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Citation for published version (APA):

Bobbert, P. A., Wieldraaijer, H., Kemerink, M., Koenraad, P. M., & Wolter, J. H. (1997). Exchange-correlation energy of a hole gas including valence band coupling. *Physical Review B: Condensed Matter*, 56(7), 3664-3671. <https://doi.org/10.1103/PhysRevB.56.3664>

DOI:

[10.1103/PhysRevB.56.3664](https://doi.org/10.1103/PhysRevB.56.3664)

Document status and date:

Published: 01/01/1997

Document Version:

Publisher's PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:

- A submitted manuscript is the version of the article upon submission and before peer-review. There can be important differences between the submitted version and the official published version of record. People interested in the research are advised to contact the author for the final version of the publication, or visit the DOI to the publisher's website.
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Exchange-correlation energy of a hole gas including valence band coupling

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(Received 1 November 1996)

We have calculated an accurate exchange-correlation energy of a hole gas, including the complexities related to the valence band coupling as occurring in semiconductors like GaAs, but excluding the band warping. A parametrization for the dependence on the density and the ratio between light- and heavy-hole masses is given. We apply our results to a hole gas in an $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ quantum well and calculate the two-dimensional band structure and the band-gap renormalization. The inclusion of the valence band coupling in the calculation of the exchange-correlation potentials for holes and electrons leads to a much better agreement between theoretical and experimental data than when it is omitted. [S0163-1829(97)03931-3]

I. INTRODUCTION

Electron gases have been used as model systems to study many-body effects for almost half a century. Very accurate results, for, e.g., the total energy, have been obtained analytically, numerically, or with quantum Monte Carlo techniques. Because of the effects of impurity scattering, it is hard to realize an ideal electron gas in a doped isotropic semiconductor. However, since the beginning of the eighties, it is possible to realize almost ideal electron gases in doped semiconductor heterostructures. Being laterally confined, these electron gases are quasi-two-dimensional, but if the lateral width of the electron gas is not too small, successful use can be made of the local density approximation (LDA) of density functional theory to relate the electron potential to the exchange-correlation energy of the three-dimensional homogeneous electron gas. This approach has been widely used and with great success.

The theoretical description of many-body effects in hole gases in III-V or row IV semiconductors such as GaAs or Ge is complicated by the structure of the top valence band region, leading to so-called valence band coupling. The most obvious complication is the simultaneous occurrence of heavy and light holes. Often, these complications are simply ignored and the hole gas is treated in the same way as an electron gas, with the electron mass replaced by some effective hole mass, usually the heavy-hole mass. One could argue that because of the highly different Fermi wave vectors of heavy and light holes in GaAs about 80% of the holes is heavy and that hence the complications of the valence band coupling will not play a big role in the calculation of the exchange-correlation potential. However, this argument overlooks the fact that the Coulomb interaction is nondiagonal with respect to the hole character (heavy or light). One of the consequences of this fact is that even in a hypothetical situation with an infinitesimally small light-hole mass, when 100% of the holes is heavy, the valence band coupling has a large influence.

In the context of exciton condensation, the exchange-correlation energy of the hole component of an electron-hole plasma in germanium was studied by Combescot and Nozières.¹ The band warping was neglected. An explicit expression was given for the exchange energy, which we will

quote below. Because of the rather large numerical difficulties involved, the correlation energy could only be estimated by these authors using several approximations and interpolation schemes. The main purpose of the present work is to systematically evaluate the correlation energy as a function of the density and the ratio between light- and heavy-hole mass.

Band-gap renormalization (BGR) in silicon and gallium arsenide due to many-body effects was studied theoretically by Abram, Childs, and Saunderson.² The self-energy operator, needed to calculate the BGR, was evaluated in the Hedin *GW* approximation.³ The screened interaction was modeled by a plasmon pole approximation. For the case of *p* doping, leading to a hole gas, the plasmon poles were taken from the aforementioned work of Combescot and Nozières,¹ hence including the valence band coupling. A similar approach, applied to modulation-doped quantum wells, was followed by Bauer and Ando.⁴ Although their approach is the preferred one for quasi-two-dimensional systems, these authors remark that in most cases density functional theory in the LDA yields accurate results. The valence band coupling, however, is omitted in their work, as, to our knowledge, in most other work on many-body effects in two-dimensional systems (see Refs. 5 and 6 references therein). Two recent attempts^{7,8} to take into account the effects of valence coupling are incorrect. We will briefly comment on them in Sec. IV.

There is clearly a need for a simple, yet accurate, way to account for many-body effects in hole gases in various systems. As we have tried to argue above, the use of the local density approximation is often justified, but the effects of valence band coupling need to be taken into account. What is needed then is an accurate exchange-correlation energy of homogeneous hole gases in bulk semiconductors as a function of the hole density for various ratios between the light- and heavy-hole masses. From this exchange-correlation energy, we can construct an exchange-correlation potential for holes in, e.g., a quantum well and without much effort calculate the band structure and properties like the BGR.

In the next section, we will discuss the theory behind the calculation of our exchange-correlation energy. As regards the exchange energy, we simply reproduce the result of Combescot and Nozières.¹ As regards the correlation energy, we use an adapted version of the theory of Vashishta and

Singwi,⁹ originally developed for electron gases. Those only interested in the results and the parametrization can skip this section and directly go to Sec. III. Section IV contains an application to a hole gas in an $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ quantum well.

II. THEORY

The system we consider is a homogeneous hole gas in a bulk semiconductor like GaAs. We are interested in holes created at the top of the valence band near the quadruplet of Γ_8 symmetry, which is a manifold of eigenstates of the square of the total angular momentum $\mathbf{J}^2 = (\mathbf{L} + \mathbf{S})^2$ with eigenvalue $\hbar^2 J(J+1)$, with $J = \frac{3}{2}$. The hole density is assumed to be small enough in order to neglect nonparabolic effects and the influence of the spin-orbit split-off band ($J = \frac{1}{2}$) and more remote bands. Apart from an interaction term due to the background potential, the Hamiltonian, in SI units, is

$$H = \int d^3r \sum_{m,m'} \psi_m^\dagger(\mathbf{r}) D_{m,m'} \psi_{m'}(\mathbf{r}) + \frac{e^2}{8\pi\epsilon_{\text{int}}\epsilon_0} \int d^3r_1 \int d^3r_2 \times \sum_{m_1,m_2} \frac{\psi_{m_1}^\dagger(\mathbf{r}_1) \psi_{m_2}^\dagger(\mathbf{r}_2) \psi_{m_2}(\mathbf{r}_2) \psi_{m_1}(\mathbf{r}_1)}{|\mathbf{r}_1 - \mathbf{r}_2|}, \quad (1)$$

where e is the electron charge, ϵ_0 the dielectric vacuum permittivity, and ϵ_{int} the static, long wavelength dielectric constant of the intrinsic semiconductor. The creation and annihilation operators $\psi_m^\dagger(\mathbf{r})$ and $\psi_m(\mathbf{r})$ create and annihilate holes at position \mathbf{r} in eigenstates of the total angular momentum along the z axis J_z with eigenvalue $\hbar m$ ($m = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$). The matrix $D_{m,m'}$ is given by¹⁰

$$D_{3/2,3/2} = -\frac{\hbar^2}{2m_0} \left[(\gamma_1 - 2\gamma_2) \frac{\partial^2}{\partial z^2} + (\gamma_1 + \gamma_2) \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \right],$$

$$D_{1/2,1/2} = -\frac{\hbar^2}{2m_0} \left[(\gamma_1 + 2\gamma_2) \frac{\partial^2}{\partial z^2} + (\gamma_1 - \gamma_2) \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \right],$$

$$D_{3/2,-1/2} = -\frac{\hbar^2}{2m_0} \sqrt{3} \left[-\gamma_2 \left(\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right) + 2i\gamma_3 \frac{\partial}{\partial x} \frac{\partial}{\partial y} \right],$$

$$D_{3/2,1/2} = -\frac{\hbar^2}{m_0} \sqrt{3} \left[-\gamma_3 \left(\frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right) \frac{\partial}{\partial z} \right], \quad (2)$$

and $D_{-3/2,-3/2} = D_{3/2,3/2}$, $D_{-1/2,-1/2} = D_{1/2,1/2}$, $D_{1/2,-3/2} = -D_{3/2,-1/2}$, $D_{3/2,-3/2} = D_{1/2,-1/2} = 0$, $D_{m,m'} = D_{m',m}^*$. Here m_0 is the bare electron mass and γ_1 , γ_2 , and γ_3 are the Luttinger parameters, which characterize the semiconductor.

The band warping is determined by the difference between the Luttinger parameters γ_2 and γ_3 . In order to keep things tractable, we need to neglect the band warping, i.e., we need to set $\gamma_2 = \gamma_3$. A good choice is to set both parameters equal to the following average:¹¹

$$\bar{\gamma} = \sqrt{\frac{2\gamma_2^2 + 3\gamma_3^2}{5}}. \quad (3)$$

Neglecting the band warping means that we are not only dealing with a homogeneous, but also an isotropic hole gas. We will see that the dependence of the exchange and the correlation energy on the light-hole/heavy-hole mass ratio is not very strong, giving an *a posteriori* justification for this approximation. Without the interaction term in Eq. (1), the one-particle energies are easily found to be

$$E_l(k) = \frac{\hbar^2}{2m_0} (\gamma_1 + 2\bar{\gamma}) k^2 \equiv \frac{\hbar^2}{2m_l} k^2,$$

$$E_h(k) = \frac{\hbar^2}{2m_0} (\gamma_1 - 2\bar{\gamma}) k^2 \equiv \frac{\hbar^2}{2m_h} k^2, \quad (4)$$

defining the light- and heavy-hole effective masses m_l and m_h . We introduce a parameter w for the ratio between the light- and heavy-hole Fermi wave vectors:

$$w \equiv \frac{k_{\text{Fl}}}{k_{\text{Fh}}} = \sqrt{\frac{m_l}{m_h}}. \quad (5)$$

Furthermore, we define an effective Bohr radius \bar{a}_0 , an effective Rydberg $\bar{\mathcal{R}}$ and a dimensionless Wigner-Seitz radius r_s by

$$\bar{a}_0 = \frac{4\pi\epsilon_{\text{int}}\epsilon_0\hbar^2}{m_h e^2}, \quad (6)$$

$$\bar{\mathcal{R}} = \frac{\hbar^2}{2m_h \bar{a}_0^2}, \quad (7)$$

$$r_s = \frac{1}{\left(\frac{4\pi}{3}\right)^{1/3} \frac{\bar{a}_0 \rho^{1/3}},} \quad (8)$$

with ρ the hole density. We have chosen to base these definitions on the heavy-hole mass.

The exchange energy of a hole gas with valence band coupling was evaluated in Ref. 1. In effective Rydbergs, the result for the exchange energy per hole is

$$\epsilon_x = -\zeta(w) \frac{3}{2} \left(\frac{9}{4\pi^2} \right)^{1/3} \frac{1}{r_s} \bar{\mathcal{R}}, \quad (9)$$

where the numerical function $\zeta(w)$ is given by

$$\zeta(w) = \frac{w^4 + 3w^3 + 3w + 1 - \frac{3}{4}(1-w^2)^2 \ln \left| \frac{1+w}{1-w} \right| + \frac{3}{4}(1-w^4) \int_w^1 dx \frac{1}{x} \ln \left| \frac{1+x}{1-x} \right|}{4(1+w^3)^{4/3}}. \quad (10)$$

Hence, apart from this numerical function, the exchange energy is equal to that of an electron gas at the same density. For $w=0$ and $w=1$ we find $\zeta(0)=1/4+3\pi^2/64\approx 0.7126$, $\zeta'(0)=0$ and $\zeta(1)=2^{-1/3}\approx 0.7937$, $\zeta'(1)=0$, so this function is of the order of, but smaller than, unity and depends rather weakly on the mass ratio.

In order to evaluate an accurate correlation energy, we apply the theory of Vashishta and Singwi,⁹ suitably adapted to the case of a hole gas. Following general many-body arguments, as can, e.g., be found in Ref. 12, one can relate the exchange-correlation energy to the dielectric function. First, the sum of the exchange and correlation energy per hole is related to the average potential energy $V(r_s)$ per hole by

$$\epsilon_c(r_s) + \epsilon_x(r_s) = \frac{1}{r_s^2} \int_0^{r_s} r'_s V(r'_s) dr'_s. \quad (11)$$

The potential energy in its turn is related to the structure factor $S(q, r_s)$ by

$$V(r_s) = \frac{2}{\pi} \frac{1}{\alpha_0 r_s} \frac{1}{(1+w^3)^{1/3}} \int_0^\infty [S(q, r_s) - 1] dq \bar{\mathcal{R}}, \quad (12)$$

with $\alpha_0 = (4/9\pi)^{1/3} \approx 0.5211$ and with the wave vector q in units of the heavy-hole Fermi wave vector $k_{\text{Fh}} = [3\rho\pi^2/(1+w^3)]^{1/3}$. Finally, the structure factor is related to the wave vector and frequency dependent dielectric function $\epsilon(q, \omega)$ by

$$\begin{aligned} S(q, r_s) &= -\frac{3q^2}{8\alpha_0 r_s} \frac{1}{(1+w^3)^{4/3}} \int_0^\infty d\omega \text{Im} \left(\frac{1}{\epsilon(q, \omega)} \right), \\ &= \frac{3q^2}{8\alpha_0 r_s} \frac{1}{(1+w^3)^{4/3}} \int_0^\infty d\omega \left[1 - \frac{1}{\epsilon(q, i\omega)} \right], \end{aligned} \quad (13)$$

where the frequency ω is in units of $\hbar k_{\text{Fh}}^2/2m_h$. Following Vashishta and Singwi,⁹ we write the dielectric function as

$$\epsilon(q, \omega) = 1 + \frac{Q_0(q, \omega)}{1 - G(q)Q_0(q, \omega)}, \quad (14)$$

with

$$Q_0(q, \omega) = -\phi(q)\chi_0(q, \omega), \quad (15)$$

with $\phi(q) = e^2/\epsilon_{\text{int}}\epsilon_0 q^2$ the Fourier transform of the Coulomb interaction and $\chi_0(q, \omega)$ the random phase approximation (RPA) of the polarizability. The function $G(q)$ in Eq. (14) is the so-called local field correction, which in an approximate fashion takes into account the vertex corrections to the RPA, i.e., the effects of the interaction between excited holes and electrons, which are left out of the RPA. The evaluation of the function $Q_0(q, \omega)$ is again straightforward, but quite involved. The reason is that one has to account for four different kinds of excitations, namely, heavy-hole-heavy electron, heavy-hole-light electron, light-hole-heavy electron, and light-hole-light electron excitations (a heavy/light electron is interpreted as a missing heavy/light hole). The result can be cast in the following form:

$$\begin{aligned} Q_0(q, i\omega) &= -\frac{2}{\pi} \frac{\alpha_0 r_s}{q^2} (1+w^3)^{1/3} \left\{ f_1(q, \omega) + w^3 f_1\left(\frac{q}{w}, \omega\right) \right. \\ &\quad + \frac{3}{2}(1-w)(1-w^2) - \frac{3}{16q} \\ &\quad \times \int_0^1 dq' [f_2^{(1,1)}(q, q', \omega) - f_2^{(1,w)}(q, q', \omega) \\ &\quad \left. - f_2^{(w,1)}(q, q', \omega) + f_2^{(w,w)}(q, q', \omega) \right\}, \end{aligned} \quad (16)$$

with

$$\begin{aligned} f_1(q) &= 1 - \frac{1}{2q} \left(1 + \frac{\omega^2}{4q^2} - \frac{q^2}{4} \right) \ln \left(\frac{\omega^2/4q^2 - (1-q/2)^2}{\omega^2/4q^2 - (1+q/2)^2} \right) \\ &\quad - \frac{\omega}{2q} \left\{ \arctan \left(\frac{q(2+q)}{\omega} \right) + \arctan \left(\frac{q(2-q)}{\omega} \right) \right\}, \end{aligned} \quad (17)$$

and

$$\begin{aligned} f_2^{(\alpha, \beta)}(q, q', \omega) &= \left(\frac{q'(\alpha^2 q'^2 - q^2)^2}{q'^4 + \omega^2} - (2\alpha^2 - \beta^2)\beta^2 q' - \frac{2\beta^2 q^2}{q'} \right) \\ &\quad \times \ln \left(\frac{[(\alpha q' - q)^2 - \beta^2 q'^2]^2 + \beta^4 \omega^2}{[(\alpha q' + q)^2 - \beta^2 q'^2]^2 + \beta^4 \omega^2} \right) \\ &\quad - \frac{2\omega}{q'} \left(\frac{(\alpha^2 q'^2 - q^2)^2}{q'^4 + \omega^2} - \beta^4 \right) \\ &\quad \times \left\{ \arctan \left(\frac{\beta^2 \omega}{(\alpha q' - q)^2 - \beta^2 q'^2} \right) \right. \\ &\quad \left. - \arctan \left(\frac{\beta^2 \omega}{(\alpha q' + q)^2 - \beta^2 q'^2} \right) \right\}, \end{aligned} \quad (18)$$

where both q and q' are in units of k_{Fh} . Still following Vashishta and Singwi, we take for the local field correction $G(q)$

$$\begin{aligned} G(q) &= G(k/k_{\text{Fh}}) = \left(1 + a\rho \frac{\partial}{\partial \rho} \right) \\ &\quad \times \left\{ -\frac{1}{\rho} \int \frac{d^3 k'}{(2\pi)^3} \frac{\mathbf{k} \cdot \mathbf{k}'}{k'^2} \left[S\left(\frac{|\mathbf{k} - \mathbf{k}'|}{k_{\text{Fh}}}, r_s\right) - 1 \right] \right\} \\ &= G_I(q, r_s) + a \left(-\frac{q}{3} \frac{\partial}{\partial q} G_I(q, r_s) - \frac{r_s}{3} \frac{\partial}{\partial r_s} G_I(q, r_s) \right), \end{aligned} \quad (19)$$

where

$$\begin{aligned} G_I(q, r_s) &= -\frac{3}{4} \int_0^\infty q'^2 [S(q', r_s) - 1] \\ &\quad \times \left(1 + \frac{q^2 - q'^2}{2qq'} \ln \left| \frac{q+q'}{q-q'} \right| \right) dq'. \end{aligned} \quad (20)$$

TABLE I. Correlation energy, in effective Rydbergs per hole, of a hole gas for different values of the density parameter r_s and light-hole/heavy-hole Fermi wave vector ratios w . In each entry, the upper number is the RPA result and the lower the result including local field corrections. For the electron gas, the corresponding values (upper and middle numbers) are taken from Ref. 9. The lower number in this case is calculated with the parametrization of Ref. 15 of the quantum Monte Carlo results of Ref. 14.

		r_s					
		1	2	3	4	5	6
w	0.0	-0.095	-0.071	-0.058	-0.051	-0.045	-0.041
		-0.091	-0.067	-0.055	-0.047	-0.042	-0.038
	0.5	-0.164	-0.124	-0.104	-0.091	-0.081	-0.074
		-0.154	-0.115	-0.095	-0.082	-0.073	-0.066
	1.0	-0.225	-0.168	-0.140	-0.121	-0.109	-0.098
		-0.207	-0.152	-0.123	-0.105	-0.093	-0.083
e -gas	-0.157	-0.124	-0.105	-0.094	-0.085	-0.078	
	-0.112	-0.089	-0.075	-0.065	-0.058	-0.052	
	-0.119	-0.090	-0.074	-0.064	-0.057	-0.051	

The latter equality in Eq. (19) is obtained by realizing that $q=k/k_{\text{Fh}}$ depends on the density ρ through k_{Fh} . With $a=0$ in Eq. (19) correspondence is obtained with the theory of Singwi *et al.*,¹³ in which the density correlation function in the presence of an external weak field is approximated by an expression containing the equilibrium pair correlation function. With nonzero a allowance is made for the change in the pair correlation function in an external field through the density derivative of the equilibrium pair correlation function. The parameter a can be chosen such that the compressibility sum rule is obeyed. This sum rule states that the compressibility as calculated from the density dependence of the total energy should be equal to that following from the large wavelength and small frequency behavior of the dielectric function. For details we refer to Ref. 9. For the electron gas the value $a=\frac{2}{3}$ guarantees almost satisfaction of this sum rule in a very broad density range. For the hole gas, we have fixed the value of a for each mass ratio such that the compressibility sum rule is exactly obeyed at $r_s=1$. Again, the sum rule is almost obeyed in a density range comparable to that in Ref. 9. The electron gas correlation energies of Ref. 9 agree very well with the best known values, which are the quantum Monte Carlo results of Ceperley and Alder,¹⁴ as parametrized by Perdew and Zunger¹⁵ (see Table I, discussed in the next section). We expect the same degree of accuracy in our case. The values of a in our case vary slightly from 1.021 for $w=0$ (infinitesimally small light hole mass) to 1.164 for $w=1$ (equal masses). Note that Eqs. (13), (14), (19), and (20) constitute a self-consistency problem, which in practice is solved by iteration, starting from the RPA result with $G(q)=0$. In all cases, sufficient convergence is obtained after not more than 12 iterations (for $r_s \leq 10$). In the next section, we will present the results of our calculations and a parametrization.

III. RESULTS AND PARAMETRIZATION

The exchange energy of the hole gas is given by the closed expression Eq. (9). The numerical function Eq. (10) of the Fermi wave vector ratio w of light and heavy holes, appearing as a prefactor in this expression, can be param-

etrized with an accuracy of better than 0.1% by the polynomial

$$\zeta(w) \approx 2^{-1/3} + (1-w)^2 [w^2(aw+b) + c(4w^3 + 3w^2 + 2w + 1)], \quad (21)$$

with $a=0.679$, $b=-0.0686$, and $c=1/4 + 3\pi^2/64 - 2^{-1/3} \approx -0.0811$. The qualitative reason why the exchange energy is smaller in magnitude than that for the electron gas [$\zeta(w)$ is smaller than unity] is the fact that, besides the spatial degrees of freedom, there are four instead of two internal degrees of freedom. Consequently, the Pauli exclusion principle has less of an effect. We note that for the — hypothetical — case $w=0$, the exchange energy is *not* equal to that of an electron gas, despite the fact that there is just one kind of hole, the heavy ones. This is a consequence of the fact that the Coulomb interaction couples heavy and light holes (i.e., the Coulomb interaction is nondiagonal with respect to the hole character).

In Table I we give the results for the correlation energy of the hole gas, for several values of the density parameter r_s [see Eq. (8)] and light-hole/heavy-hole Fermi wave vector ratios w . The numerical errors are smaller than an effective milli-Rydberg. The correlation energy is calculated with a RPA dielectric constant and with a dielectric constant including the local field correction in the way described in the previous section [Eq. (14) without and with local field correction $G(q)$]. For comparison, we also include the comparable results for the electron gas, taken from Ref. 9, and the quantum Monte Carlo results for the electron gas,¹⁴ as parametrized in Ref. 15. The inclusion of the local field correction in the hole gas has less influence on the RPA results than in the electron gas. The reason is the relatively larger dielectric constant for the hole gas, caused by the larger number of possibilities to create hole-electron pairs. The larger dielectric constant leads to a better screening of the interaction between excited hole-electron pairs. As a consequence, RPA, in which this interaction is neglected, becomes a better approximation. As can be understood without much

effort, the RPA results for the electron gas are related to those for the hole gas with $w=1$ by the transformation $\epsilon_c^{e\text{-gas}}(r_s) = \epsilon_c^{h\text{-gas}}(2^{-4/3}r_s)/2$ (this is not true for the results including local field corrections). Again, we note that the hole-gas results for $w=0$ (only heavy holes) are not equal to the electron-gas results.

The correlation energies in Table I, including the local field effects, can quite adequately be parametrized by

$$\epsilon_c(w, r_s) \approx a(w)f(b(w)r_s)\overline{\mathcal{R}}, \quad (22)$$

with the function $f(r_s)$ fitting the correlation energy for $w=0.5$:

$$f(r_s) = \begin{cases} -0.1358 - 0.0179r_s + 0.0752\ln r_s + 0.0024r_s \ln r_s & (r_s \leq 1) \\ 1/(-2.2568 - 3.5742\sqrt{r_s} - 0.7017r_s) & (r_s > 1). \end{cases} \quad (23)$$

The functions $a(w)$ and $b(w)$ were determined such that the approximation Eq. (22) and its derivative with respect to r_s have the correct values at $r_s=1$. Fitting polynomials for $a(w)$ and $b(w)$ are

$$a(w) \approx 1 + 0.960(w-0.5) - 0.112(w-0.5)^2 - 0.454(w-0.5)^3 + 2.106(w-0.5)^4, \quad (24)$$

$$b(w) \approx 1 + 0.364(w-0.5) + 1.056(w-0.5)^2 - 1.667(w-0.5)^3 + 1.865(w-0.5)^4. \quad (25)$$

The parametrizations Eqs. (22), (23), (24), and (25) reproduce the numbers in Table I, and calculated numbers for several intermediate values for w that are not included in this table, with errors of at most one effective milli-Rydberg.

IV. APPLICATION TO A HOLE GAS IN A $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ QUANTUM WELL

As a demonstration, we will apply our results for the exchange-correlation energy to a hole gas in a $\text{Al}_x\text{Ga}_{1-x}/\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}$ quantum well, with $x=0.45$ and grown in the [001] direction. We will calculate the two-dimensional band structure, and compare the BGR we obtain with an experimentally determined value. For the Luttinger parameters and intrinsic dielectric constants of GaAs and AlAs we take $\gamma_1=6.85$, $\gamma_2=2.10$, $\gamma_3=2.90$, and $\gamma_4=3.45$, $\gamma_2=0.68$, $\gamma_3=1.29$, and $\epsilon_{\text{int}}=12.79$ and 10.06 ,¹⁶ respectively. We apply the virtual crystal approximation to obtain the corresponding values for $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}$. For the direct band gaps we take $E_g^{\text{GaAs}}=1.519$ eV (Ref. 16) and $E_g^{\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}}=2.176$ eV.¹⁷ For the conduction and valence band offset we take 0.460 and 0.197 eV, respectively (according to the 7:3 rule). The precise values of the band gaps and offsets are not critical for our calculations.

The sample used in the experiments is a single p -type GaAs quantum well, confined between two $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}$ barriers. The sample is symmetrically doped in the barriers with Be and has a nominal well width of 95 Å. The low temperature (1.4 K) carrier density, obtained from Shubnikov–de Haas and Hall measurements, is $9.0 \times 10^{15} \text{ m}^{-2}$. Experimentally, the BGR was determined from a com-

parison between measured and calculated absorption energies at zero wave vector. Experimental absorption energies are obtained from photo-luminescence excitation (PLE) spectra, taken at 4.2 K, using perpendicularly incident light from a tunable Ti:sapphire laser. The laser power was kept below 0.5 W/cm^2 to prevent significant changes in the carrier density or carrier temperature due to the exciting light. The absorption energies were corrected for the binding energies of the screened $L0\text{-}E0$ and $H1\text{-}E1$ excitons (see Fig. 2 for this terminology), which were determined from magneto-PL spectra by a method outlined in a forthcoming publication.¹⁸ Excitonic effects on the $H0\text{-}E0$ transition can be neglected. They only influence the intensity, but not the energy position of the emission peak related to this transition, as was shown by several authors.^{4,19,20}

In order to make a meaningful comparison with the calculations, it is essential to know the real well width, which usually deviates somewhat from its nominal value. The energy difference between the $H0\text{-}E0$, $L0\text{-}E0$, and $H1\text{-}E1$ transitions strongly depends on the actual well width but hardly on the BGR, since the BGR almost cancels in these energy differences.²¹ We therefore calculated these differences as a function of the well width from a simple one-dimensional Schrödinger equation, including the band offsets and the Hartree potential, using as effective two-dimensional binding masses $m_0/(\gamma_1-2\gamma_2)$, $m_0/(\gamma_1+2\gamma_2)$, and $0.0665m_0$ (Ref. 16) for the heavy holes, light holes, and electrons, respectively. The electron binding energy was corrected for nonparabolicity along the lines of Ref. 22. We found that at a well width of 88 ± 2 Å, all calculated energy differences were, within experimental errors, equal to their experimental counterparts. In order to obtain the correct value for the $H0\text{-}E0$ transition at zero wave vector, a BGR of 17 ± 2 meV is required. It is important to note that this method for obtaining well widths has yielded results that were in exact agreement with results from high-resolution x-ray diffraction measurements for an empty ten-period $\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ multiple-quantum-well sample.¹⁸ Unfortunately, x-ray diffraction spectra are very insensitive to the width of single quantum wells.

To calculate the two-dimensional band structure of the quantum well we solve the Luttinger-Kohn Hamiltonian for the four envelope functions $f_{m\mathbf{k}_\parallel}(z)$ ($m = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}$) related to the top of the valence band region near the point of Γ_8 symmetry [cf. Eq. (2)].¹⁰

$$\mathcal{H}_{\Gamma_8} = \begin{pmatrix} \mathcal{H}_h & b & c & 0 \\ b^* & \mathcal{H}_l & 0 & c \\ c^* & 0 & \mathcal{H}_l & -b \\ 0 & c^* & -b^* & \mathcal{H}_h \end{pmatrix}, \quad (26)$$

where

$$\begin{aligned} \mathcal{H}_h &= -\frac{1}{2m_0} p_z (\gamma_1 - 2\gamma_2) p_z + V(z) - \frac{\hbar^2 k_{\parallel}^2}{2m_0} (\gamma_1 + \gamma_2), \\ \mathcal{H}_l &= -\frac{1}{2m_0} p_z (\gamma_1 + 2\gamma_2) p_z + V(z) - \frac{\hbar^2 k_{\parallel}^2}{2m_0} (\gamma_1 - \gamma_2), \\ c &= \frac{\hbar^2 \sqrt{3}}{m_0} \frac{1}{2} [\gamma_2 (k_x^2 - k_y^2) - 2i\gamma_3 k_x k_y], \\ b &= \frac{\hbar}{m_0} \frac{\sqrt{3}}{2} (k_x - ik_y) (\gamma_3 p_z + p_z \gamma_3). \end{aligned} \quad (27)$$

The z axis is chosen perpendicular to the quantum well, $p_z = (\hbar/i) \partial/\partial z$ and $\mathbf{k}_{\parallel} = (k_x, k_y, 0)$ is the wave vector parallel to the quantum well. At the interfaces between GaAs and $\text{Al}_x\text{Ga}_{1-x}\text{As}$ we require continuity of the envelope functions and continuity of the derivatives of the envelope functions divided by the effective heavy-hole (for $m = \pm \frac{3}{2}$) or light-hole mass (for $m = \pm \frac{1}{2}$).²³ The potential $V(z)$ in Eq. (27) contains the valence band offset, the electrostatic Hartree potential $V_H(z)$ and the exchange-correlation potential V_{xc} . In the local density approximation, the exchange-correlation potential is related to the exchange-correlation energy $\epsilon_{xc}(\rho)$ per hole of a homogeneous hole gas of density ρ by²⁴

$$\begin{aligned} V_{xc}(z) &= -\frac{d}{d\rho} [\rho \epsilon_{xc}(\rho)](z) \\ &= -\epsilon_{xc}(\rho(z)) - \rho(z) \frac{d}{d\rho} [\epsilon_{xc}(\rho)](z). \end{aligned} \quad (28)$$

The minus sign in this equation is due to the fact that the Luttinger-Kohn Hamiltonian gives the energy of the valence band electrons, which is minus the energy of the holes. In the exchange-correlation energy we have neglected the effects of band warping (see Sec. II) but we do not neglect the band warping in the Luttinger-Kohn Hamiltonian Eq. (26). The neglect of band warping in the calculation of the exchange-correlation potentials seems justified. The variations of the heavy-hole mass in GaAs in different directions are of the order of 20%,¹⁰ leading to variations in the light-hole/heavy-hole Fermi wave vector ratio w [Eq. (5)] of the order of 10%. This in turn leads to variations in the exchange-correlation potential of only a few percent, due to the rather weak dependence of the exchange-correlation potential on w . According to the criterion of Langreth and Mehl,²⁵ the use of the local density approximation for an electron gas in a quantum well is justified as long as $r_s a_0 \ll 5d$,²⁶ with d the width of the quantum well. We expect the range of validity of the LDA for the hole gas to be even wider. Since the dielectric constant for the hole gas is larger than that for the electron gas (see Sec. III), the nonlocality of the self-energy, as, e.g., calculated in the GW approximation,³ is smaller, leading to a

better performance of the LDA.²⁷ In our case we have $r_s \approx 5$, $a_0 \approx 11 \text{ \AA}$, and $d \approx 88 \text{ \AA}$, so that the above criterion is indeed satisfied. Nevertheless, the LDA is probably the weakest point in our calculation and could, with corrections of the order of $r_s a_0 / 5d$, lead to errors of the order of 10%, which is the size of error we observe (see further on). The agreement between the theoretical results of the Vashishta-Singwi theory and the quantum Monte Carlo results for the electron gas for $r_s \approx 5$ is very good (deviations of the order of 2%, see Table I) and we expect the same to be true for the hole gas. Finally, because of the roughly $\rho^{1/3}$ dependence of the BGR on the density, the well width is not a critical parameter in the calculation of the theoretical BGR. The well width we adopted for those calculations is 88 \AA.

Reboredo and Proetto, in dealing with a two-dimensional hole gas in acceptor δ -doped GaAs,⁷ construct a LDA exchange-correlation potential by making an analogy with the spin-density functional formalism.²⁸ Instead of taking the same $V(z)$ in the diagonal elements \mathcal{H}_h and \mathcal{H}_l [Eqs. (27)], they take different potentials $V_h(z)$ and $V_l(z)$, depending only on the local ‘‘heavy-hole’’ and ‘‘light-hole density,’’ respectively. These local ‘‘heavy- and light-hole densities’’ are obtained from the envelope functions $f_{\pm(3/2), \mathbf{k}_{\parallel}}(z)$ and $f_{\pm(1/2), \mathbf{k}_{\parallel}}(z)$, respectively. However, no physical meaning can be attached to these definitions. It is easy to verify that taking, e.g., the x axis as quantization axis for the total angular momentum will change the densities defined in this way. Hence, the approach of these authors is not invariant under a change of quantization axis. Sipahi *et al.*, in dealing with a similar system,⁸ use a complicated procedure to construct an exchange-correlation matrix. Their procedure does have the above invariance property, but is, apart from that, rather *ad hoc* and misses the essential physics involved.

In order to calculate the band gap renormalization, we also need the potential for the electrons. There is of course no exchange contribution to this potential, but there is a correlation contribution. Again we apply the local density approximation. We proceed in the same way as in Ref. 2 and approximate the potential of an electron in a homogeneous hole gas by the GW self-energy.³ The differences with Ref. 2 is that we take into account the full energy dependence of the screened interaction W , instead of using a plasmon pole model, and that we use the dielectric function of Sec. II, including the local field correction, instead of the RPA dielectric function. We take an effective electron mass in GaAs of $m_e = 0.0665m_0$.¹⁶ The resulting potential in GaAs can quite accurately (2.5% accuracy in the density range around $r_s = 5$, which is relevant here) be reproduced by the expression

$$V_c^e(r_s) \approx -\frac{1}{C \sqrt{r_s} [1 + A r_s^{1/4} + B r_s^{1/8}]} \bar{\mathcal{R}}, \quad (29)$$

with $A = 4.526$, $B = 1.956$ and $C = 0.273$. The effective Rydberg $\bar{\mathcal{R}}$ and the density parameter r_s are defined by Eqs. (7) and (8). The parametrization Eq. (29) is of the same kind as that used by Bauer and Ando.⁴ The correlation potential Eq. (29) differs very little from the result of Abram *et al.*² In the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ barriers of the well we also use the potential Eq. (29). The error made by doing this is extremely small,

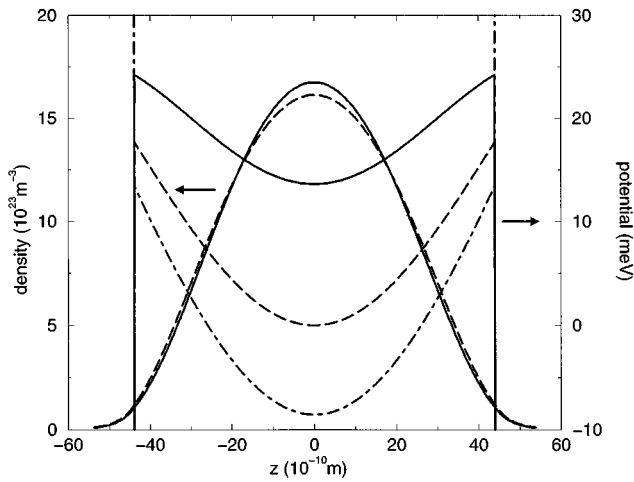


FIG. 1. Self-consistent hole density distribution and hole and electron potentials of a hole gas in a $\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}/\text{GaAs}/\text{Al}_{0.45}\text{Ga}_{0.55}\text{As}$ quantum well without (dashed) and with (solid for the case of holes and dash-dotted for the case of electrons) an exchange-correlation potential. The potential is measured relative to the Hartree potential in the middle of the well ($z=0$). The band edge energies in GaAs are subtracted. The total hole density is $9 \times 10^{15} \text{ m}^{-2}$ and the width of the well is 88 \AA .

because the band offset is very much larger than the possible error in the electron correlation potential.

Another popular quantum well system is $\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$ between $\text{Al}_{0.48}\text{In}_{0.52}\text{As}$ barriers. Both materials are lattice matched to InP. The electron correlation potential for $\text{Ga}_{0.47}\text{In}_{0.53}\text{As}$ was also calculated and fitted with the expression Eq. (29). The fitting parameters are $A=4.382$, $B=1.956$, and $C=0.300$. For the effective masses we took $m_e=0.043m_0$, $m_h=0.581m_0$, $m_l=0.053m_0$. These effective masses were obtained by linear interpolation of the effective masses of GaAs and InAs, obtained from the Luttinger parameters of Ref. 16 and neglecting the band warping by using Eq. (3).

As usual, the eigenstates of the Hamiltonian Eq. (26), which depend in a self-consistent way on the density and hence on the (occupied) eigenstates themselves, are found by iteration. In Fig. 1 we give the self-consistent density and total hole and electron potentials for the case without and with inclusion of the exchange-correlation potential. The inclusion of the exchange-correlation potential leads to a considerable upward shift and a flattening of the hole potential. The hole density distribution changes only slightly. The change in the electron potential has an opposite trend. In Fig. 2 we give the two-dimensional band structure of the top valence (Γ_8) region and the lowest conduction subband (Γ_6) in the quantum well in the [110] and [100] direction for the case without and with exchange-correlation potential. From this figure one can readily read off the BGR of 19.9 meV . We have also calculated the BGR neglecting the valence coupling in the calculation of the exchange-correlation potential of the holes and assuming all the holes to be heavy. However, we still used the Luttinger-Kohn Hamiltonian Eq. (26). The corresponding correlation potential for the electrons is taken from Ref. 4. The result is a BGR of 21.8 meV . We see that our correctly calculated exchange-correlation potentials yields a result which is closer to the experimental

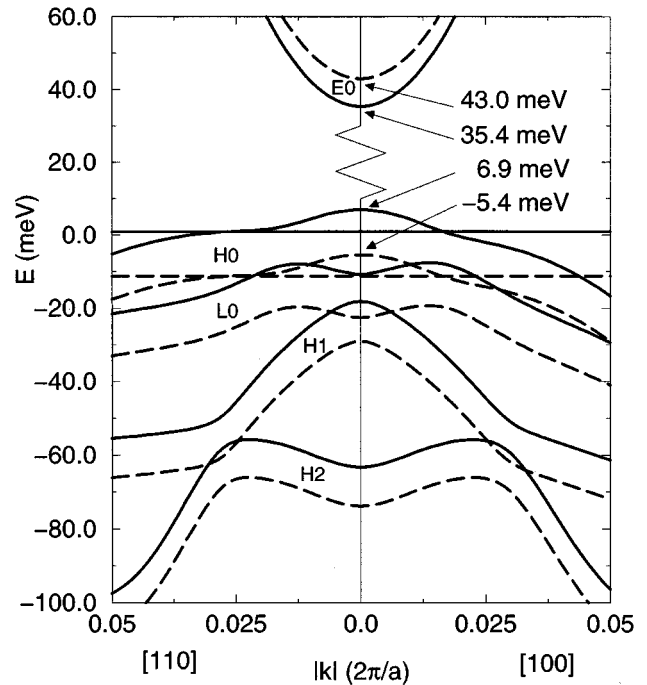


FIG. 2. Two-dimensional valence band structure in the [110] and [100] directions of the hole gas in the $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ quantum well without (dashed) and with (solid) exchange-correlation potential. The corresponding quasi-Fermi energies are indicated by horizontal lines. Also the lowest conduction subband for the two cases is plotted. The energy is measured relative to the Hartree potential in the middle of the well and the band edge energies in GaAs are subtracted.

value of $17 \pm 2 \text{ meV}$. It is not clear what the remaining small difference between our theoretical and experimental results should be attributed to. One could think of corrections to the LDA or corrections to the exchange-correlation energy due to the band warping. Corrections of only a few percent could bring the theoretical value within the experimental uncertainty range. However, these corrections are extremely difficult to estimate.

Surprisingly good agreement between experimental and theoretical BGR in n - and p -doped $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ quantum wells was reported by Haacke *et al.*²⁹ However, these authors obtained the BGR for p -doped wells by interchanging the roles of holes and electrons in all their calculations, i.e., they did not only neglect the effects of valence band coupling on the exchange-correlation potentials, but did not even use the Luttinger-Kohn Hamiltonian Eq. (26). Apparently, the errors made almost cancel and the final result is, fortuitously, rather close to the experimental data.

Summarizing, we have evaluated and parametrized an accurate exchange-correlation energy for a hole gas, including the effects of valence band coupling, but excluding the band warping. Using the local density approximation to obtain the exchange-correlation potential for holes, we calculated the band structure of a p -doped $\text{Al}_x\text{Ga}_{1-x}\text{As}/\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ quantum well. In addition, we constructed a correlation potential for electrons for this system. We obtain a band-gap renormalization which is in much better agreement with experiment than what is obtained if the valence band coupling is omitted in the calculation of these potentials.

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