) + (2\pi / A) \partial E_{\text{xc}} / \partial \varepsilon_{\mathbf{k}\sigma}^\sigma \), \( \Delta V_{\text{xc}}^{\mathbf{k}\sigma}(z) = V_{\text{xc}}^{\mathbf{k}\sigma}(z) - u_{\mathbf{k}\sigma}^{\mathbf{k}\sigma}(z) \), \( u_{\mathbf{k}\sigma}^{\mathbf{k}\sigma}(z) = 4\pi / A (k_{\mathbf{k}p})^2 \xi_{\mathbf{k}\sigma}^\sigma(z)^* \delta E_{\text{xc}} / \delta \varepsilon_{\mathbf{k}\sigma}^\sigma(z) \), and mean values are defined as

\[
\langle \mathcal{O} \rangle = \int dz \xi_{\mathbf{k}\sigma}^\sigma(z)^* \mathcal{O}(z) \xi_{\mathbf{k}\sigma}^\sigma(z). \tag{6}
\]

Eqs. (4) determine the local \( V_{\text{xc}}^{\mathbf{k}\sigma}(z) \) corresponding to an orbital and eigenvalue-dependent approximation for \( E_{\text{xc}} \). Eqs. (4) and (2) have to be solved self-consistently.

Some comments are necessary here: \( a) \) Our treatment corresponds to an open system, and this is the origin of the term \( V_{\text{xc}}^{\mathbf{k}\sigma}(z) \) in \( \langle \mathcal{O} \rangle \) on the r.h.s. of Eq. (3). This term gives a finite (\( \neq 0 \)) contribution under the replacement \( V_{\text{xc}}^{\mathbf{k}\sigma}(z) \rightarrow V_{\text{xc}}^{\mathbf{k}\sigma}(z) + \alpha^\sigma \), with \( \alpha^\sigma \) an arbitrary constant. As a consequence Eq. (2) is not invariant if \( V_{\text{xc}}^{\mathbf{k}\sigma}(z) \) is shifted by a constant, and \( V_{\text{xc}}^{\mathbf{k}\sigma}(z) \) is strictly determined. For closed systems, this term is absent and the corresponding OEP expression gives \( V_{\text{xc}}^{\mathbf{k}\sigma}(z) \) up to an additive constant. \( [3] \) \( b) \) Using Eq. (3) it can be found that the \( \psi_{\mathbf{k}\sigma}^\sigma(z) \) (denoted as “shifts”) satisfy the orthogonality constraint \( \int dz \xi_{\mathbf{k}\sigma}^\sigma(z)^* \psi_{\mathbf{k}\sigma}^\sigma(z) = 0 \). Application of \( \hat{h}_{K-S}^{\mathbf{k}\sigma}(z) \) to the \( \psi_{\mathbf{k}\sigma}^\sigma(z) \) in Eq. (1) yields an inhomogeneous differential equation, which can be considered as an alternative definition of the shifts. \( [10, 11] \) \( c) \) Integrating Eq. (2) and using the orthogonality constraint, we obtain the important property \( \sum_{i} \text{occ.} C_{\mathbf{k}\sigma}^{\mathbf{k}\sigma}(z) = 0 \).
Consequently, all that for \( z \) in Fig. 2. The top panel corresponds to the inter-subband energy \( \varepsilon \) given until this point include both exchange and correlation. In the open case to find a self-consistent solution of Eq. (1) with \( \rho = 1 \). Using Eqs. (1) and (2), and dropping spin indices by assuming a paramagnetic situation, \( V_{xc}(z) \) could be formally expressed for real \( \xi_i(z) \)'s (as is our case) as

\[
V_{xc1}(z) = \sum_i^{\text{occ.}} \frac{k_i^2 \xi_i(z)}{2\pi n(z)} \left[ u_i^1(z) + \Delta \mathbf{A}_{xc}^1 \right],
\]

\[
V_{xc2}(z) = \sum_i^{\text{occ.}} \frac{(k_i^2)^2 S_i(z)}{[2\pi n(z)]},
\]

\[
V_{xc3}(z) = \sum_i^{\text{occ.}} \frac{(k_i^2)^2 \psi_i'(z) \xi_i'(z) - C_{xc}^i \xi_i'(z)^2}{2\pi n(z)},
\]

with primes denoting derivation with respect to \( z \). It can be shown that if the shifts in \( V_{xc}(z) \) are forced to be zero, the only term left is \( V_{xc1}(z) \). This truncated expression for \( V_{xc}(z) \) is identical to the one obtained in Ref. [12] for closed systems (KLI approximation). Accordingly, we identify here that \( V_{xc}^{KLI}(z) \equiv V_{xc1}(z) \). In the 1S regime \( V_{xc2}(z) = V_{xc3}(z) \equiv 0 \) [13] and \( V_{xc}^{(1S)}(z) = V_{xc}^{KLI}(z) \). A KLI calculation in the many-subband situation, requires in our open case to find a self-consistent solution of Eq. 1 with \( V_{xc}(z) = V_{xc1}(z) \), constrained by the exact condition \( \sum_i^{\text{occ.}} C_{xc}^i = 0 \). This procedure univocally determines \( V_{xc1}(z) \). It is important to realize however, that what we call KLI approximation is not the same as previously considered [12]. While the expressions for \( V_{xc}^{KLI} \) are identical in both cases, the boundary conditions are different. In our case, we use \( \sum_i^{\text{occ.}} C_{xc}^i = 0 \). In previous studies, the physical boundary condition \( \mathbf{V}_{xc} = \mathbf{v}_{xc}^{\text{macro}} \) was imposed in order to satisfy the correct asymptotic behavior (\( m \) denoting the index of the highest-occupied subband). All results given until this point include both exchange and correlation. In the \( x \)-only version of the OEP method, \( V_{xc} \to V_x \) [6, 11, 12]

We plot in Fig. 1 the \( x \)-only OEP for several fillings. It is noticeable the large difference for \( V_x(z) \) as calculated for \( \Delta = \mu - z \to 0^- \) (A) or \( \Delta \to 0^+ \) (B), as well as the “hump” that \( V_x(z) \) develops for incipient population of the second subband, and the fast decay of this “hump” after macroscopic occupation of the band (C).

The \( x \)-only eigenvalue spectra, in the neighborhood of the 1S \( \to \) 2S transition, is shown in Fig. 2. The top panel corresponds to the inter-subband energy \( \epsilon_{01} \equiv \epsilon_1 - \epsilon_0 \) calculated in three different ways: OEP, KLI and LDA. The lower panel displays the asymptotic values of the \( x \)-only potential. We notice an abrupt increase of \( \epsilon_{01}^{\text{OEP}} \) when the system passes from the 1S to the 2S regime. This should be contrasted with the abrupt decrease of \( \epsilon_{01}^{\text{KLI}} \), and the continuity of \( \epsilon_{01}^{\text{LDA}} \). Also noticeable is the abrupt jump of \( V_x(z) \to \infty \) in OEP and KLI at \( \Delta = 0 \).

In what follows we will provide a brief explanation for each of the striking results shown in previous figures. We start with the asymptotic behavior of \( V_x(z) \), for the many-subband case \( m > 1 \). Following the analysis of Ref. [13], and based on the fact that \( \xi_i(z \to \infty) \to e^{-\beta_i z} \) (disregarding factors involving powers of \( z \)) with \( \beta_i > 0 \) and \( \beta_i < \beta_j \) if \( \epsilon_i > \epsilon_j \), one can derive from the asymptotic limit of the differential equation for the shifts that \( \psi_{i<m}(z \to \infty) \to e^{-\beta_m z} \). From the asymptotic analysis of Eq. (2), we obtain \( \psi_{m}(z \to \infty) \to [C_{xc}^m/(k_F^m)^2] e^{-\beta_m z} \). Consequently, all the shifts corresponding to occupied subbands decay exponentially at the same rate. Inserting this result in the asymptotic expression for \( V_x(z) \), which amounts to restrict the sum over the occupied subbands to the last one \( (i = m) \), it can be checked that \( V_{x2}(z) \) and \( V_{x3}(z) \) vanish to leading order, while the contribution from \( V_{x1}(z) \) remains finite,
Fig. 1 – Thin lines: exchange-only OEP for \( \Delta = -0.1(A), 0.01(B), 0.1, 0.3 \) and 10 meV (C). Thick line: \( V_{x2}(z) \) in the limit \( \varepsilon_1 \to 0^+ \) (see text below). The arrows on the right denote the asymptotic value of the exchange potential for selected subband fillings. Inset: schematic view of our model for the modulation-doped QW. The thick vertical stripe on the left represents the ionized donor impurities region. The thin vertical line on the right represents a distant metallic plane which induces a charge-transfer field along \( z \) included in \( V_{ext}(z) \). If the metallic plate is positively (negatively) charged more (less) electrons are transferred towards the well.

Fig. 2 – Exchange-only energy spectra by different methods. Top panel: inter-subband energy spacing \( \varepsilon_{01} \) and \( \mu - \varepsilon_0 \). Lower panel: asymptotic value of the exchange potential \( V_x(z \to \infty) = \Delta V_\text{x}^0 \) (see Eq. (8)). The KLI approximation coincides with the exact result (OEP) in the 1S regime. Open circles: same as above, but including correlation \textit{a la} LDA.
\[ V_x(z \to \infty) \to V_{x1}(z \to \infty) \to u^m_x(z \to \infty) + \Delta V^m_x, \]  

where \( u^m_x(z \to \infty) \to -1/z \). \[15\] Eq. \[5\] coincides with the asymptotic result found in standard applications of the OEP method to closed systems. \[3\] In such a case, as discussed above, \( V_x(z) \) is determined up to an additive constant, which is fixed arbitrarily choosing \( \Delta V^m_x = 0 \). In our open configuration, however, the constant is automatically generated by the self-consistent solution of Eqs. \[1\] - \[2\]. Remembering that \( \Delta V^m_x = V^m_x - \Pi^m_x \), we have no reason to expect a smooth change in the value of the asymptotic constant at the \( 1S \to 2S \) transition. This explains the abrupt jump at \( \Delta = 0 \) in Fig. \[2\]. The KLI approximation preserves this jump in \( \Delta V^m_x \), but fails quantitatively, giving a jump a 23 % larger than the exact one. \( V^LDA_x(z \to \infty) \) is concentrated, it affects mainly the electrons in the second subband, resulting in an increase of the inter-subband spacing \( \varepsilon_{xc} \) as the number of electrons is allowed to vary from \( N \) to \( N + \delta \) where \( \delta \) is a positive infinitesimal. This non-analytic behavior of \( V_{xc} \) leads in turn to discontinuities on the \( N \)-dependence of the eigenvalues, which

\[ V_{xc}(z \to \infty) \to V_{xc1}(z \to \infty) \to u^m_{xc}(z \to \infty) + \Delta \varepsilon_{xc} \]

Let us concentrate now on the the “hump” effect observed in Fig. \[1\]. This effect is due to the contribution \( V_{xc2}(z) \) in \( V_{xc}(z) \). To see this, let us analyze \( V_{xc2}(z) \) in the limit \( k_{F}^2 \to 0^+ \). In this almost depleted \( 2S \) regime, we can approximate \( V_{xc2}(z) \approx C^0_{xc} - (k_{F}^2)^2 \psi_0(z)/\xi_0(z) \). Using \( S_0(z) + S_1(z) = 0 \), and \( C^0_{xc} + C^1_{xc} = 0 \), we find that \( \psi_0(z) \approx C^0_{xc} \xi_0(z)^2 - \xi_1(z)^2 \)/\xi_0(z)(k_{F}^2)^2 \). Replacing \( \psi_0(z) \) in the latter expression for \( V_{xc2}(z) \), we obtain \( V_{xc2}(z) \approx C^0_{xc} [\xi_1(z)/\xi_0(z)]^2 \).

We plot this approximation for \( V_{xc2}(z) \) in Fig. \[1\] (thick line), showing that it is the “limiting” value of the full \( V_{xc}(z) \) if \( \Delta \to 0^+ \) in the region where the ratio \( \xi_1(z)/\xi_0(z) \) is large, excluding the asymptotic region, which is dominated by \( V_{x1}(z) \). Since \( V_{xc2} \) and \( V_{xc3} \) are neglected in the KLI approximation (as defined above), the “hump” effect is also lost. From this point of view, our KLI is not a good approximation for slight occupancies of excited subbands.

To further clarify the role played by the different contributions to the \( x \)-only OEP, we display them in Fig. \[3\]. It is clear from this figure that the “hump” effect is due to \( V_{xc2}(z) \), while \( V_{x1}(z) \) dominates in the high-density region and gives also the main contribution to \( V_{xc}(z) \) in the asymptotic region, according to the result of Eq. \[8\]. The contribution from \( V_{x3}(z) \) has been found to be small in all the analyzed situations.

The building of this significant barrier explains, in turn, the abrupt increase of \( \varepsilon_{01}^{OEP} \) under second subband occupation: as the barrier lies about the same zone where the weight of \( \xi_1(z) \) is concentrated, it affects mainly the electrons in the second subband, resulting in an increase of the inter-subband spacing \( \varepsilon_{01}^{OEP} \). However this increase is the result of two opposite contributions: the barrier building, which tends to increase \( \varepsilon_{01}^{OEP} \), and the abrupt jump in the value of \( V_{x}(z \to \infty) \), which tends to decrease \( \varepsilon_{01}^{OEP} \). \[16\] The fact that the sum of the two contributions result in a net increase of \( \varepsilon_{01}^{OEP} \), implies that the repulsive barrier effect overcomes the decrease of \( V_{x}(z \to \infty) \). This latter effect is the only one included in \( \varepsilon_{01}^{KLI} \), that leads to an abrupt decrease of \( \varepsilon_{01}^{KLI} \) at the \( 1S \to 2S \) transition. Finally \( \varepsilon_{01}^{LDA} \), lacking from the “hump” and asymptotic value effects, displays a smooth transition at \( \Delta = 0 \). Several works in the past have addressed the (surprising) issue of the discontinuity of the exact \( V_{xc}(r) \) as a function of the electron number. \[12,17-19\] Such a \( V_{xc} \), for a filled-subshell system with \( N \) electrons, must essentially jump by a constant for finite \( r \) as the number of electrons is allowed to vary from \( N - \delta \) to \( N + \delta \) where \( \delta \) is a positive infinitesimal. This non-analytic behavior of \( V_{xc} \) leads in turn to discontinuities on the \( N \)-dependence of the eigenvalues, which
are reminiscent of the results presented in Fig. 2. In our case, $V_x$ can also in principle change discontinuously by a constant at the $1S \rightarrow 2S$ transition. Instead, our calculation predicts that the system shows another type of discontinuous behavior, replacing $V_x(z)$ (curve A in Fig. 1) by another function $V_z(z)$ (curve B in Fig. 1). The resulting $V_z(z)$ induces a charge transfer from the minority subband to the other optimizing the exchange energy by maximizing overlaps. A constant shift in the exchange potential does not favor such transfer. We have assumed that exchange is the dominant contribution although correlations could contribute subband discontinuities \[19\]. In order to estimate the importance of correlation on the $x$-only results, and considering the good agreement between $V_x$ and $V_x^{\text{LDA}}$ in the high density region inside the quantum well displayed in Fig. 3, we show in Fig. 2 with open circles the effect of replacing $V_x^{\text{OEP}}(z)$ by $V_x^{\text{OEP}}(z) + V_x^{\text{LDA}}(z)$, both on $\varepsilon_{01}^{\text{OEP}}$ and $V_x^{\text{OEP}}(z \rightarrow \infty)$. This amounts to re-calculate the self-consistent solutions of Eqs. (1) and (2) for all $\Delta$, with $V_x^{\text{OEP}}(z)$ obtained according to the OEP procedure, while $V_x^{\text{LDA}} \equiv \delta E_c^{\text{LDA}} / \delta n(z)$. \[9\] The correction on $\varepsilon_{01}^{\text{OEP}}$ is extremely small ($\sim 0.1$ meV for all values of $\Delta$), and could be understood as resulting from a shift of the $x$-only value of $\varepsilon_{01}$ under a small (perturbative) correlation potential. The impact of LDA correlation on the discontinuity at $\Delta = 0$ in $\varepsilon_{01}^{\text{OEP}}$ and $V_x^{\text{OEP}}(z \rightarrow \infty)$ is negligible.

Let us discuss the results for this system, in the more general context of the semiconductor gap problem. \[19\] Note that if the gap is defined as the energy difference of exchanging an electron or hole between a given system and a reservoir \[2, 3\] then, i) it is necessary to consider an open system, and ii) the gap will be affected by a sudden change of $V_x(r)$ under an infinitesimal occupation of the conduction band as observed in this work. This study also suggest that going beyond KLI might be required to describe exchange contributions to the gap. The strong decrease of the barrier-like component on $V_x(z)$ in Fig. 1 for $\Delta \simeq 0.01 \text{ meV} \rightarrow 0.3 \text{ meV}$ implies a significant reduction of the exchange contribution to $\varepsilon_{01}^{\text{OEP}}$. This reduction of $\varepsilon_{01}^{\text{OEP}}$ resembles the one observed in the gap of semiconductors under intense photo-excitation (band-gap renormalization). The $\varepsilon_{01}^{\text{OEP}}$ results of Fig. 2 for $\Delta \gtrsim 0$ suggest an
exchange contribution to the band-gap renormalization of the same order of magnitude than the $\Delta = 0$ gap discontinuity itself. This should be contrasted with the smaller reduction rate with increasing density displayed by $\varepsilon_{0}^{KLI}$ and $\varepsilon_{0}^{LDA}$.

In summary, we have shown that the $x$-only OEP has a number of interesting properties when applied to an open 2DEG: i) under depopulation of the highest-occupied subband, $V_{x}(z)$ develops a barrier-like structure in the spatial region where the density starts to be dominated by electrons in that subband; ii) the size of the barrier increases dramatically when the highest subband occupation is tuned to complete depletion; iii) $V_{x}(z \to \infty)$ strongly depends on subband filling, showing an abrupt jump at the $1S \to 2S$ transition; and iv) as a consequence of the combined effect of ii) and iii), the inter-subband energy is discontinuous at the $1S \to 2S$ transition. Correlation effects, estimated $a la$ LDA, are found to be very small for this system, giving hope for its rigorous and systematic consideration following the lines of the KS perturbative approach. [20] The results for the present system offer insights into fundamental problems related to the band-gap in semiconductors.

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