# Theoretical study of interacting hole gas in *p*-doped bulk III-V semiconductors

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We study the homogeneous interacting hole gas in *p*-doped bulk III-V semiconductors. The structure of the valence band is modeled by Luttinger's Hamiltonian in the spherical approximation, giving rise to heavy and light hole dispersion branches, and the Coulomb repulsion is taken into account via a self-consistent Hartree-Fock treatment. As a nontrivial feature of the model, the self-consistent solutions of the Hartree-Fock equations can be found in an almost purely analytical fashion, which is not the case for other types of effective spin-orbit coupling terms. In particular, the Coulomb interaction renormalizes the Fermi wave numbers for heavy and light holes. As a consequence, the ground state energy found in the self-consistent Hartree-Fock approach and the result from lowest-order perturbation theory do not agree. We discuss the consequences of our observations for ferromagnetic semiconductors, and for the possible observation of the spin Hall effect in bulk *p*-doped semiconductors. Finally, we also investigate elementary properties of the dielectric function in such systems.

## I. INTRODUCTION

Over the last years, effects of spin-orbit coupling in semiconductors have moved into the very focus of both experimental and theoretical solid-state research, mainly within the large and still rapidly growing field of spintronics.[1] In the *p*-type valence band of III-V zinc-blende semiconductors spin-orbit interaction is particularly strong. Important examples of *p*-doped semiconductor systems with itinerant charge carriers in the valence band include ferromagnetic semiconductors with $Ga_{1-x}Mn_x As$ being the most intensively studied material, for an overview see Refs. [2–4]. In $Ga_{1-x}Mn_x As$ and related systems, the substitutional Mn dopants form local moments with spin $S=5/2$ from its five *d* electrons, while they also act as acceptors providing holes in the valence band interacting with the local moments. This interaction between charge carriers and local spin moments then leads, at low enough temperatures, to ferromagnetic order, giving rise to the notion of *carrier-induced ferromagnetism*. So far, Curie temperatures as high as $T_c \approx 160$–170 K have been observed.[5,6] There is vast literature on the theoretical description of ferromagnetic semiconductors taking into account realistic band structure parametrizations for the valence band, for an early key publication see Ref. [7]. However, what is most often neglected in the treatment of models for ferromagnetic semiconductors is the Coulomb interaction *among* the holes. A (semi-)phenomenological way to account for Coulomb repulsion is to introduce appropriate Fermi liquid parameters.[8] Exceptions to these heuristic approaches include numerical works based on dynamical mean-field theory,[9] and a numerical Hartree-Fock study of a disordered two-band model, neglecting spin-orbit coupling.[13] For further dynamical-mean-field studies of models for ferromagnetic semiconductors not incorporating Coulomb repulsion see Refs. [10–12].

Moreover, *p*-doped semiconductors have also attracted interest with respect to the recently predicted intrinsic spin Hall effect;[14–16] for a recent overview see also Ref. [17]. In fact, the pioneering paper by Murakami, Nagaosa, and Zhang studies a *p*-doped bulk III-V semiconductor taking into ac-

count heavy and light hole bands around the Γ point.[14] However, the Coulomb repulsion between holes was also neglected here.

In summary, in light of the above challenges and activities, it is certainly desirable to develop a deeper and possibly least partially analytical understanding of the effects of Coulomb interaction in *p*-doped semiconductors taking into account spin-orbit coupling. In the present work we study interacting holes in the valence band of a III-V semiconductor. The band structure is modeled by Luttinger's Hamiltonian in the spherical approximation leading to heavy and light hole dispersion branches.[18] The Coulomb repulsion between holes is treated via Hartree-Fock theory. As a nontrivial feature of the model, the self-consistent solutions of the Hartree-Fock equations can be found in an almost purely analytical fashion, which is not the case for other types of effective spin-orbit coupling terms. In particular, the Coulomb interaction renormalizes the Fermi wave numbers for heavy and light holes. As a consequence, the ground state energy found in the self-consistent Hartree-Fock approach and the result from lowest-order perturbation theory do not agree. In other words, the self-consistent Hartree-Fock treatment contains contributions beyond lowest-order perturbation theory, which is a result of the nontrivial band structure. We discuss the consequences of our observations for ferromagnetic semiconductors, and for the possible observation of the spin-Hall effect in bulk *p*-doped semiconductors. Moreover, we also investigate elementary properties of the dielectric function in such systems.

This paper is organized as follows. In Sec. II we introduce the single-particle Hamiltonian and basic properties of the noninteracting system. In particular, the structure of the single-particle eigenstates will be of importance for the Hartree-Fock study in Sec. III. The self-consistent solution of the Hartree-Fock equations for Coulomb repulsion is presented in Sec. III A. In Sec. III B we compare our findings for the three-dimensional hole gas with the situation in other generic semiconductor structures where spin-orbit coupling plays an important role. We then return to the three-dimensional hole gas and investigate its ground state energy and pair correlation functions in Hartree-Fock theory. In Sec.

III E we also discuss elementary properties of the dielectric function within random phase approximation. We close with a discussion and outlook in Sec. IV.

## II. THE NONINTERACTING HOLE GAS

A good approximative description of heavy and light hole states around the $\Gamma$ point in III-V zinc-blende semiconductors is given by Luttinger's Hamiltonian (Ref. 18)

$$\mathcal{H} = \frac{1}{2m_0}\left[\left(\gamma_1 + \frac{5}{2}\gamma_2\right)\vec{p}^2 - 2\gamma_2(\vec{p}\cdot\vec{S})^2\right]. \qquad (1)$$

Here $m_0$ is the bare electron mass, $\vec{p}$ is the hole lattice momentum, and $\vec{S}$ are spin-3/2 operators, resulting from adding the $l=1$ orbital angular momentum to the $s=1/2$ electron spin. The dimensionless Luttinger parameters $\gamma_1$ and $\gamma_2$ describe the valence band of the specific material with effects of spin-orbit coupling being included in $\gamma_2$. The above Hamiltonian is rotationally invariant and commutes with the helicity operator $\lambda = (\vec{k}\cdot\vec{S})/k$, where $\vec{k}=\vec{p}/\hbar$ is the hole wave vector.

Thus, the eigenstates of (1) can be chosen to be eigenstates of the helicity operator, which grossly facilitates analytical calculations. The heavy holes correspond to $\lambda = \pm 3/2$, while the light holes have $\lambda = \pm 1/2$. For the dispersions of $\varepsilon_{h/l}(\vec{k})$ of heavy and light hole states, respectively, one finds

$$\varepsilon_{h/l}(\vec{k}) = \frac{\hbar^2 k^2}{2m_{h/l}}, \qquad (2)$$

where the masses $m_{h/l}$ of heavy and light holes are given by

$$m_{h/l} = \frac{m_0}{\gamma_1 \mp 2\gamma_2}. \qquad (3)$$

Well established values for the Luttinger parameters, among other band structure parameters, can be found in the literature.[19] For example, for GaAs one has $\gamma_1 \approx 7.0$ and $\gamma_2 \approx 2.5$ giving $m_h \approx 0.5 m_0$ and $m_l \approx 0.08 m_0$.

The corresponding eigenstates of the Hamiltonian (1) are given by

$$\langle \vec{r} | \vec{k}, \lambda \rangle = \frac{e^{i\vec{k}\vec{r}}}{\sqrt{V}} |\chi_\lambda(\vec{k})\rangle, \qquad (4)$$

where $V$ is the volume of the system. Using the conventional basis of eigenstates of $S^z$ and introducing the usual parametrization $\vec{k}=k(\cos\varphi\sin\vartheta, \sin\varphi\sin\vartheta, \cos\vartheta)$ in terms of polar coordinates, the eigenspinors $|\chi_\lambda(\vec{k})\rangle$ of the helicity operator $\lambda = (\vec{k}\cdot\vec{S})/k$ read explicitly

$$|\chi_{\frac{3}{2}}(\vec{k})\rangle = \begin{pmatrix} \cos^3\dfrac{\vartheta}{2}e^{-(3i/2)\varphi}, \\[2mm] \sqrt{3}\cos^2\dfrac{\vartheta}{2}\sin\dfrac{\vartheta}{2}e^{-(i/2)\varphi}, \\[2mm] \sqrt{3}\cos\dfrac{\vartheta}{2}\sin^2\dfrac{\vartheta}{2}e^{+(i/2)\varphi}, \\[2mm] \sin^3\dfrac{\vartheta}{2}e^{+(3i/2)\varphi} \end{pmatrix}, \qquad (5)$$

$$|\chi_{\frac{1}{2}}(\vec{k})\rangle = \begin{pmatrix} -\sqrt{3}\cos^2\dfrac{\vartheta}{2}\sin\dfrac{\vartheta}{2}e^{-(3i/2)\varphi}, \\[2mm] \cos\dfrac{\vartheta}{2}\left(\cos^2\dfrac{\vartheta}{2} - 2\sin^2\dfrac{\vartheta}{2}\right)e^{-(i/2)\varphi}, \\[2mm] \sin\dfrac{\vartheta}{2}\left(2\cos^2\dfrac{\vartheta}{2} - \sin^2\dfrac{\vartheta}{2}\right)e^{+(i/2)\varphi}, \\[2mm] \sqrt{3}\cos\dfrac{\vartheta}{2}\sin^2\dfrac{\vartheta}{2}e^{+(3i/2)\varphi} \end{pmatrix} \qquad (6)$$

and the remaining eigenspinors $|\chi_{-3/2}(\vec{k})\rangle$, $|\chi_{-1/2}(\vec{k})\rangle$ can be obtained from the above ones by shifting $\vartheta \mapsto \pi - \vartheta$, $\varphi \mapsto \varphi + \pi$, corresponding to a spatial inversion $\vec{k} \mapsto -\vec{k}$. Note that $|\chi_{\pm\frac{3}{2}}(\vec{k})\rangle$ is just a usual spin-coherent state of spin length $S = 3/2$ polarized along the direction $\pm\vec{k}/k$. In what follows, we will also need the mutual overlaps squared between spinors which are given by

$$|\langle\chi_{\frac{3}{2}}(\vec{k}_1)|\chi_{\frac{3}{2}}(\vec{k}_2)\rangle|^2 = \left[\frac{1}{2}\left(1 + \frac{\vec{k}_1\vec{k}_2}{k_1 k_2}\right)\right]^3, \qquad (7)$$

$$|\langle\chi_{\frac{1}{2}}(\vec{k}_1)|\chi_{\frac{1}{2}}(\vec{k}_2)\rangle|^2 = \frac{1}{8}\left(1 + \frac{\vec{k}_1\vec{k}_2}{k_1 k_2}\right)\left(3\frac{\vec{k}_1\vec{k}_2}{k_1 k_2} - 1\right)^2, \qquad (8)$$

$$|\langle\chi_{\frac{3}{2}}(\vec{k}_1)|\chi_{\frac{1}{2}}(\vec{k}_2)\rangle|^2 = \frac{3}{8}\left(1 + \frac{\vec{k}_1\vec{k}_2}{k_1 k_2}\right)^2\left(1 - \frac{\vec{k}_1\vec{k}_2}{k_1 k_2}\right). \qquad (9)$$

These expressions can be derived easily from Eqs. (5) and (6) by putting one of the wave vectors along the $z$ direction and writing the resulting overlap squared in an explicitly rotationally invariant fashion as above.

Let us now consider a noninteracting hole gas in an infinite system. Then the ground state is characterized by the Fermi wave numbers

$$k_{h/l} = \sqrt{\frac{2m_{h/l}}{\hbar^2}\varepsilon_f}, \qquad (10)$$

where $\varepsilon_f$ is the Fermi energy. These wave numbers are related to the density $n=N/V$, $N$ being the number of holes, via

$$n = \frac{1}{3\pi^2}(k_h^3 + k_l^3). \qquad (11)$$

The kinetic energy per particle is straightforwardly obtained as follows:

$$\frac{E_{kin}}{N} = \frac{1}{5\pi^2 n}\left(\frac{\hbar^2}{2m_h}k_h^5 + \frac{\hbar^2}{2m_l}k_l^5\right). \tag{12}$$

The above expression suggests to introduce an averaged mass $\tilde{m}$ by defining

$$\tilde{m}^{3/2} = \frac{1}{2}(m_h^{3/2} + m_l^{3/2}) \tag{13}$$

along with an averaged Fermi wave number

$$\tilde{k} = \sqrt{\frac{\tilde{m}}{m_{h/l}}}k_{h/l} \tag{14}$$

fulfilling

$$n = \frac{2}{3\pi^2}\tilde{k}^3 \tag{15}$$

and

$$\tilde{k} = \sqrt{\frac{2\tilde{m}}{\hbar^2}\varepsilon_f}. \tag{16}$$

The kinetic energy per particle can then be rewritten

$$\frac{E_{kin}}{N} = \frac{3}{10}\frac{\hbar^2}{\tilde{m}}\tilde{k}^2, \tag{17}$$

which exactly resembles the familiar expression for the usual spin-1/2 electron gas.[20,21] In circumstances of Coulomb interaction between the holes, the above finding suggests to introduce a density parameter $r_s$ and a Bohr radius $\tilde{a}_B$ by defining

$$\frac{1}{n} = \frac{4\pi}{3}(r_s\tilde{a}_B)^3 \tag{18}$$

and

$$\tilde{a}_B = \frac{\hbar^2}{\tilde{m}e^2}\varepsilon_r, \tag{19}$$

where $e$ is the electron charge, where we have included a static dielectric constant $\varepsilon_r$ to account for screening from electrons in remote bands. Then the kinetic energy per particle can be rewritten

$$\frac{E_{kin}}{N} = \frac{3}{5}\left(\frac{9\pi}{8}\right)^{2/3}\frac{1}{r_s^2}\frac{e^2}{2\tilde{a}_B\varepsilon_r}, \tag{20}$$

where $e^2/2\tilde{a}_B\varepsilon_r$ is the Rydberg energy unit. Up to a slight difference in the prefactor, the above expression is again completely analogous to the result for the usual electron gas.[20,21] However, as we shall see below, the exchange contribution from Coulomb interaction cannot be casted in a form immediately analogous to the spin-degenerate electron gas.

### III. THE INTERACTING HOLE GAS IN SELF-CONSISTENT HARTREE-FOCK APPROXIMATION

We now consider an infinite system with a repulsive interaction between the holes which is naturally assumed to be translationally and rotationally invariant. Later on it will be specified to be the Coulomb repulsion. Moreover, we assume a homogeneous neutralizing background ensuring charge neutrality and canceling all direct (or Hartree) contributions from Hartree-Fock expressions.

The eigenstates (4) of the single-particle Hamiltonian (1) solve the Hartree-Fock equations

$$\varepsilon_\lambda^{HF}(\vec{k})\langle\vec{r}|\vec{k},\lambda\rangle = \frac{\hbar^2 k^2}{2m_\lambda}\langle\vec{r}|\vec{k},\lambda\rangle$$
$$- \frac{e^{i\vec{k}\vec{r}}}{\sqrt{V}}\frac{1}{(2\pi)^3}\sum_{\lambda'}\int_{k\le q_{\lambda'}}d^3k'\langle\chi_{\lambda'}(\vec{k}')|\chi_\lambda(\vec{k})\rangle$$
$$\times V(|\vec{k}-\vec{k}'|)|\chi_{\lambda'}(\vec{k}'), \tag{21}$$

where $V(|\vec{k}|)$ is the Fourier transform of the interaction potential, and $m_\lambda$ stands for $m_h$ ($m_l$) if $\lambda=\pm3/2$ ($\lambda=\pm1/2$), a notation scheme which we will also use in the following. The Hartree-Fock eigenenergies are given by

$$\varepsilon_{h/l}^{HF}(\vec{k};q_h,q_l)$$
$$= \frac{\hbar^2 k^2}{2m_{h/l}} - \frac{1}{(2\pi)^3}\int_{k'\le q_{h/l}}d^3k'\frac{1}{4}\left[1 + 3\left(\frac{\vec{k}\vec{k}'}{kk'}\right)^2\right]V[|\vec{k}-\vec{k}'|]$$
$$- \frac{1}{(2\pi)^3}\int_{k'\le q_{l/h}}d^3k'\frac{3}{4}\left[1 - \left(\frac{\vec{k}\vec{k}'}{kk'}\right)^2\right]V(|\vec{k}-\vec{k}'|). \tag{22}$$

To see that the eigenstates (4) solve the above Hartree-Fock equations, one can, again without loss of generality, take the wave vector $\vec{k}$ in Eq. (21) to point along the $z$ direction. Using the explicit parametrizations (5) and (6) of the eigenspinors in terms of polar coordinates, one easily sees that the integration over the azimuthal angle $\varphi'$ ensures that the integral in Eq. (21) is indeed proportional to $|\chi_\lambda(\vec{k})\rangle$. This result holds for any interaction potential since $|\vec{k}-\vec{k}'|$ is independent of $\varphi'$. The eigenvalues (22) are then derived by performing the summation over $\lambda'$ in Eq. (21) and using Eqs. (7)–(9). The first integral in Eq. (22) stems from the contributions with $|\lambda|=|\lambda'|$ whereas the second integral results from the cases $|\lambda|\ne|\lambda'|$. As explicitly shown in the notation of Eq. (22), these eigenvalues are functions of the integration boundaries $q_h$, $q_l$ arising in Eq. (21). In the presence of interactions, these quantities will in general not coincide with the Fermi wave numbers $k_h$, $k_l$ of the noninteracting system, as we shall see below.

### A. Self-consistent Hartree-Fock solution for Coulomb interaction: Renormalization of Fermi wave numbers

Let us now specify the interaction to be the Coulomb repulsion, i.e.,

$$V(k) = \frac{e^2}{\varepsilon_r}\frac{4\pi}{k^2}. \tag{23}$$

The Hartree-Fock eigenenergies read explicitly

$$\varepsilon_{h/l}^{HF}(\vec{k};q_h,q_l)$$

$$= \frac{\hbar^2 k^2}{2m_{h/l}} - \frac{e^2}{\varepsilon_r} \frac{q_{h/l}}{4\pi} \left[ \frac{11}{8} - \frac{3}{8} \frac{q_{h/l}^2}{k^2} + \frac{3}{4} \frac{k}{q_{h/l}} h\left(\frac{q_{h/l}}{k}\right) \right.$$

$$+ \frac{k}{q_{h/l}} \left( \frac{5}{4} \frac{q_{h/l}^2 - k^2}{k^2} + \frac{3}{16} \frac{q_{h/l}^4 - k^4}{k^4} \right) \log \left| \frac{q_{h/l} + k}{q_{h/l} - k} \right| \Bigg]$$

$$- \frac{e^2}{\varepsilon_r} \frac{q_{l/h}}{4\pi} \left[ \frac{21}{8} + \frac{3}{8} \frac{q_{l/h}^2}{k^2} - \frac{3}{4} \frac{k}{q_{l/h}} h\left(\frac{q_{l/h}}{k}\right) \right.$$

$$+ \frac{k}{q_{l/h}} \left( \frac{3}{4} \frac{q_{l/h}^2 - k^2}{k^2} - \frac{3}{16} \frac{q_{l/h}^4 - k^4}{k^4} \right) \log \left| \frac{q_{l/h} + k}{q_{l/h} - k} \right| \Bigg],$$

$$(24)$$

where the function $h(x)$ is defined by

$$h(x) = \begin{cases} 2\sum_{n=0}^{\infty} \dfrac{x^{2n+1}}{(2n+1)^2} & x \leq 1 \\[2em] \dfrac{\pi^2}{2} - 2\sum_{n=0}^{\infty} \dfrac{\left(\dfrac{1}{x}\right)^{2n+1}}{(2n+1)^2} & x \geq 1 \end{cases}. \quad (25)$$

Note that $h(1)$ is simply related to Riemann's $\zeta$ function, $h(1) = (3/2)\zeta(2) = \pi^2/4$.

The two dispersions branches (24) coincide at zero wave vector,

$$\varepsilon_{h/l}^{HF}(0;q_h,q_l) = -\frac{e^2}{\varepsilon_r \pi}(q_h + q_l) \quad (26)$$

for any values of $q_h$, $q_l$. However, when evaluated for the Fermi wave numbers $k_h$, $k_l$, they differ at the corresponding wave numbers,

$$\varepsilon_h^{HF}(k_h;k_h,k_l) \neq \varepsilon_l^{HF}(k_l;k_h,k_l). \quad (27)$$

Of course the Fermi energies for heavy and light holes have to be the same since otherwise a redistribution of occupation numbers would take place. Therefore, in order to obtain a truly self-consistent solution to the Hartree-Fock equations, the Fermi wave numbers $q_h$, $q_l$ have to be adjusted such that

$$\varepsilon_h^{HF}(q_h;q_h,q_l) = \varepsilon_l^{HF}(q_l;q_h,q_l) \quad (28)$$

under the constraint of a fixed density,

$$n = \frac{1}{3\pi^2}(q_h^3 + q_l^3). \quad (29)$$

Thus, in fact just a single parameter, say $q_h$, has to be determined numerically, which is technically a very simple task. Figure 1 shows the ratios $q_{h/l}/k_{h/l}$ of renormalized to unrenormalized Fermi wave numbers as a function of hole density for the III-V semiconductors GaAs, InAs, and InSb. The relevant parameters for these materials are summarized in Table I. As seen from the figure, for realistic parameters one always has $q_h < k_h$ and $q_l > k_l$, i.e., due to Coulomb interaction heavy hole states which get depopulated in favor of light hole states. Moreover, the renormalization of Fermi wave numbers affects primarily the light hole wave number at low
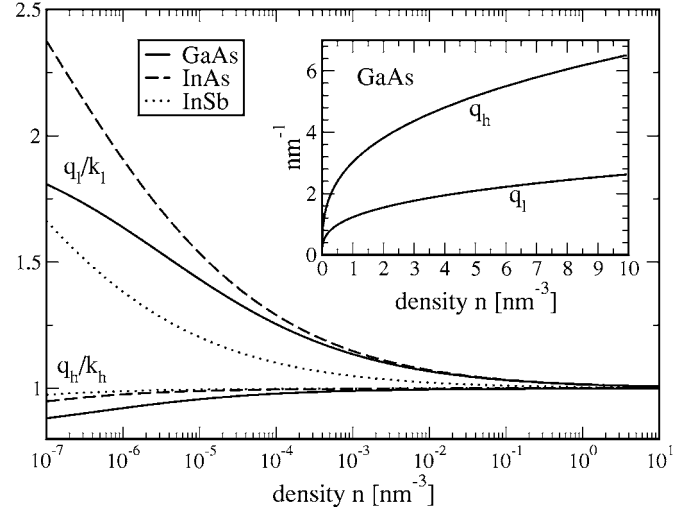


FIG. 1. The ratios of renormalized and unrenormalized Fermi wave numbers, $q_{h/l}$ and $k_{h/l}$, respectively, as a function of hole density for different III-V semiconductors. The renormalization of Fermi wave numbers affects primarily the light hole wave number at low densities. The inset shows $q_h$ and $q_l$ as a function of density for GaAs.

densities. The inset of Fig. 1 shows $q_h$ and $q_l$ as a function of density for GaAs.

In Fig. 2 we have plotted the Hartree-Fock dispersions $\varepsilon_{h/l}^{HF}(k;q_h,q_l)$ for GaAs at a hole density of $n=5 \times 10^{-4}$ nm$^{-3}$. The solid lines show the dispersion including Coulomb exchange for renormalized Fermi wave number $q_{h/l}$, while the dashed lines represent the dispersions of the free hole gas in the absence of interactions. As seen from Eqs. (24) the first derivative of the dispersions $\varepsilon_{h/l}^{HF}(k;q_h,q_l)$ with respect to $k$ diverges both at $k=q_h$ and $k=q_l$ giving rise to a vertical tangent at these points. In Fig. 2 these singularities are clearly pronounced for $\varepsilon_{h/l}^{HF}(k;q_h,q_l)$ at $k=q_{h/l}$ while they are weaker and hardly visible in the plot at $k=q_{l/h}$. The fact that weak singularities occur in the derivative $\varepsilon_{h/l}^{HF}(k;q_h,q_l)$ also at $k=q_{l/h}$ is due to the mixing of heavy and light holes, i.e., the mutual overlap between heavy and light hole states at different wave vectors. Such an effect would be absent if one just had two spin-1/2 species of different mass, say electrons and muons, living in strictly different Hilbert spaces.

### B. Comparison with the two-dimensional electron gas and other systems

As seen in Eq. (21), the eigenstates (4) of the noninteracting system provide solutions to the Hartree-Fock equations

TABLE I. The Luttinger parameters $\gamma_1$, $\gamma_2$, effective hole masses $m_{h/l}$, and static dielectric constants $\varepsilon_r$ for the III-V semiconductors GaAs, InAs, and InSb.

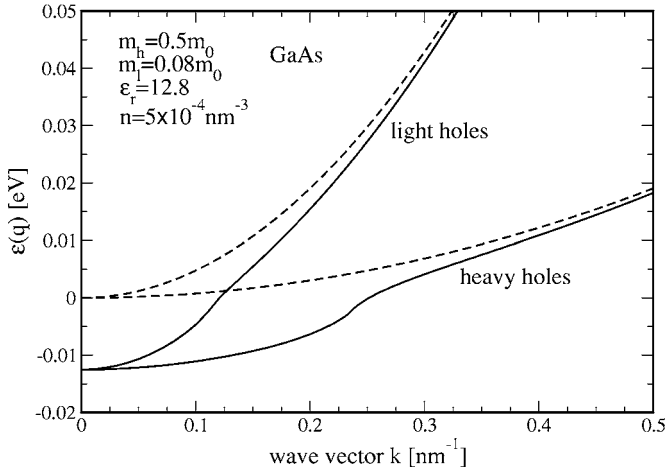| | $\gamma_1$ | $\gamma_2$ | $m_h/m_0$ | $m_l/m_0$ | $\varepsilon_r$ |
|---|---|---|---|---|---|
| GaAs | 7 | 2.5 | 0.5 | 0.08 | 12.8 |
| InAs | 20 | 9 | 0.5 | 0.026 | 14.5 |
| InSb | 35 | 15 | 0.2 | 0.015 | 18.0 |

FIG. 2. The Hartree-Fock dispersions $\varepsilon_{h/l}^{HF}(k; q_h, q_l)$ for GaAs at a hole density of $n = 5 \times 10^{-4}$ nm$^{-3}$. The solid lines show the dispersion including Coulomb exchange for renormalized Fermi wave number $q_{h/l}$, while the dashed lines represent the dispersions of the free hole gas in the absence of interactions. The singularities in $\varepsilon_{h/l}^{HF}(k; q_h, q_l)$ at $k = q_{h/l}$ are clearly pronounced while the singularities at $k = q_{l/h}$ are weaker and hardly visible in the plot.

for a general pair interaction. This observation is familiar from the usual spin-1/2 electron gas without spin-orbit coupling.[20,21] If spin-orbit interaction is present, however, such a simple structure cannot be taken for granted, and the solutions to the Hartree-Fock equations can in general become more complicated. As an example, consider a two-dimensional electron gas in a quantum well being subject to Rashba spin-orbit coupling (Ref. 22),

$$\mathcal{H} = \frac{\vec{p}^2}{2m} + \frac{\alpha}{\hbar}(p_x \sigma^y - p_y \sigma^x), \tag{30}$$

where $m$ is an effective band mass, and $\alpha$ is the Rashba parameter being tunable by an electric gate across the quantum well. $\vec{\sigma}$ are the usual Pauli matrices describing the electron spin. We note that many-body effects in this type of system have recently attracted considerable interest.[23–29] The above Hamiltonian has two energy branches,

$$\varepsilon_\pm(\vec{k}) = \frac{\hbar^2 k^2}{2m} \pm \alpha k \tag{31}$$

with eigenstates

$$\langle \vec{r} | \vec{k}, \pm \rangle = \frac{e^{i\vec{k}\vec{r}}}{\sqrt{A}} \frac{1}{\sqrt{2}} \begin{pmatrix} 1, \\ \pm(-k_y + ik_x)/k \end{pmatrix}, \tag{32}$$

where $A$ is the area of the system. Now consider an arbitrary pair interaction. Since the total Hamiltonian is still translationally invariant, the solutions to the Hartree-Fock equations can always be chosen to have a form similar as above, i.e., a plane wave factor times a two-component spinor. However, it is easy to see that the eigenstates (32) do not provide solutions to the Hartree-Fock equations for a general interaction potential. This observation is due to the fact that the angular integration in this two-dimensional case is different from the three-dimensional situation of Eq. (21). Only for

a pure contact interaction (having a constant Fourier transform), the eigenstates (32) solve the Hartree-Fock equations.

The same conclusions apply to bulk valence-band electrons being subject to the three-dimensional Dresselhaus spin-orbit coupling term,[30] and to heavy holes in asymmetric quantum wells.[31,32] In both cases, the effective spin-orbit interaction is trilinear in the particle momentum.

The situation of the two-dimensional electron gas becomes even more complicated if also Dresselhaus spin-orbit coupling is considered which reads in its two-dimensional approximation (Ref. 33)

$$\mathcal{H}_D = \frac{\beta}{\hbar}(p_y \sigma^y - p_x \sigma^x) \tag{33}$$

with a coupling parameter $\beta$. However, in the case when the Rashba parameter is of equal magnitude as the Dresselhaus parameter, $\alpha = \pm \beta$, the corresponding eigenstates of the noninteracting system solve the Hartree-Fock equations for an arbitrary interaction potential. This is due to the additional conserved quantity arising at this point[34] which cancels the effects of spin-orbit coupling in many respects.[34,35]

### C. Total ground state energy

Let us come back to the case heavy and light holes interacting via Coulomb repulsion in the valence band of bulk III-V semiconductors. With the renormalized Fermi wave numbers $q_h$, $q_l$, the total kinetic energy per particle in the ground state reads

$$\frac{E_{kin}(q_h, q_l)}{N} = \frac{1}{5\pi^2 n}\left(\frac{\hbar^2}{2m_h}q_h^5 + \frac{\hbar^2}{2m_l}q_l^5\right) \tag{34}$$

with the density $n$ given by Eq. (29), and for the total exchange energy per particle one finds

$$\frac{E_{ex}(q_h, q_l)}{N} = -\frac{e^2}{\varepsilon_r}\frac{1}{16\pi^3 n}[4(q_h^4 + q_l^4) - 3(q_h^3 - q_l^3)(q_h - q_l)], \tag{35}$$

resulting in a total energy per hole

$$\frac{E_{tot}(q_h, q_l)}{N} = \frac{E_{kin}(q_h, q_l)}{N} + \frac{E_{ex}(q_h, q_l)}{N}. \tag{36}$$

To obtain the corresponding results for the unrenormalized Fermi wave numbers, one just has to replace in the above expressions $q_{h/l}$ with $k_{h/l}$. Note that the unrenormalized expression $E_{tot}(k_h, k_l)$ is the equivalent to first-order perturbation theory in the Coulomb repulsion where one just computes the expectation value of the interaction with respect to the ground state of the noninteracting system characterized by the Fermi wave numbers $k_{h/l}$.

Figure 3 shows the ground state energy per particle $E_{tot}(q_h, q_l)/N$ from the self-consistent Hartree-Fock treatment and the result $E_{tot}(k_h, k_l)/N$ from lowest-order perturbation theory as a function of the density for GaAs. As seen in the figure, it is always $E_{tot}(q_h, q_l) < E_{tot}(k_h, k_l)$, i.e., the self-consistent Hartree-Fock approach gives the lower ground state energy. This is clear since the ground state ob-
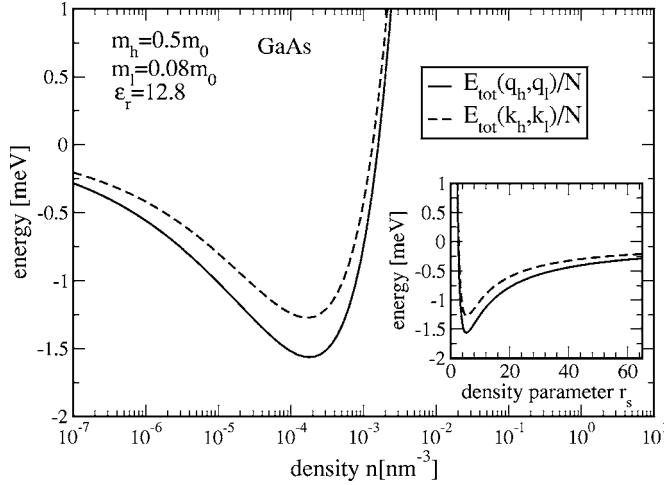
FIG. 3. The ground state energy per particle $E_{tot}(q_h, q_l)/N$ from the self-consistent Hartree-Fock treatment (with renormalized Fermi wave numbers) and the result $E_{tot}(k_h, k_l)/N$ from lowest-order perturbation theory (with unrenormalized Fermi wave numbers) as a function of the density for GaAs. The inset shows the same data as the main panel but as a function of the density parameter $r_s$.

tained from a self-consistent solution of the Hartree-Fock equations is by construction the Slater determinant of lowest energy in the Hilbert space of the many-particle system. Thus, any other Slater determinant state has to have a higher energy expectation value. In fact, the renormalized Fermi wave numbers can alternatively be obtained by minimizing $E_{tot}(q_h, q_l)/N$ with respect to $q_h$, $q_l$ under the constraint of a fixed density $n$. In the absence of interactions the minimization of $E_{kin}(q_h, q_l)/N$ immediately reproduces the results of Sec. II (as it has to be), whereas for $E_{tot}(q_h, q_l)/N$ one ends up with a coupled system of polynomial equations which does not seem to allow for an explicit analytical solution.

The hole densities usually occurring in realistic samples lie at $n = 0.01-1.0$ nm$^{-3}$. At such densities, the difference between $E_{tot}(q_h, q_l)/N$ and $E_{tot}(k_h, k_l)/N$ is indeed very small (cf. Fig. 3), and the density parameter $r_s$ as defined in Eqs. (18) and (19) is of order unity, giving confidence to the validity of the Hartree-Fock approach.[20,21] At smaller densities like $n < 0.001$ nm$^{-3}$, $E_{tot}(q_h, q_l)/N$, and $E_{tot}(k_h, k_l)/N$ differ appreciably. However, at these densities Hartree-Fock theory cannot be expected to give accurate results. On the other hand, it is common in many-body perturbation theory to refer to all contributions to the ground state energy beyond the lowest-order exchange term as correlation contributions.[20,21] In this sense the difference between $E_{tot}(q_h, q_l)/N$ and $E_{tot}(k_h, k_l)/N$ (resulting from the renormalization of Fermi momenta) can be viewed as a correlation effect.

The inset of Fig. 3 shows the same data as the main panel, but as a function of the density parameter $r_s$. The minimum of the Hartree-Fock ground state energy lies at about $r_s \approx 5$, similar to the case of the usual spin-1/2 electron gas.[20,21] Note that the maximum difference between $E_{tot}(q_h, q_l)/N$ and $E_{tot}(k_h, k_l)/N$ is also achieved around this value.

### D. Pair distribution function

It is instructive to also investigate the pair distribution function $g(r)$ defined by

$$n^2 g(|\vec{r} - \vec{r}'|) = \left\langle \sum_{I \neq J} \delta(\vec{r} - \vec{r}_I) \delta(\vec{r}' - \vec{r}_J) \right\rangle, \quad (37)$$

where $I, J$ label the particles in the system and $\langle \cdot \rangle$ denotes the expectation value within the ground state. The ground state obtained from self-consistent Hartree-Fock theory is a single Slater determinant. Here the pair distribution function can be formulated

$$g(r) = 1 - [g_{hh}^{ex}(r) + g_{ll}^{ex}(r) + g_{hl}^{ex}(r)], \quad (38)$$

where $g_{hh}^{ex}$ ($g_{ll}^{ex}$) are the exchange contributions from heavy (light) hole states only, whereas $g_{hl}^{ex}$ stems from exchange between heavy and light holes. It is straightforward to calculate these contributions explicitly using Eqs. (7)–(9). The results can be formulated as follows:

$$g_{hh}^{ex}(r) = \left(\frac{m_h}{\tilde{m}}\right)^3 \left\{ \frac{9}{32}[I_1(q_h r)]^2 + \frac{27}{16}[I_2(q_h r)]^2 \right.$$
$$\left. + \frac{27}{8}[I_3(q_h r)]^2 \right\}, \quad (39)$$

$$g_{ll}^{ex}(r) = \left(\frac{m_l}{\tilde{m}}\right)^3 \left\{ \frac{9}{32}[I_1(q_l r)]^2 + \frac{27}{16}[I_2(q_l r)]^2 + \frac{27}{8}[I_3(q_l r)]^2 \right\}, \quad (40)$$

$$g_{ll}^{ex}(r) = \left(\frac{m_h}{\tilde{m}}\right)^{3/2} \left(\frac{m_l}{\tilde{m}}\right)^{3/2} \left\{ \frac{27}{16}[I_1(q_h r)][I_1(q_l r)] \right.$$
$$\left. - \frac{27}{8}[I_2(q_h r)][I_2(q_l r)] - \frac{27}{4}[I_3(q_h r)][I_3(q_l r)] \right\}, \quad (41)$$

where we have defined

$$I_1(x) = -\frac{\cos x}{x^2} + \frac{\sin x}{x^3}, \quad (42)$$

$$I_2(x) = -\frac{\sin x}{x^3} + \frac{1}{x^3}\int_0^x dy \frac{\sin y}{y}, \quad (43)$$

$$I_3(x) = -\frac{1}{2}\frac{\cos x}{x^2} + \frac{3}{2}\frac{\sin x}{x^3} - \frac{1}{x^3}\int_0^x dy \frac{\sin y}{y}. \quad (44)$$

Note that $g(0) = 3/4$, corresponding to a fermionic gas with four spin components. In the absence of spin-orbit coupling, $q_h = q_l$, the contributions involving $I_2$, $I_3$ cancel and one obtains the well-known exchange terms of the usual electron gas.[20,21] Figure 4 shows the pair distribution function in GaAs for three different densities. At high enough hole density one can see Friedel-type modulations of $g(r)$ whose period is essentially given by twice the heavy hole Fermi wave number $q_h$.
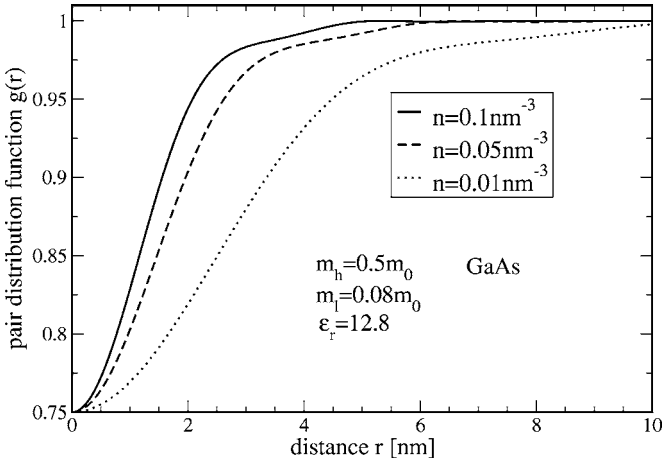
FIG. 4. The pair distribution function $g(r)$ for GaAs at three different densities.

### E. The dielectric function in random phase approximation

Within random phase approximation (RPA), the dielectric function is given by (Refs. 20 and 21)

$$\varepsilon^{RPA}(\vec{k},\omega) = 1 - V(\vec{k})\chi_0(\vec{k},\omega), \tag{45}$$

where $\chi_0(\vec{k},\omega)$ is the susceptibility of the noninteracting system. Its real part has the form

$$\chi_0(\vec{k},\omega) = \frac{1}{(2\pi)^3} \sum_{\lambda_1,\lambda_2} \int d^3k' \left[ |\langle \chi_{\lambda_1}(\vec{k}')|\chi_{\lambda_2}(\vec{k}'+\vec{k})\rangle|^2 \right.$$
$$\left. \times \frac{f(\vec{k}',\lambda_1) - f(\vec{k}'+\vec{k},\lambda_2)}{\hbar\omega - [\varepsilon_{\lambda_2}(\vec{k}'+\vec{k}) - \varepsilon_{\lambda_1}(\vec{k}')]} \right] \tag{46}$$

$$= \frac{2}{(2\pi)^3} \sum_{\lambda_1,\lambda_2} \int d^3k' \left[ |\langle \chi_{\lambda_1}(\vec{k}')|\chi_{\lambda_2}(\vec{k}'+\vec{k})\rangle|^2 \right.$$
$$\left. \times \frac{f(\vec{k}',\lambda_1)[\varepsilon_{\lambda_2}(\vec{k}'+\vec{k}) - \varepsilon_{\lambda_1}(\vec{k}'))]}{(\hbar\omega)^2 - [\varepsilon_{\lambda_2}(\vec{k}'+\vec{k}) - \varepsilon_{\lambda_1}(\vec{k}')]^2} \right]. \tag{47}$$

Here $f(\vec{k},\lambda_1)$ are Fermi functions, and to obtain Eq. (46) from Eq. (47) we have used elementary properties of the spinor overlaps and the dispersion relations of the noninteracting system. In particular, in the static limit one has

$$\chi_0(\vec{k},0) = \frac{2}{(2\pi)^3} \sum_{\lambda_1,\lambda_2} \int d^3k' \left[ |\langle \chi_{\lambda_1}(\vec{k}')|\chi_{\lambda_2}(\vec{k}'+\vec{k})\rangle|^2 \right.$$
$$\left. \times \frac{f(\vec{k}',\lambda_1)}{\varepsilon_{\lambda_1}(\vec{k}') - \varepsilon_{\lambda_2}(\vec{k}'+\vec{k})} \right]. \tag{48}$$

By construction, $\chi_0(\vec{k},\omega)$ is entirely determined by the properties of the noninteracting system. In particular, at zero temperature, the integration boundaries in the above expressions are given by the unrenormalized Fermi wave numbers $k_h$, $k_l$. However, in order to be consistent with the self-consistent Hartree-Fock treatment, one may use the renormalized wave numbers $q_h$, $q_l$ instead. As seen above, at high enough densities, the difference is negligible.

For early work on dielectric response in zero-gap semiconductors we refer to Refs. 36 and 37. An evaluation of the static expression (48) for the case of the two-dimensional electron gas with Rashba spin-orbit interaction has been given by Chen and Raikh.[23] Their findings have recently been challenged by Pletyukhov and Gritsev.[28] The main technical obstacle there is posed by nonelementary integrals. In the present case of the three-dimensional hole gas, however, the occurring integrations are mostly elementary but often very tedious.

Analogously as for the three-dimensional electron gas the static dielectric function for the hole system at zero temperature can be formulated

$$\varepsilon^{RPA}(\vec{k},0) = 1 + \frac{k_{TF}^2}{k^2} L\left( \frac{k}{2q_h}, \frac{k}{2q_l} \right), \tag{49}$$

where

$$k_{TF} = \sqrt{\frac{6\pi e^2 n}{\varepsilon_r \varepsilon_f}} \tag{50}$$

is the usual Thomas-Fermi screening wave number. The function $L$ is the analogue of the well-known Lindhard correction for the electron gas. The explicit form of $L$ for the hole system, however, is rather lengthy and tedious and shall not be given here. For a long wavelength, $k \to 0$, $L$ approaches unity. In this limit terms mixing heavy and light holes do not contribute to the dielectric function. A similar finding is valid for the plasma frequency which characterizes collective excitations at zero wave vector.[20,21] Here contributions mixing heavy and light holes are also absent, and the plasma frequency $\omega_p$ is given by

$$\omega_p^2 = \frac{4\pi e^2}{\varepsilon_r} \left( \frac{n_h}{m_h} + \frac{n_l}{m_l} \right), \tag{51}$$

where $n_h$, $n_l$ are the densities of heavy and light holes, respectively.

## IV. DISCUSSION AND OUTLOOK

We have studied the homogeneous interacting hole gas in $p$-doped bulk III-V semiconductors modeled by Luttinger's Hamiltonian in the spherical approximation. The Coulomb repulsion is taken into account via a self-consistent Hartree-Fock treatment. As a nontrivial feature of the model, the self-consistent solutions of the Hartree-Fock equations can be found in an almost purely analytical fashion. As we have discussed in detail in Sec. III B this is not the case for other types of effective spin-orbit coupling terms. As an important qualitative feature, the Coulomb repulsion renormalizes the Fermi wave numbers for heavy and light holes: The interaction leads to a redistribution of occupation numbers from heavy holes to light holes compared to the noninteracting case. As a consequence, the ground state energy found in the self-consistent Hartree-Fock approach and the result from lowest-order perturbation theory differ from each other. By

construction, the self-consistent Hartree-Fock result gives the lower ground state energy.

The three-dimensional III-V semiconductor hole gas is particularly relevant for ferromagnetic semiconductors which are usually *p*-doped materials. In the theoretical description of these materials, the interaction between itinerant charge carriers is most often neglected,[2–4] or absorbed in effective Fermi liquid parameters.[8] The typical hole densities in Mn-doped GaAs, the most prominent and best-studied ferromagnetic semiconductor, are of order $n \approx 0.1$ nm$^{-3}$. For such carrier concentrations, the density parameter $r_s$ is of order unity, giving confidence to the validity of the Hartree-Fock approach.[20,21] Moreover, as seen in the present investigation, the renormalization of Fermi wave numbers is negligible at such densities, i.e., the interacting ground state in Hartree-Fock approximation and the noninteracting ground state are practically the same. In this sense, the above mentioned models for ferromagnetic semiconductors neglecting the Coulomb interaction are supported by the present study. However, the single-particle Hamiltonian used there is a simplified one which does not take into account the split-off band. A more complete description of the valence band including these states is given by the six-band Kohn-Luttinger model[38] as used in Refs. 7 and 8. In fact, the influence of the split-off band is known to be important for the stability of the ferromagnetic order.[39] However, for the full six-band Kohn-Luttinger Hamiltonian mainly analytical progress as in the present work is certainly not possible, and one would need to resort to more complicated numerics.

During the last years various predictions and subsequent experiments regarding spin Hall transport in semiconductor systems have attracted a remarkable amount of interest;[14–16] for a recent overview see also Ref. 17. The first work opening the field of intrinsic spin Hall effect was a paper by Murakami, Nagaosa, and Zhang who considered a *p*-type bulk III-V semiconductor.[14] The single-particle Hamiltonian used in Ref. 14 is the same as here with the Coulomb repulsion between the holes being neglected.[14] For a disorder-free system, the spin Hall conductivity is given by (Refs. 17 and 40)

$$\sigma^S(q_h, q_l) = \frac{e}{4\pi^2} \frac{\gamma_1 + 2\gamma_2}{\gamma_2} (q_h - q_l), \tag{52}$$

where the direction of the spin current, its polarization direction, and the direction of the electric field are mutually per-
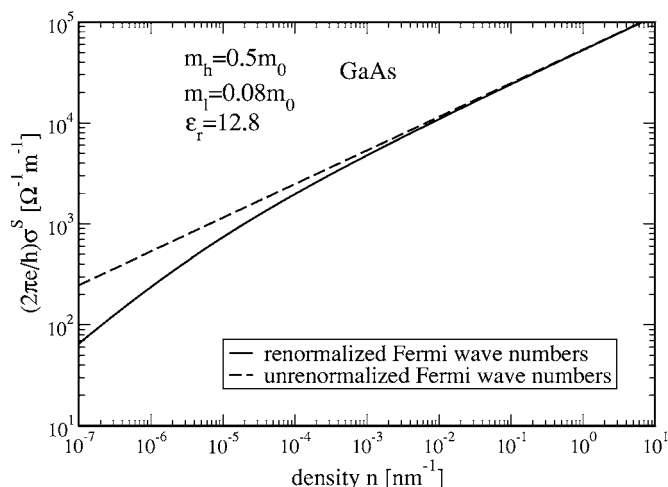


FIG. 5. The spin Hall conductivity $\sigma^S$ (converted to units of charge transport) as a function of hole density $n$ for GaAs.

pendicular. In the above expression we have used the renormalized Fermi wave numbers $q_h$, $q_l$. Figure 5 shows a spin Hall conductivity as a function of hole density for GaAs both for renormalized and unrenormalized Fermi wave numbers. To facilitate the comparison to the usual charge conductivity, we have converted the spin Hall conductivity to units of charge transport by multiplying with a factor of $e/\hbar$. As shown in the figure, at densities $n \gtrsim 0.01$ nm$^{-3}$ typical for realistic samples, the difference between the case of renormalized and unrenormalized wave numbers is negligible. Appreciable discrepancies occur only at small densities, where the validity of the Hartree-Fock treatment becomes questionable anyway.

Finally, we hope that the present study will initiate further investigations on interacting III-V semiconductor hole systems. One possible direction is to perform (presumably numerical) Hartree-Fock calculations for more complex band structure models as mentioned above. Another obvious goal for future studies is to investigate many-body effects beyond the Hartree-Fock level.

## ACKNOWLEDGMENT

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