Rashba spin splitting in two-dimensional electron and hole systems

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(Received 25 January 2000; revised manuscript received 17 May 2000)

In two-dimensional (2D) hole systems the inversion asymmetry induced spin splitting differs remarkably from its familiar counterpart in the conduction band. While the so-called Rashba spin splitting of electron states increases linearly with in-plane wave vector $k_\parallel$, the spin splitting of heavy-hole states can be of third order in $k_\parallel$ so that spin splitting becomes negligible in the limit of small 2D hole densities. We discuss consequences of this behavior in the context of recent arguments on the origin of the metal-insulator transition observed in 2D systems.

At zero magnetic field, B spin splitting in quasi two-dimensional (2D) semiconductor quantum wells (QW's) can be a consequence of the bulk inversion asymmetry (BIA) of the underlying crystal (e.g., a zinc-blende structure) and of the structure inversion asymmetry (SIA) of the confinement potential. This $B=0$ spin splitting[1,2] is the subject of considerable interest because it concerns details of energy-band structure that are important in both fundamental research and electronic device applications (Refs. 3–23 and references therein).

Here we want to focus on the SIA spin splitting that is usually the dominant part of $B=0$ spin splitting in 2D systems.[3,4] To lowest order in $k_\parallel$ SIA spin splitting in 2D electron systems is given by the so-called Rashba model,[5] which predicts a spin splitting linear in $k_\parallel$. For small in-plane wave vector $k_\parallel$, this is in good agreement with more accurate numerical computations.[6] For 2D hole systems, on the other hand, the situation is more complicated because of the fourfold degeneracy of the topmost valence band Γ_8^v, and so far only numerical computations on hole spin splitting have been performed.[7–9] In the present paper we will develop an analytical model for the SIA spin splitting of 2D hole systems. We will show that in contrast to the familiar Rashba model the spin splitting of heavy-hole (HH) states is basically proportional to $k_\parallel^3$. This result was already implicitly contained in several numerical computations.[7–9] But a clear analytical framework was missing. We will discuss consequences of this behavior in the context of recent arguments on the origin of the metal-insulator transition observed in 2D systems.[10,11]

First we want to review the major properties of the Rashba model[5]

$$H_{6c}^{\mathrm{SO}}=\alpha\mathbf{k}\times\mathbf{E}\cdot\boldsymbol{\sigma}. \tag{1}$$

Here $\boldsymbol{\sigma}=(\sigma_x,\sigma_y,\sigma_z)$ denotes the Pauli spin matrices, α is a material-specific prefactor,[12,13] and $\mathbf{E}$ is an effective electric field that results from the built-in or external potential V as well as from the position dependent valence-band edge.[14] For $\mathbf{E}=(0,0,E_z)$, Eq. (1) becomes (using explicit matrix notation)

$$H_{6c}^{\mathrm{SO}}=\alpha E_z\begin{pmatrix}0 & k_-\\ k_+ & 0\end{pmatrix} \tag{2}$$

with $k_\pm=k_x\pm ik_y$. By means of perturbation theory we obtain for the spin splitting of the subband dispersion to lowest order in $\mathbf{k}_\parallel=(k_x,k_y,0)$

$$\mathcal{E}_{6c}^{\mathrm{SO}}(\mathbf{k}_\parallel)=\pm\langle\alpha E_z\rangle k_\parallel. \tag{3}$$

Using this simple formula several groups determined the prefactor $\langle\alpha E_z\rangle$ by analyzing Shubnikov-de Haas (SdH) oscillations.[15–18]

Equation (3) predicts an SIA spin splitting that is linear in $k_\parallel$. For small $k_\parallel$, Eq. (3) thus becomes the dominant term in the energy dispersion $\mathcal{E}_\pm(\mathbf{k}_\parallel)$, i.e., SIA spin splitting of electron states is most important for small 2D densities. In particular, we get a divergent van Hove singularity of the density-of-states (DOS) at the bottom of the subband,[6] which is characteristic for a k linear spin splitting. As an example, we show in Fig. 1 the self-consistently calculated[6] subband dispersion $\mathcal{E}_\pm(k_\parallel)$, DOS effective mass m^*/m_0, and spin splitting $\mathcal{E}_+(k_\parallel)-\mathcal{E}_-(k_\parallel)$ for a metal-oxide semiconductor (MOS) inversion layer on InSb obtained by means of the 8×8 Hamiltonian in Ref. 24. For small $k_\parallel$, the spin splitting increases linearly as a function of $k_\parallel$, in agreement with Eq. (3). Due to nonparabolicity, the spin splitting for larger $k_\parallel$ converges toward a constant.[6]

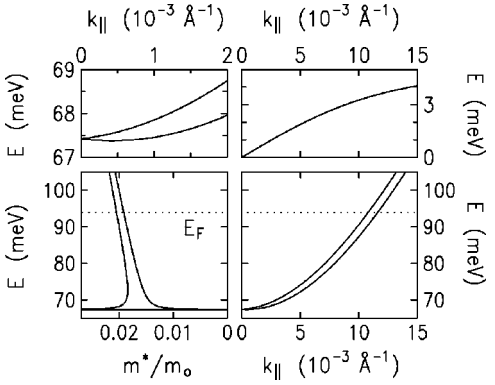

FIG. 1. Self-consistently calculated subband dispersion $\mathcal{E}_\pm(k_\parallel)$ (lower right), DOS effective mass m^*/m_0 (lower left), spin splitting $\mathcal{E}_+(k_\parallel)-\mathcal{E}_-(k_\parallel)$ (upper right) and subband dispersion $\mathcal{E}_\pm(k_\parallel)$ in the vicinity of $k_\parallel=0$ (upper left) for an MOS inversion layer on InSb with $N_s=2\times10^{11}$ cm^{-2} and $|N_A-N_D|=2\times10^{16}$ cm^{-2}. The dotted line indicates the Fermi energy E_F.

The spin splitting results in unequal populations $N_\pm$ of the two branches $\mathcal{E}_\pm(k_\parallel)$. For a given total density $N_s=N_+ +N_-$ and a subband dispersion $\mathcal{E}_\pm(k_\parallel)=\langle\mu\rangle k_\parallel^2 \pm\langle\alpha E_z\rangle k_\parallel$ with $\mu=\hbar^2/2m^*$ we obtain

$$N_\pm=\frac{1}{2}N_s\pm\frac{\langle\alpha E_z\rangle}{8\pi\langle\mu\rangle^2}\sqrt{8\pi\langle\mu\rangle^2 N_s-\langle\alpha E_z\rangle^2}. \tag{4}$$

This equation can be directly compared with, e.g., the results of SdH experiments.[15–18]

The Rashba model (1) can be derived by purely group-theoretical means. The electron states in the lowest conduction band are *s* like (orbital angular momentum $l=0$). With spin-orbit (SO) interaction we have total angular momentum $j=1/2$. Both $\mathbf{k}$ and $\mathbf{E}$ are polar vectors and $\mathbf{k}\times\mathbf{E}$ is an axial vector (transforming according to the irreducible representation Γ_4 of T_d).[13,24] Likewise, $\boldsymbol{\sigma}$ is an axial vector. The dot product (1) of $\mathbf{k}\times\mathbf{E}$ and $\boldsymbol{\sigma}$ therefore transforms according to the identity representation Γ_1, in accordance with the theory of invariants.[25] In the Γ_6^c conduction band the scalar triple product (1) is the only term of first order in $\mathbf{k}$ and $\mathbf{E}$ that is compatible with the symmetry of the band.

Now we want to compare the Rashba model (1) with the SIA spin splitting of hole states. The topmost valence band is *p* like ($l=1$). With SO interaction we have $j=3/2$ for the HH/light-hole (LH) states (Γ_8^v) and $j=1/2$ for the SO states (Γ_7^v). For the Γ_8^v valence band there are two sets of matrices that transform like an axial vector, namely, $\mathbf{J}=(J_x,J_y,J_z)$ and $\boldsymbol{\mathcal{J}}=(J_x^3,J_y^3,J_z^3)$ (Refs. 24 and 26). Here J_x, J_y, and J_z are the angular momentum matrices for $j=3/2$. Thus we get[27]

$$H_{8v}^{\mathrm{SO}}=\beta_1\mathbf{k}\times\mathbf{E}\cdot\mathbf{J}+\beta_2\mathbf{k}\times\mathbf{E}\cdot\boldsymbol{\mathcal{J}}. \tag{5}$$

Similar to the Rashba model, the first term has axial symmetry with the symmetry axis being the direction of the electric field $\mathbf{E}$. The second term is anisotropic, i.e., it depends on both the crystallographic orientation of $\mathbf{E}$ and $\mathbf{k}$. Using $\mathbf{k}\cdot\mathbf{p}$ theory we find that the prefactor β_2 is always much smaller than β_1, i.e., the dominant term in Eq. (5) is the first term. This is due to the fact that the $\mathbf{k}\cdot\mathbf{p}$ coupling between Γ_8^v and Γ_6^c is isotropic, so that it contributes to β_1 but not to β_2. The prefactor β_2 stems from $\mathbf{k}\cdot\mathbf{p}$ coupling to more remote bands such as the higher conduction bands Γ_8^c and Γ_7^c.

For $\mathbf{E}=(0,0,E_z)$, Eq. (5) becomes (using explicit matrix notation with $j=3/2$ eigenstates in the order $j_z=+3/2$, $+1/2,-1/2,-3/2$)

$$H_{8v}^{\mathrm{SO}}=\beta_1 E_z\begin{pmatrix} 0 & \frac{1}{2}\sqrt{3}k_- & 0 & 0\\ \frac{1}{2}\sqrt{3}k_+ & 0 & k_- & 0\\ 0 & k_+ & 0 & \frac{1}{2}\sqrt{3}k_-\\ 0 & 0 & \frac{1}{2}\sqrt{3}k_+ & 0\end{pmatrix}$$
$$+\beta_2 E_z\begin{pmatrix} 0 & \frac{7}{8}\sqrt{3}k_- & 0 & 3/4k_+\\ \frac{7}{8}\sqrt{3}k_+ & 0 & 5/2k_- & 0\\ 0 & 5/2k_+ & 0 & \frac{7}{8}\sqrt{3}k_-\\ 3/4k_- & 0 & \frac{7}{8}\sqrt{3}k_+ & 0\end{pmatrix}. \tag{6}$$

Here the first term couples the two LH states ($j_z=\pm1/2$) and the HH states ($j_z=\pm3/2$) to the LH states. But there is no *k* linear splitting of the HH states proportional to β_1. The second matrix in Eq. (6) contains a *k* linear coupling of the HH states.

We want to emphasize that H_{6c}^{SO} and H_{8v}^{SO} are *effective* Hamiltonians for the spin splitting of electron and hole subbands, which are implicitly contained in the full multiband Hamiltonian for the subband problem[6,14]

$$H=H_{\mathbf{k}\cdot\mathbf{p}}(\mathbf{k}_\parallel,k_z=-i\partial_z)+eE_z z\mathbb{1}. \tag{7}$$

Here $H_{\mathbf{k}\cdot\mathbf{p}}$ is a $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian for the bulk band structure (i.e., $H_{\mathbf{k}\cdot\mathbf{p}}$ does not contain H_{6c}^{SO} or H_{8v}^{SO}) and we have restricted ourselves to the lowest-order term in a Taylor expansion of the confining potential $V(z)=V_0+eE_z z+\mathcal{O}(z^2)$ which reflects the inversion asymmetry of $V(z)$. The effective Hamiltonians (2) and (6) stem from the combined effect of $H_{\mathbf{k}\cdot\mathbf{p}}$ and the term $eE_z z$. For a systematic investigation of the importance of the different terms in H we have developed an analytical approach based on a perturbative diagonalization of H using a suitable set of trial functions and Löwdin partitioning.[25,28] Though we cannot expect accurate numerical results from such an approach it is an instructive complement for numerical methods, as we can clearly identify in the subband dispersion $\mathcal{E}(\mathbf{k}_\parallel)$ the terms proportional to E_z that are breaking the spin degeneracy. Neglecting in $H_{\mathbf{k}\cdot\mathbf{p}}$ remote bands like Γ_8^c and Γ_7^c we obtain for the HH spin splitting to lowest order in $\mathbf{k}_\parallel$

$$\mathcal{E}_{\mathrm{HH}}^{\mathrm{SO}}(k_\parallel)\propto\pm\langle\beta_1 E_z\rangle k_\parallel^3. \tag{8a}$$

In particular, we have no *k* linear splitting (and $\beta_2\equiv0$) if we restrict ourselves to the Luttinger Hamiltonian,[26] which includes Γ_8^c and Γ_7^c by means of second-order perturbation theory.[7,29] Accurate numerical computations[6] show that the dominant part of the *k* linear splitting of the HH states is due to BIA. However, for typical densities this *k* linear splitting is rather small. For the LH states we have to lowest order in $\mathbf{k}_\parallel$

$$\mathcal{E}_{\mathrm{LH}}^{\mathrm{SO}}(k_\parallel)\propto\pm\langle\beta_1 E_z\rangle k_\parallel. \tag{8b}$$

Thus we have a qualitative difference between the spin splitting of electron and LH states that is proportional to $k_\parallel$ and the splitting of HH states that essentially is proportional to $k_\parallel^3$. The former is most important in the low-density regime whereas the latter becomes negligible for small densities. Note that for 2D hole systems the first subband is usually HH like so that for low densities the SIA spin splitting is given by Eq. (8a). In Eq. (8) the lengthy prefactors depend on the geometry of the QW. But the order of the terms with respect to $k_\parallel$ is independent of such details. It is crucial that, basically, we have

$$\alpha,\beta_1,\beta_2\propto\Delta_0 \tag{9}$$

with Δ_0 the SO gap between the bulk valence bands Γ_8^v and Γ_7^v, i.e., we have no SIA spin splitting for $\Delta_0=0$.[13] This can be most easily seen if we express $H_{\mathbf{k}\cdot\mathbf{p}}$ in a basis of orbital angular momentum eigenstates.

A more detailed analysis of our analytical model shows that both H_{6c}^{SO} and H_{8v}^{SO} stem from a third-order perturbation

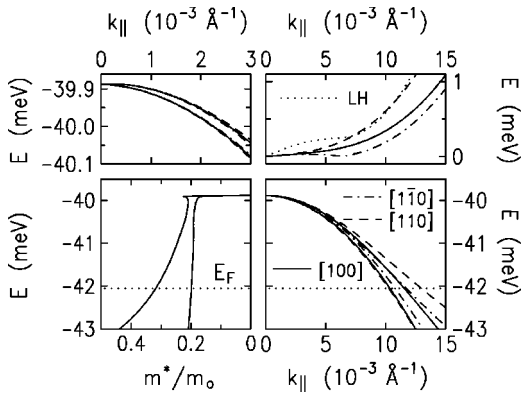

FIG. 2. Self-consistently calculated anisotropic dispersion $\mathcal{E}_{\pm}(\mathbf{k}_{\|})$ (lower right), DOS effective mass m^*/m_0 (lower left), spin splitting $\mathcal{E}_{+}(\mathbf{k}_{\|})-\mathcal{E}_{-}(\mathbf{k}_{\|})$ (upper right), and dispersion $\mathcal{E}_{\pm}(\mathbf{k}_{\|})$ in the vicinity of $k_{\|}=0$ (upper left) of the topmost HH subband of a [001] grown GaAs/$Al_{0.5}Ga_{0.5}$As heterostructure with $N_s=2\times10^{11}$ cm^{-2} and $|N_A-N_D|=2\times10^{16}$ cm^{-2}. Different line styles correspond to different directions of the in-plane wave vector $\mathbf{k}_{\|}$ as indicated. In the lower-right figure, the dotted line indicates the Fermi energy E_F. In the upper-right part, the dotted line shows the spin splitting of the first LH subband for $\mathbf{k}_{\|}\|[100]$.

theory for $k_{\pm}$, $k_z=-i\partial_z$ and eE_zz. This seems to be a rather high order. Nevertheless, the resulting terms are fairly large.[30] In agreement with Refs. 3,6, and 14 this is a simple argument to resolve the old controversy based on an argument by Ando[31] that spin splitting in 2D systems ought to be negligibly small because for bound states in first order we have $\langle E_z\rangle=0$. We note that the present ansatz for the prefactors α and β_1,β_2 is quite different from the ansatz in Ref. 12. We obtain H_{6c}^{SO} and H_{8v}^{SO} by means of Löwdin partitioning of the Hamiltonian (7) whereas in Ref. 12 the authors explicitly introduced H_{6c}^{SO} into their model. Moreover, we evaluate the matrix elements of eE_zz with respect to envelope functions for the bound states whereas in Ref. 12 the authors considered matrix elements of eE_zz with respect to bulk Bloch functions. The latter quantities are problematic because they depend on the origin of the coordinate frame.

As an example, we show in Fig. 2 the self-consistently calculated[6] anisotropic dispersion $\mathcal{E}_{\pm}(\mathbf{k}_{\|})$, DOS effective mass m^*/m_0, and spin splitting $\mathcal{E}_{+}(\mathbf{k}_{\|})-\mathcal{E}_{-}(\mathbf{k}_{\|})$ of the topmost HH subband of a GaAs/$Al_{0.5}Ga_{0.5}$As heterostructure. The calculation was based on a 14×14 Hamiltonian (Γ_8^c, Γ_7^c, Γ_6^c, Γ_8^v, and Γ_7^v). It fully took into account both SIA and BIA. The weakly divergent van Hove singularity of the DOS effective mass at the subband edge indicates that the k linear splitting is rather small. [Its dominant part is due to BIA (Refs. 4 and 24).] Basically, the spin splitting in Fig. 2 is proportional to $k_{\|}^3$. For comparison, in the upper-right part of Fig. 2, the dotted line shows the spin splitting of the first LH subband. For small $k_{\|}$, the splitting is linear in $k_{\|}$, but for larger $k_{\|}$, due to both HH-LH mixing and nonparabolicity, it is dominated by terms of higher order in $k_{\|}$.

Only for the crystallographic growth directions [001] and [111] the hole subband states at $k_{\|}=0$ are pure HH and LH states. For low-symmetry growth directions like [113] and [110] we have mixed HH-LH eigenstates even at $k_{\|}=0$, though often the eigenstates can be labeled by their dominant spinor components.[32] The HH-LH mixing adds a k linear term to the splitting (8a) of the HH states, which often exceeds $\langle\beta_2E_z\rangle k_{\|}$. However, this effect is still small when compared with the cubic splitting. Note that HH-LH mixing[7] at nonzero $k_{\|}$ does not affect our general conclusions concerning the HH spin splitting because for larger $k_{\|}$ the cubic term always dominates. A significant $k_{\|}$ linear spin splitting in 2D hole systems can be obtained in strained QW's, where the order of the topmost HH and LH subbands can be reversed.[33]

For a HH subband dispersion $\mathcal{E}_{\pm}(k_{\|})=\langle\mu\rangle k_{\|}^2\pm\langle\beta_1E_z\rangle k_{\|}^3$ we obtain for the densities $N_{\pm}$ in the spin-split subbands

$$N_{\pm}=\frac{1}{2}N_s\pm\frac{\langle\beta_1E_z\rangle N_s}{\sqrt{2}\langle\mu\rangle X}\sqrt{\pi N_s(6-4/X)} \tag{10a}$$

with

$$X=1+\sqrt{1-4\pi N_s(\langle\beta_1E_z\rangle/\langle\mu\rangle)^2}. \tag{10b}$$

The spin splitting according to Eq. (10) is substantially different from Eq. (4). For electrons and a fixed electric field E_z but varying N_s the difference $\Delta N=N_+-N_-$ increases like $N_s^{1/2}$ whereas for HH subbands it increases like $N_s^{3/2}$. Using a fixed density N_s but varying E_z it is more difficult to detect the difference between Eqs. (4) and (10). In both cases a power expansion of ΔN gives $\Delta N=a_1|E_z|+a_3|E_z|^3+\mathcal{O}(|E_z|^5)$ with $a_3<0$ for electrons and $a_3>0$ for HH subbands.

The proportionality (9) is completely analogous to the effective g factor in bulk semiconductors.[34] Lassnig[14] pointed out that the $B=0$ spin splitting of electrons can be expressed in terms of a position dependent effective g factor $g^*(z)$. In the following we want to discuss the close relationship between Zeeman splitting and $B=0$ spin splitting from a more general point of view. Note that in the presence of an external magnetic field $\mathbf{B}$ we have $\mathbf{k}\times\mathbf{k}=(-ie/\hbar)\mathbf{B}$ and the Zeeman splitting in the Γ_6^c conduction band can be expressed as[24]

$$H_{6c}^{Z}=\frac{i\hbar}{e}\frac{g^*}{2}\mu_B\mathbf{k}\times\mathbf{k}\cdot\boldsymbol{\sigma}=\frac{g^*}{2}\mu_B\mathbf{B}\cdot\boldsymbol{\sigma} \tag{11}$$

with μ_B the Bohr magneton. Thus apart from a prefactor we obtain the Rashba term (1) from Eq. (11) by replacing one of the $\mathbf{k}$'s with $i\mathbf{E}$. In the Γ_8^v valence band we have two invariants for the Zeeman splitting[24,26]

$$H_{8v}^{Z}=2\kappa\mu_B\mathbf{B}\cdot\mathbf{J}+2q\mu_B\mathbf{B}\cdot\boldsymbol{\mathcal{J}}. \tag{12}$$

Here, the first term is the isotropic contribution, and the second term is the anisotropic part. It is well-known that in all common semiconductors for which Eq. (12) is applicable, the dominant contribution to H_{8v}^{Z} is given by the first term proportional to κ whereas the second term is rather small.[24,26] Analogous to β_1 and β_2 the isotropic $\mathbf{k}\cdot\mathbf{p}$ coupling between Γ_8^v and Γ_6^c contributes to κ but not to q. The latter stems from $\mathbf{k}\cdot\mathbf{p}$ coupling to more remote bands such as Γ_8^c and Γ_7^c.

Several authors[10,17–19] used an apparently closely related intuitive picture for the $B=0$ spin splitting that was based on the idea that the velocity $v_{\|}=\hbar k_{\|}/m^*$ of the 2D electrons is perpendicular to the electric field E_z. In the electron's rest frame, E_z is Lorentz transformed into a magnetic field B so

that the $B=0$ spin splitting becomes a Zeeman splitting in the electron's rest frame. However, this magnetic field is given by $B=(v_\parallel/c^2)E_z$ (SI units) and for typical values of E_z and $v_\parallel$ we have $B\sim 2\ldots 20\times 10^{-7}$ T which would result in a spin splitting of the order of 5×10^{-9}–5×10^{-5} meV. On the other hand, the experimentally observed spin splitting is of the order of 0.1–10 meV. The $B=0$ spin splitting requires the SO interaction caused by the atomic cores. In bulk semiconductors this interaction is responsible for the SO gap Δ_0 between the valence bands Γ_8^v and Γ_7^v that appears in Eq. (9). The SO interaction is the larger the larger the atomic number of the constituting atoms. In Si we have $\Delta_0=44$ meV whereas in Ge we have $\Delta_0=296$ meV. Therefore, SIA spin splitting in Si quantum structures is rather small.[9]

Recently, spin splitting in 2D systems has gained renewed interest because of an argument by Pudalov[10] that relates the metal-insulator transition (MIT) in low-density 2D systems with the SIA spin splitting. Based on the Rashba model[5] it was argued that the SIA spin splitting ''results in a drastic change of the internal properties of the system even without allowing for the Coulomb interaction.''[11] In the low-density regime required for the MIT, however, this argument holds only for electron and LH states. As noted above, spin splitting in low-density HH systems is rather small. The MIT has been observed also in pure HH systems in, e.g., Si/SiGe QW's[35,36] for which already the bulk SO interaction is very small. Therefore it appears unlikely that here the broken inversion symmetry of the confining potential is responsible for the MIT. We note that in Si 2D electron systems the effective g factor is enhanced due to many-body effects.[31,37] It can be expected that similar effects are also relevant for the $B=0$ spin splitting, though this will not affect our general conclusions.

The author wants to thank O. Pankratov, S. J. Papadakis, and M. Shayegan for stimulating discussions and suggestions.

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[30] For a third-order term such as $\langle h_i|k_\pm|c_j\rangle\langle c_j|k_z|h_k\rangle\langle h_k|E_z z|h_i\rangle$ we have only one energy denominator of the order of the fundamental gap E_g; the second denominator is given by the subband spacing. Note that $1/m^*\propto 1/E_g$, i.e., both spin splitting and $\hbar^2k_\parallel^2/(2m^*)$ scale like E_g^{-1}. If we restrict ourselves to the Luttinger Hamiltonian we get Eq. (6) from a second-order perturbation theory for $E_z z$ and the off-diagonal terms $\gamma_3 k_\pm k_z$. Here, the energy denominator E_g is contained in the Luttinger parameter γ_3.
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