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Interface states in inhomogeneous semiconductor structures

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Contents

Abstract. The conditions for the appearance and the spectrum of localised electron states are reviewed for various inhomogeneous structures made of narrow-gap semiconductors with mutually inverted energy bands. The methods of supersymmetry and factorisation are used to solve Dirac-type equations with inhomogeneous external potentials in one-dimensional, two-dimensional, and three-dimensional systems.

1. Classification of inhomogeneities in two-band semiconductor structures

The $\boldsymbol{k}\cdot\boldsymbol{p}$ approximation is used widely in the description of the properties of narrow-gap semiconductors. In the simplest two-band approximation for IV – VI compounds the $\boldsymbol{k}\cdot\boldsymbol{p}$ scheme leads to the Dirac-type Hamiltonian in which the matrix element of the rate of interband transitions plays the role of the matrix element of the velocity of light [1].

This approach can be used to describe the various types of inhomogeneous semiconductor structures by including external fields in the appropriate Hamiltonian. In the case of the Dirac Hamiltonian these fields are represented by covariant bilinear forms and the Dirac equation is

$$\left[v\gamma^0\boldsymbol{\gamma}\cdot(\boldsymbol{p}-e\boldsymbol{A})+\gamma^0\Delta+\boldsymbol{\Sigma}\cdot\boldsymbol{M}+\gamma^0\boldsymbol{\Sigma}\cdot\boldsymbol{B}+\mathrm{i}\boldsymbol{\gamma}\cdot\boldsymbol{u}+\gamma^0\gamma_5 P+\mathrm{i}\gamma^5 M_0+G\right]\hat{\Psi}=E\hat{\Psi}\,, \tag{1.1}$$

where γ^μ are the Dirac matrices; $\gamma_5=\gamma_0\gamma_1\gamma_2\gamma_3$, $\boldsymbol{\Sigma}$ is the diagonal spin matrix; $\boldsymbol{p}=-\mathrm{i}\nabla$ is the momentum operator; v is the matrix element of an interband transition, which is regarded as a constant. The wave function is a column of Ψ_1 and Ψ_2 spinors, representing two adjacent terms forming the conduction and the valence bands of a semiconductor structure.

The quantities G and $\boldsymbol{A}$ are the usual scalar and vector potentials of an electromagnetic field. The role of $G(\boldsymbol{r})$ may also be played by the work function which varies in space. The field $2\Delta(\boldsymbol{r})$ represents variation of the band gap [2, 3].

The interaction $\mathrm{i}\boldsymbol{\gamma}\cdot\boldsymbol{u}$, due to the polar vector $\boldsymbol{u}$, appears in IV – VI semiconductors which undergo a ferroelectric phase transition. The vector $\boldsymbol{u}$ is proportional to the polarisation [4] and, in view of the anisotropy of the optical deformation potential g, the interaction $\mathrm{i}\boldsymbol{\gamma}\cdot\boldsymbol{u}$ should be written in the form $\mathrm{i}g_z\gamma_3 u_z+\mathrm{i}g_\perp\gamma_\perp\boldsymbol{u}_\perp$ (this is true, for example, of $Pb_{1-x}Ge_xTe$ and $Pb_{1-x}Sn_xTe$, where the z axis is parallel to the [111] crystallographic direction). In a sample containing ferroelectric domains the field $\boldsymbol{u}$ varies in space. The field M_0 may also appear in semiconducting ferroelectrics and it is due to an additional contribution, associated with the loss of a centre of inversion, to the spin – orbit interaction.

The diagonal terms $\boldsymbol{\Sigma}\cdot\boldsymbol{M}$ and $\gamma^0\boldsymbol{\Sigma}\cdot\boldsymbol{B}$ correspond to the Zeeman interaction ($H_z=\mu_B\boldsymbol{\Sigma}\cdot\boldsymbol{H}$, where μ_B is the Bohr magneton) in which the contribution of the distant bands to the g factors is taken into account [5]. The exchange interaction H_{ex} with magnetic impurities is of the same form if the spin density is even. This situation is encountered in semimagnetic IV – VI semiconductors, such as

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$Pb_{1-x}Mn_xTe$ and $Pb_{1-x}Eu_xTe$ [6, 7]. The matrix element $\gamma^0\gamma_5 P$ also appears because of the exchange interaction with magnetic impurities. However, in this case the impurities should be antiferromagnetically ordered and should be located at interstices (when the spin density is odd and the matrix element $\langle L^-|H_{ex}|L^+\rangle$ between L bands with opposite parities differs from zero, which corresponds to the appearance of the field $\gamma^0\gamma_5 P$).

It follows that all these fields may be encountered, in principle, in IV–VI semiconductors. Various heterojunctions can be formed by varying the composition of solid solutions. The ferroelectric phase transition in $Pb_{1-x}Ge_xTe$ and $Pb_{1-x}Sn_xTe$ makes it possible to simulate the vector field $\boldsymbol{u}$ and the pseudoscalar field M_0. The high solubility of magnetic impurities can be used to create the fields $\boldsymbol{M}$, $\boldsymbol{B}$, and P.

We shall be interested only in those fields which may give rise to bound electron states of inhomogeneities of the system. It has been shown [2–4, 8] that this condition is satisfied by the fields $\Delta, \boldsymbol{u}$, and P. When only these fields as well as the potentials $G(\boldsymbol{r})$ and A are retained in the Hamiltonian (1.1), the result is

$$\hat{H}\hat{\Psi} = \{v\gamma^0\boldsymbol{\gamma}\cdot(\boldsymbol{p}-e\boldsymbol{A}) + \gamma^0\Delta(\boldsymbol{r}) + \mathrm{i}\boldsymbol{\gamma}\cdot\boldsymbol{u}(\boldsymbol{r}) + \gamma^0\gamma_5 P + G(\boldsymbol{r})\}\hat{\Psi} = E\hat{\Psi}. \tag{1.2}$$

Eqns (1.1) and (1.2), corresponding to the cases when $\Delta = \text{const}$, $P = P(\boldsymbol{r})$ (antiferromagnetic domain wall) and $P = \text{const}$, $\Delta = \Delta(\boldsymbol{r})$ (heterojunction with a variable band gap in a homogeneous ferromagnet) are mathematically equivalent [8] in the absence of the field $\boldsymbol{u}(\boldsymbol{r})$. In fact, the Hamiltonian

$$H_1\hat{\Psi} = \{v\gamma^0\boldsymbol{\gamma}\cdot(\boldsymbol{p}-e\boldsymbol{A}) + \gamma^0\Delta(\boldsymbol{r}) + \gamma^0\gamma_5 P + G(\boldsymbol{r})\}\hat{\Psi} = E\hat{\Psi} \tag{1.3}$$

subjected to the unitary transformation $\hat{\Psi} = \hat{U}\hat{\Phi} = \exp(\gamma^5\pi/4)\hat{\Phi} = (1+\gamma^5)\hat{\Phi}/\sqrt{2}$, becomes

$$\hat{H}_2\hat{\Phi}\{v\boldsymbol{\gamma}^0\gamma\cdot(\boldsymbol{p}-e\boldsymbol{A}) - \gamma^0 P + \gamma^0\gamma_5\Delta(\boldsymbol{r}) + G(\boldsymbol{r})\}\hat{\Phi} = E\hat{\Phi}, \tag{1.4}$$

A comparison of the Hamiltonians (1.3) and (1.4) shows that $\hat{H}_1$ is identical with $\hat{H}_2$ when the substitutions $\Delta(\boldsymbol{r}) \to P$, $P \to \Delta(\boldsymbol{r})$ and $\hat{\Psi} \to \hat{\Phi}$ are made. We shall therefore consider only the fields $\Delta(\boldsymbol{r})$, $\boldsymbol{U}(\boldsymbol{r})$, $G(\boldsymbol{r})$ and $\boldsymbol{A}(\boldsymbol{r})$.

A Dirac-type Hamiltonian with inhomogeneous external potentials can be analysed conveniently by the supersymmetry and factorisation methods. The procedure of reducing a given Hamiltonian to the supersymmetric form is described in the Appendix. It is shown there that diagonalisation of the Hamiltonian (1.2) is possible only if the spatial dependence of the potentials is described by the same function $f(\boldsymbol{r})$:

$$\Delta(\boldsymbol{r}) = \Delta_1 + \Delta_0 f(\boldsymbol{r}), \quad u(\boldsymbol{r}) = u_1 + u_0 f(\boldsymbol{r}), \quad G(\boldsymbol{r}) = g_0 f(\boldsymbol{r}) \tag{1.5}$$

Since any inhomogeneity generally alters not only the band gap, but also the work function and the polarisation, this assumption is fully justified.

2. One-dimensional semiconductor heterostructures

In this section we shall demonstrate the use of the supersymmetry method in investigations of the electron spectra of heterostructures: this corresponds to a one-dimensional dependence $f = f(z)$. The condition for the existence of the zeroth mode of the supersymmetric Hamiltonian $\hat{H}_s$ imposes certain constraints on the parameters of a semiconductor structure. The first of these constraints is [on condition that the superpotential $W_\lambda(z)$ given by expression (5.11) is real]

$$\Delta_0^2 + u_0^2 - g_0^2 > 0 \tag{2.1}$$

The other constraints on the parameters of a semiconductor structure can be identified if the asymptotic values of the functional dependence of these parameters are known. It is convenient to rewrite condition (5.19) of normalisation of the wave function of the zeroth mode in the form

$$\text{sign}\,[W_\lambda(\pm\infty)] = -\text{sign}\,[W_\lambda(\mp\infty)] \tag{2.2}$$

and to use the explicit expression for the superpotential $W_\lambda(z)$ [expressions (5.11) and (5.12) in the Appendix]. In general, these expressions are quite cumbersome [9], so that we shall consider only some special cases.

2.1. Symmetric heterojunction

In an inhomogeneous structure in the form of a symmetric heterojunction only the band gap varies. Among the potentials described by formulas (1.5), we have only the potential $\Delta(z)$ ($u_0 = u_1 = g_0 = 0$), and the expression for the superpotential has the simple form (5.11):

$$W(z) = \Delta_0 f(z) + \Delta_1 \equiv \Delta(z). \tag{2.3}$$

The asymptotes of the function $f(z)$ at $z = \pm\infty$ will be denoted by μ_1 and μ_2 (specifically, it will be assumed that $\mu_1 < \mu_2$). It follows from expressions (2.2) and (2.3) that the zeroth mode of the Hamiltonian $\hat{H}_s$ exists only if

$$\mu_1\mu_2 < 0 \quad \text{and} \quad \mu_1\Delta_0 > \Delta_1 \tag{2.4}$$

In other words, the condition for the appearance of the zeroth mode is the mutual inversion of the bands of the semiconductors forming a heterojunction. Such a heterojunction is known as an inverted contact [2].

It then follows from general theorems of supersymmetric quantum mechanics [10] that a bound state appears only in the case of particles with one spin direction. The spectrum of these states is linear (all the energy parameters are assumed to be normalised to $\hbar v$)

$$E_\lambda = \lambda k_\perp \tag{2.5}$$

and the wave functions are

$$\hat{\Psi}^0_\lambda = C\begin{pmatrix} 1 \\ 0 \\ 0 \\ \lambda\exp(\mathrm{i}\theta) \end{pmatrix} \exp\left[\int_0^z W(x)\,\mathrm{d}x + \mathrm{i}\boldsymbol{k}_\perp\cdot\boldsymbol{r}\right] \tag{2.6}$$

where $\exp(\mathrm{i}\theta) \equiv (k_x + \mathrm{i}k_y)/|\boldsymbol{k}_\perp|$; $\boldsymbol{k}_\perp = (k_x, k_y, 0)$ is the wave vector. In the (x, y) plane the functions $\hat{\Psi}^0_\lambda$ satisfy the Dirac equation with zero mass. This equation is unitarily equivalent to the Weyl equation describing a neutrino [2]. Therefore, electrons localised in the plane of an inverted contact behave as a two-dimensional gas of

charged neutrinos. Such states exist irrespective of the actual form of $\Delta(z)$ and, therefore, are unaffected by fluctuations of the composition of the semiconductors forming a heterojunction. The only requirement is that the signs of the asymptotes $\Delta(\pm\infty)$ should be opposite.

2.2. Asymmetric inverted contact

If the change in the work function of the two semiconductors in contact is taken into account, it is found that two-dimensional electron states exist in a limited range of energies and transverse momenta [3]. In fact, in this case ($g_0 \neq 0$) the superpotential given by formula (5.11) is

$$W_\lambda(z) = \left(\Delta_0^2 - g_0^2\right)^{1/2} f(z) + \frac{\Delta_1\Delta_0 + Eg_0}{\left(\Delta_0^2 - g_0^2\right)^{1/2}} \tag{2.7}$$

which is energy-dependent. The spectrum of the bound states is limited because the superpotential of expression (2.7) becomes constant in sign as the energy $|E|$ is increased, and the wave function described by formula (2.6) becomes unrenormalisable. The existence of the field $g(z)$ limits the energies in the spectrum of the interface states, but the zero-mass (linear) energy spectrum of the states

$$E_\pm^0 = -\frac{\Delta_1 g_0}{\Delta_0} \pm k_\perp \left[1 - \left(\frac{g_0}{\Delta_0}\right)^2\right]^{1/2} \tag{2.8}$$

and the absence of degeneracy (in respect of the pseudoparity) are retained. The points of contact of linear and bulk spectra are given by the following relationships [3]

$$(k_\perp^\pm)_{\max} = (\mu_{1,2}\Delta_0 - \Delta_1)\left[\left(\frac{\Delta_0}{g_0}\right)^2 - 1\right]^{1/2}. \tag{2.9}$$

Here, μ_1 and μ_2 on the right of the above expression correspond to $k_\perp^+$ and $k_\perp^-$ on the left-hand side.

It follows from the expression (2.7) for the superpotential that the Weyl interface states exist only if $|\Delta_0| < |g_0|$ (i.e. if the change in the band gap in a heterostructure is greater than the change in the work function of the semiconductors forming this structure).

The existence of a finite work function g_0 leads to the appearance of interface states also in conventional unin-verted heterojunctions. This is demonstrated in Refs [11, 12] for abrupt functions. However, it is also true of graded (linear-gradient) junctions, as is clear from expression (2.7). In fact, if the asymptotes of the function $f(z)$ at $z = \pm\infty$ have the same sign, but different magnitudes (asymmetric heterojunction without band inversion), there is a finite interval of the energies E where the corresponding asymptotes of the superpotential described by expression (2.7) have opposite signs. Therefore, the states localised at an interface should exist irrespective of the form of the transition layer. The energies of these states overlap either the valence band (if $g_0 > 0$) or the conduction band (if $g_0 < 0$).

2.3. Ferroelectric domain wall

If there is a ferroelectric domain wall ($\Delta_0 = g_0 = 0$, $u_{0,1} \neq 0$) in a semiconductor heterostructure, the superpotential described by expression (5.11) becomes

$$W_\lambda(z) = u_0 f(z) + u_1 - \lambda k_\perp, \tag{2.10}$$

and expression (5.12) is equivalent to

$$E_s = E^2 - \Delta_1^2. \tag{2.11}$$

Subsitution of expression (2.10) in (2.2) leads to the conclusion that in this case the conditions for the appearance of the zeroth mode are the opposite signs of the asymptotes of the function $f(z)$ at $z = \pm\infty$ (it is assumed specifically that $u_0 > u_1$).

The solutions corresponding to the zeroth mode,

$$\chi^- = c\exp\left\{-\int_0^z \left[u(x) \pm k_\perp\right] \mathrm{d}x\right\}, \tag{2.12}$$

correspond to two-dimensional electron states whose energy is $E = +\Delta_1$, and which are localised at a domain wall [4]. These solutions can be normalised for $k_\perp < |u(\pm\infty)|$. In the opposite case when $u(+\infty) < 0$, $u(-\infty) > 0$, there are no bound states with $E = +\Delta_1$, but there is a level with $E = -\Delta_1$.

2.4. Degenerate interface states

We have considered so far the solutions corresponding to the zeroth mode of the supersymmetric Hamiltonian $\hat{H}_s$ given by expression (5.10). However, in addition to the states represented by these solutions there may be ordinary degenerate interface states at a contact between two semiconductors. The whole spectrum of the interface states can be investigated provided we know the specific form of the functional dependence of the heterostructure parameters. We can select this dependence to be the function $f(z) = \tanh(z/l)$, where l is the thickness of the transition layer. We shall use here the results given in Section 5.1.

In the simplest case of a symmetric inverted contact ($l_0 = 1/\Delta_0$) expression (5.30) for the spectrum becomes

$$E^\pm = \pm\frac{[l^2k_\perp^2 - n(n - 2l/l_0)]^{1/2}}{l}, \tag{2.13}$$

which is identical with the results given in Ref. [2]. It follows from expression (2.13) that n should vary in the interval $0 < n < 2l/l_0$. If $l < l_0$, only the zeroth mode ($n = 0$) exists. If $l > l_0$, additional two-dimensionally degenerate branches of interface states ($m, \lambda = +1$) and ($m = +1$, $\lambda = -1$) appear. If $l \gg l_0$ the discrete levels given by expression (2.13) form a quasicontinuous spectrum, which fills the whole band gap [2, 13].

Whenever l reaches an integral multiple of l_0, a pair of interface states splits from the Dirac bands. This is due to the fact that the parameter $a = l/l_0$ then assumes values which are integers and the sequence of potentials $U_\pm(\alpha_n, z)$ [described by expressions (5.23) and (5.24)] reduces to the potential $U(a, z) = 0$ for $n = a$ (the point from which the energy E_s is measured is shifted by the amount $\Delta_0/l = 1/ll_0$). In other words, the potential given by expression (5.28) becomes reflection-free. This means that the asymptotes of the delocalised wave functions do not contain a reflected wave and a contact of this kind is absolutely transparent for the Dirac-spectrum electrons.

When the asymmetry of the contact ($g_0 \neq 0$) is taken into account, the results given above are not affected in a qualitative sense. The number N of the Dirac levels within the band gap is determined by the thickness of the contact:

$$N = 2l\left(\Delta_0^2 - g_0^2\right)^{1/2} - \frac{1+\lambda}{2}. \tag{2.14}$$

In the case of a ferroelectric domain wall only the coefficients u_1, u_0, and Δ_1 differ from zero. It follows from expression (5.30) that

$$E^{\pm}=\pm\left\{\Delta_1^2+\frac{n(2u_0l-n)}{l^2}\left[1-\frac{(u_1-\lambda k_{\perp})^2l^2}{(u_0l-n)^2}\right]\right\}^{1/2}, \quad (2.15)$$

which shows that the condition for the appearance of a Dirac level with the serial number n is

$$l>\frac{n\left[\left(u_0^2+\Delta_1^2\right)^{1/2}-u_0\right]}{\Delta_1^2}. \quad (2.16)$$

We thus reach the conclusion, which also remains valid for the general form of the potential described by expression (5.11), that in the case of graded heterostructures the band gap contains not only the zeroth mode, but also a finite number of doubly degenerate Dirac levels. These levels correspond to states localised at the interface and the number of these levels is governed by the transition layer thickness l and by the semiconductor structure parameters. If the contact (junction) is abrupt, so that the thickness l is less than a certain critical value at which the first 'Dirac' level appears, only the zeroth mode (known as the 'Weyl' branch) is observed.

3. One-dimensional size-quantised semiconductor structures

3.1 Rectangular quantum well formed by inverted contacts

Let us consider a rectangular quantum well of width $2a$ formed by a semiconductor with inverted bands and surrounded by two different semiconductors with uninverted bands. The function $f(z)$ for this structure can be selected in the form

$$f(z)=1+\mu_L+\mu_R-(1+\mu_L)\theta(a+z)-(1+\mu_R)\theta(a-z). \quad (3.1)$$

Here, θ are the step functions and the parameters $(1+\mu_L)$ and $(1+\mu_R)$ give the height of the left- and right-hand barriers, respectively.

The supersymmetry method described in the Appendix is inapplicable to the dependence $f(z)$ of the type described by formula (3.1). However, then expression (5.10) (or its quadrature analogue) can be solved separately in each region, bearing in mind that the logarithmic derivative of χ has jumps at the interfaces:

$$\left.\frac{d\chi_{\mp}^{(2)}}{dz}\right|_{z=-a}-\left.\frac{d\chi_{\mp}^{(1)}}{dz}\right|_{z=-a}=\mp(1+\mu_L)\varkappa\chi_{\mp}(-a),$$
$$\left.\frac{d\chi_{\mp}^{(3)}}{dz}\right|_{z=+a}-\left.\frac{d\chi_{\mp}^{(2)}}{dz}\right|_{z=+a}=\pm(1+\mu_R)\varkappa\chi_{\mp}(a). \quad (3.2)$$

This leads to the following dispersion equation

$$\tanh(2qa)=\frac{q(q_L+q_R+\varkappa_L-\varkappa_R)}{(\varkappa+\varkappa_L)(\varkappa+\varkappa_R)-q^2-q_Lq_R+q_L(\varkappa+\varkappa_R)-q_R(\varkappa+\varkappa_L)}, \quad (3.3)$$

where

$$q_{L,R}^2=(W_{\lambda}+\varkappa_{L,R})^2-(W_{\lambda}-\varkappa)^2+q^2,$$
$$q^2=(W_{\lambda}-\varkappa)^2-\tilde{E}^2=(\Delta_1-\Delta_0)^2$$
$$+(u_1-u_0-\lambda k_{\perp})^2-(E+g_0)^3, \quad (3.4)$$
$$\varkappa_{L,R}=\varkappa\mu_{L,R}.$$

Let us assume that $u_1=u_0=g_0=\Delta_1=0$, $\Delta_0\equiv\varkappa$. Then, expressions (3.4) become

$$q^2=\varkappa^2+k_{\perp}^2-E^2,$$
$$q_{L,R}^2=\varkappa_{L,R}^2+q^2-\varkappa^2 \quad (3.5)$$

Let us consider specifically that $|\varkappa|<|\varkappa_{L,R}|$. The real values of q in the dispersion equation (3.3) then correspond to levels localised at the walls of a quantum well, the imaginary values of q when the real values are q_L and q_R correspond to size-quantisation levels in the well, and the imaginary values of q, q_L, and q_R represent delocalised states in the continuous spectrum. We shall be interested in the localised states which are of the same origin as the Weyl branch in the case of a single inverted contact.

A detailed analysis of the dispersion equation (3.3) is reported in Ref. [14]. In particular, if $a\to\infty$ the solution of Eqn (3.3) is $q=\varkappa$ and $E=\pm\lambda k_{\perp}$, i.e. the zeroth mode is doubly degenerate ($\lambda=\pm1$). The wave functions of these states are localised at the opposite interfaces. If the size of the well is finite, the spectrum of the localised states becomes of the gap type:

$$E=\pm\left(\varkappa^2-q^2+k_{\perp}^2\right)^{1/2}. \quad (3.6)$$

If the size of the well is reduced to a certain critical value $a=a_c$ (which depends on the relationship between $\varkappa$ and $\varkappa_{L,R}$), the quantity q becomes purely imaginary, i.e. both levels described by formula (3.6) transform to size-quantisation levels. It follows that the electron-like and hole-like branches of the localised states split off from the upper and lower bulk energy bands, respectively. It should therefore be stressed that even in the case of a single inverted contact the zeroth mode is truly degenerate because there is always a second interface between an 'inverted' semiconductor and, for example, vacuum.

Let us return to an analysis of the solutions of the disperison equation. In general, the expression for a_c is fairly cumbersome. The dispersion equation for a symmetric well ($\varkappa_L=\varkappa_R=\varkappa_0$) is identical with that obtained in Refs [15, 16]:

$$\mathrm{th}(2qa)=\frac{qq_0}{\varkappa(\varkappa+\varkappa_0)-q^2}, \quad (3.7)$$

which means that

$$2a_c=\frac{1}{\varkappa}\sqrt{\frac{\varkappa_0-\varkappa}{\varkappa_0+\varkappa}}. \quad (3.8)$$

In the fully symmetric case ($\varkappa=\varkappa_0$) we have $a_c=0$, i.e. there are states localised at the interfaces for any size of the well.

3.2. Inverted semiconductor film

The largest value $2a_c = 1/\varkappa$ is obtained for $\varkappa \ll \varkappa_0$, which corresponds to a film of a semiconductor with inverted bands surrounded by an insulator. An estimate of this value for a IV–VI semiconductor ($2\Delta \approx 100$ meV, $v = 3 \times 10^7$ cm s^{-1}) gives $a_c \approx 100$ A. The origin of the interface states can be demonstrated for such a film in a clear manner. In fact, in this case the spectrum of the system is completely discrete (in a transverse direction) and the dispersion equation has the simple form

$$\tanh(2qa) = \frac{q}{\varkappa} . \tag{3.9}$$

The solutions of this equation with purely imaginary values of q correspond to size-quantisation levels with $E > |\varkappa|$. The states inside the band gap ($E < |\varkappa|$) correspond to real values of q. In a semiconductor with an uninverted band structure ($\varkappa < 0$) there are only size-quantisation levels, which simply shift to the edge of the band gap when this gap is reduced. The band gap width then passes through zero and becomes negative ($\varkappa > 0$), but the levels still shift continuously to the edge, although their number does not change. Finally, when $\varkappa$ reaches a certain finite value (which depends on the film thickness $2a$), the imaginary solution with the value of q smallest in the absolute sense becomes real, i.e. the electron and hole size-quantisation levels nearest to the edge of the band gap migrate into the gap and form interface states.

The wave function also has the simplest form for a film [15]

$$\hat{\Psi}_\lambda(z) = B \begin{pmatrix} \sinh\left[q(a+z)\right] \\ i\lambda \exp(i\theta) \dfrac{\sqrt{\varkappa^2 - q^2}}{E + \lambda k_\perp} \sinh\left[q(a-z)\right] \\ -i \dfrac{\sqrt{\varkappa^2 - q^2}}{E + \lambda k_\perp} \sinh\left[q(a-z)\right] \\ \lambda \exp(i\theta) \sinh\left[q(a+z)\right] \end{pmatrix}, \tag{3.10}$$

$$B^2 = \frac{\varkappa^2 - q^2}{\varkappa - 2a(\varkappa^2 - q^2)} \frac{E + \lambda k_\perp}{2E} \tag{3.11}$$

It should be pointed out that in a state with the wave function (3.10) the maxima of the distributions of the charge and spin densities do not coincide in space. In fact, the charge density $n_\lambda(z)$ is

$$n_\lambda(z) = \hat{\Psi}^+_\lambda(z)\hat{\Psi}_\lambda(z) = \tilde{B}^2 \left\{ \frac{E + \lambda k_\perp}{2E} \sinh^2\left[q(a+z)\right] + \frac{E - \lambda k_\perp}{2E} \sinh^2\left[q(a-z)\right] \right\}, \tag{3.12}$$

where

$$\tilde{B}^2 = \frac{\varkappa^2 - q^2}{\varkappa - 2a(\varkappa^2 - q^2)} . \tag{3.13}$$

According to expression (5.4), the spin distribution $\Sigma_\lambda(z)$ is

$$\Sigma_\lambda(z) = \lambda \hat{\Psi}^+_\lambda \gamma^0 \hat{\Psi}_\lambda = \lambda \tilde{B}^2 \frac{\varkappa}{E} \left[1 - \frac{\cosh(2qz)}{\cosh(2qa)} \right]. \tag{3.14}$$

It is thus clear that the distribution of the spin density is symmetric with its maximum at the centre and it vanishes at the boundaries of a film. However, the charge density is concentrated at the boundaries and, as $k_\perp$ is increased, the 'electron' states with positive parity are driven against the right-hand boundary and those with negative parity are driven to the left-hand boundary. The reverse is true of the 'hole' states.

The existence of pseudoparity leads to certain selection rules for the optical transitions between localised states whose spectra is described by expression (3.6). In contrast to an inverted contact, the matrix element of the velocity (for an $E_\lambda - E'_{\lambda'}$ transition) is $\boldsymbol{v} = v\langle \hat{\Psi}_{\lambda'} | \gamma^0 \boldsymbol{\gamma} | \hat{\Psi}_\lambda \rangle$ and it has nonzero components both in the plane of a film and across it:

$$v_l = i\lambda v(1 - \delta_{\lambda\lambda'}) ,$$
$$v_{k_\perp} = \lambda v \delta_{\lambda\lambda'} \frac{\sqrt{\varkappa^2 - q^2}}{|E|} , \tag{3.15}$$
$$v_z = iv \frac{2(2a\varkappa - 1)}{\varkappa - 2a(\varkappa^2 - q^2)} \sqrt{\varkappa^2 - q^2}\, \mathrm{sign}(E) \delta_{\lambda\lambda'} .$$

Hence, it is clear that for light polarised along the $\boldsymbol{l} = [\boldsymbol{n} \times \boldsymbol{k}_\perp]/|\boldsymbol{k}_\perp|$ direction, only the transitions with a change in parity are allowed. The expression for v_l then becomes identical with the corresponding expression for an inverted contact [16]. In the case of light polarised in the $(\boldsymbol{k}_\perp, z)$ plane only the parity-conserving transitions are allowed. Such transitions are impossible in the case of an inverted contact when the zeroth mode is nondegenerate. It is also evident from expressions (3.15) that the components $v_{k_\perp}$ and v_l are proportional to $(\varkappa^2 - q^2)^{1/2}$, i.e. they decrease with increase in the film thickness (vanishing in the limit $a \to \infty$). This is due to the fact that the wave functions of the electron and hole states with the same parity are localised at the opposite boundaries of the film. Expressions (3.15) can be used to calculate the frequency dependence of the absorption of light with different polarisations. For example, the transmission coefficient of light polarised linearly in the film plane is [15]

$$R(\omega) = \frac{e^2}{\hbar c n_r} \pi \left[1 + \frac{E_g^2}{\hbar^2 \omega^2} \right] \theta(\hbar\omega - E_g) , \tag{3.16}$$

where $E_g = 2\hbar v(\varkappa^2 - q)^{1/2}$ is the gap in the spectrum of the localised states and n_r is the refractive index of light.

The spectrum of the surface states of a film and of a semi-infinite crystal of a narrow-gap semiconductor is determined in Ref. [17] by adopting a different approach. Eqn (5.2) is solved with a constant gap $\Delta(z) = \Delta$ (and $g = u = 0$) and the following phenomenological boundary conditions are applied:

$$\hat{\Psi} = -i\hat{A}(\boldsymbol{\gamma} \cdot \boldsymbol{n})\hat{\Psi} , \tag{3.17}$$

which require only the absence of the current across the interfaces. Here, $\boldsymbol{n}$ is the normal to the surface and $\hat{A}$ is a certain Hermitian matrix, which is defined by a single phenomenological real parameter a_0:

$$\hat{A} = \left[\left(a_0 + \frac{1}{a_0} \right) + \left(a_0 - \frac{1}{a_0} \right) \right] \gamma^0 . \tag{3.18}$$

We can show that a_0 is governed by the semiconductor structure parameters and is related to the finite work function: $g_0 \neq 0$. This can be shown by substituting $u(z) = 0$ in Eqns (5.6) and (5.7). The canonical trans-

formation operator $\hat{S}$, which diagonalises the quadrature equation (5.7), then becomes

$$\hat{S} = \cosh\left(\frac{\alpha}{2}\right) + \gamma^0 \sinh\left(\frac{\alpha}{2}\right), \quad \tanh(\alpha) = \frac{g_0}{\Delta_0}. \quad (3.19)$$

The action of the operator (3.19) on the linear equation (5.6) gives

$$\{\gamma^0[\gamma^3\hat{P}_z + w(z)] - i\gamma^3\lambda k_\perp - \tilde{E}\}\hat{\chi} = 0, \quad (3.20)$$

where

$$w(z) = \left(\Delta_0^2 - g_0^2\right)^{1/2} f(z) + \tilde{E}(g_0/\Delta_0),$$
$$\tilde{E} = E\Delta_0/\left(\Delta_0^2 - g_0^2\right)^{1/2}.$$

Hence, since the pseudoparity operator $\hat{P}$ commutes with the operator $\hat{S}$ and the function $\hat{\chi}$ satisfies the boundary conditions $\hat{\chi} = -i(\gamma n)\hat{\chi}$, we find that

$$\hat{\Psi} = -i\hat{S}(\boldsymbol{\gamma}\cdot\boldsymbol{n})\hat{S}^{-1}\hat{\Psi} = -i\hat{S}^2(\boldsymbol{\gamma}\cdot\boldsymbol{n})\hat{\Psi}, \quad (3.21)$$

i.e. the matrix $\hat{A}$ in expression (3.18) is identical with the square of the operator (3.19), which leads to

$$a_0 = \cosh(\alpha) + \sinh(\alpha) = \mathrm{sgn}(\Delta_0)\left[\frac{(1 - g_0/\Delta_0)}{(1 + g_0/\Delta_0)}\right]^{1/2}. \quad (3.22)$$

We can see that for $g_0 = 0$, we have $a_0 = \pm 1$, depending on whether the energy bands of the semiconductor film are inverted or not. For $g_0 \neq 0$, the absolute value of this parameter can be less or greater than unity, depending on the sign of g_0/Δ_0. In the case of an abrupt heterojunction the quantity g_0 represents the difference between the work functions of the two semiconductors. Therefore, for $g_0/\Delta_0 < 0$ the valence band offset at the heterojunction is less than the conduction band offset, whereas the opposite is true for $g_0/\Delta_0 > 0$.

3.3. Ferroelectric domain

We shall now consider a homogeneous intrinsic semiconductor containing one ferroelectric domain of size $2a$. Once again, we shall use the function (3.1) and assume that $\Delta_0 = g_0 = u_1 = 0$, $\mu_L = \mu_R = 1$. The dispersion equation (3.3) then becomes

$$\tanh(2qa) = \frac{q(q^2 - 4\lambda k_\perp u_0)^{1/2}}{2u_0(u_0 + \lambda k_\perp) - q^2}. \quad (3.23)$$

The roots of this equation determine the energy spectrum of localised states

$$E = \pm\left[\Delta_1^2 - (u_0 + \lambda k_\perp)^2 - q^2\right]^{1/2}. \quad (3.24)$$

In the limit $a \to \infty$ (representing two walls separated by an infinite distance), the solution of Eqn (3.23) is $q = u_0 + \lambda k_\perp$ and the spectrum consists of two degenerate branches with energies $E = \pm\Delta_1$. If the domain is of finite dimensions, the degeneracy of λ is lifted and the spectrum of localised states exhibits dispersion. An analysis of Eqns (3.23) and (3.24) shows [18] that these states exist in the range of transverse momenta $0 < k_\perp < u_0$ ($\lambda = +1$) and $0 < k_\perp < k_c$ ($\lambda = -1$), where

$$k_c = u_0\left(1 - \frac{(1 + 16a^2u_0^2)^{1/2} - 1}{8a^2u_0^2}\right). \quad (3.25)$$

In the case of negative parity states, if $k_\perp > k_c$, the solution of Eqn (3.23) becomes purely imaginary and the wave function changes from exponentially falling at the domain walls to an oscillatory function, i.e. it corresponds to the 'size-quantisation' states inside the domain. Apart from this branch, if $k_\perp > k_{n,c}$, where

$$k_{n,c} = \frac{1}{4u_0}\left(\frac{n\pi}{2a}\right)^2, \quad (3.26)$$

a whole series of negative-parity 'size-quantised' states appears. As the domain dimensions are reduced, in the limit $a \to 0$, we have $k_{n,c} \to \infty$ and these branches disappear. The surface states with $\lambda = +1$ merge with the bulk spectrum branch $E^- = \pm[\Delta_1^2 + (u_0 - k_\perp)^2]^{1/2}$, and the states with $\lambda = -1$ become size-quantised ($k_c \to 0$) and merge with the branch $E^+ = \pm[\Delta_1^2 + (u_0 + k_\perp)^2]^{1/2}$, so that we then have the usual continuous spectrum of a bulk semiconducting ferroelectric.

3.4. Spectrum of interface states in a magnetic field

Let us consider how the spectrum of the interface states is modified by a homogeneous magnetic field H, directed along the z axis. To reveal the effect of this field, we shall assume that the potentials $\boldsymbol{u}$, P, and G in the Hamiltonian (1.2) vanish and we shall select the vector potential $\boldsymbol{A}$ in the $\boldsymbol{A} = [\boldsymbol{H}\cdot\boldsymbol{\rho}]/2$ gauge, where $\boldsymbol{\rho} = (x, y)$. The Hamiltonian then becomes

$$\hat{H}_A = [v\gamma^0\gamma^3\hat{p}_z + \gamma^0\Delta(z) + v\gamma^0(\gamma_+\hat{\pi}_- + \gamma_-\hat{\pi}_+)], \quad (3.27)$$

where $\gamma_\pm = (\gamma^1 \pm i\gamma^2)$, $\hat{\pi}_\pm = (\hat{\pi}_x \pm i\hat{\pi}_y)$, $\hat{\boldsymbol{\pi}} = \hat{\boldsymbol{p}} - e\boldsymbol{A}$. We can show that this Hamiltonian commutes with the operator

$$\hat{P}_A = \gamma^5(\boldsymbol{\gamma}\,[\mathbf{n}\times\hat{\boldsymbol{\pi}}_\perp]) = i\gamma^0\gamma^3(\gamma_+\hat{\pi}_- + \gamma_-\hat{\pi}_+), \quad (3.28)$$

which represents a simple generalisation of the operator described by expression (5.3) to the case when a magnetic field is present. The eigenfunctions of the operator (3.28) are found as follows. The commutation properties of the matrices $\gamma_\pm$, lead to

$$\hat{P}_A^2 = \hat{\pi}_+\hat{\pi}_- + (1 + \hat{\Sigma}_3)\frac{\hbar^2}{L^2}, \quad (3.29)$$

where $\hat{\Sigma}_3$ is the operator of the projection of the spin onto the z axis and $L^2 = \hbar/|e|H$ is the magnetic length. The eigenfunctions of the operator $\hat{\pi}_+\hat{\pi}_-$ are the Landau oscillator functions $\Phi_n(x, y)$, where

$$\hat{\pi}_+\hat{\pi}_-\Phi_n(x, y) = 2n\frac{\hbar^2}{L^2}\Phi_n(x, y), \quad n = 0, 1, 2, \ldots \quad (3.30)$$

Since the spin operator $\hat{\Sigma}$ is diagonal, the components of the eigen bispinor $\hat{\psi}$ of the operator (3.29), and consequently also of the operator $\hat{P}_A$, can be represented in the form

$$\hat{\psi}_{1,3} = \Phi_{n-1}(x, y) f_{1,3}(z),$$
$$\hat{\psi}_{2,4} = \Phi_n(x, y) f_{2,4}(z). \quad (3.31)$$

Then, bearing in mind that

$$\hat{P}_A\hat{\psi} = \frac{\lambda\hbar}{L}\sqrt{2n}\,\hat{\psi}, \quad (3.32)$$

we obtain the Dirac equation for $\hat{\psi}$ in the form

$$\left\{\gamma^0\left[v\gamma^3\hat{P}_z+\Delta(z)\right]-i\gamma^3\lambda\hbar v\,\frac{\sqrt{2n}}{L}-E\right\}\hat{\psi}=0\,. \tag{3.33}$$

A comparison of this expression with Eqn (5.6) shows that the only difference is the replacement of $k_\perp$ with $\sqrt{2n}/L$, i.e. in a homogeneous magnetic field directed along the z axis the Landau quantisation takes place and the spectrum described by expression (3.6) becomes

$$E=\pm\left(\varkappa^2-q^2+\frac{2n}{L^2}\right)^{1/2}. \tag{3.34}$$

If $n=0$, the components are $\psi^{(0)}_{1,3}=0$, so that the zeroth Landau levels with energies $E=\pm\sqrt{\varkappa^2-q^2}$ are not degenerate. The other levels with $n=0$ remain doubly degenerate in terms of the parity $\lambda=\pm1$.

The matrix elements of the transitions between the Landau levels can be calculated by analogy with the velocity components described by expressions (3.15). If light polarised along the z axis propagates perpendicular to a magnetic field (Voigt configuration), only the transitions between the levels with the same index n are allowed (these are 'interband' transitions) and the matrix element itself is identical with the corresponding expression (3.15) for v_z. In the Faraday configuration, when light propagates along a magnetic field, it is meaningful to speak of the right- and left-handed circular polarisations in the plane of a film. In this case the transitions between the Landau levels with the numbers n and $n'=n\pm1$, are allowed and for the transitions in which n increases, the right-handed polarisation is active, whereas the left-handed polarisation is active in the transitions accompanied by a reduction in n. Both 'interband' and 'intraband' transitions are then possible.

We shall conclude by noting that the operator (3.28) commutes also with the general Hamiltonian

$$\hat{H}\hat{\Psi}=\left[v\gamma^0\boldsymbol{\gamma}\boldsymbol{\pi}+\gamma^0\Delta(z)+i\gamma^3u(z)+G(z)\right]\hat{\Psi}=E\hat{\Psi} \tag{3.35}$$

which means that in all the cases discussed above the application of a magnetic field results in a standard splitting of the spectrum into the Landau levels.

4. Two-dimensional and three-dimensional inhomogeneous structures

4.1 Localised states near linear and point defects

We shall now consider the characteristics of two-dimensional structures. We shall ignore the existence of polarisation. Mechanical stresses and strains near linear and point defects are known to decrease inversely proportionally to the distance from these defects [19, 20]. Therefore, in describing the spectrum of narrow-gap semiconductors containing such defects the spatial dependences of the potentials $\Delta(r)=\Delta_0 f(r)+\Delta_1$ and $G(r)=g_0 f(r)$ can be selected in the form $f(r)=1/r$. In Section 5.2 of the Appendix it is shown that in this (and only in this) case the Hamiltonian can be reduced to the supersymmetric form. The conditions for a real superpotential and for normalisation of the wave function of the zeroth mode are

$$M^2+\Delta_0^2-g_0^2>0\,, \tag{4.1}$$

$$\Delta_0\Delta_1+Eg_0<0\,, \tag{4.2}$$

where $M=1/2,3/2,\ldots$, in the case of a linear defect and $M=1,2,\ldots=(j+1/2)$ for a point defect (M is the projection of the angular momentum along the z axis and j is the total angular momentum). It is evident from expressions (4.1) and (4.2) that if $g_0\neq0$, localised states of both electrons and holes may appear near such defects irrespective of whether the energy bands of a semiconductor are inverted. It should also be noted that if $\Delta_0=0$, then expression (5.46) for the spectrum in the three-dimensional case ($p_z=0$) becomes identical with the familiar expression for localised states near a charged point centre, derived in Ref. [21] for two-band semiconductors:

$$E_n^{\pm}=-\mathrm{sign}(g_0)\,\frac{(c+n)\Delta_1}{\left[(c+n)^2+g_0^2\right]^{1/2}}\,,\quad c=\left[k^2-g_0^2\right]^{1/2}\,, \tag{4.3}$$

where the quantity g_0 acts as the effective charge and condition (4.2) is equivalent to the condition that the same centre captures both electrons and holes.

4.2. Interface states in two-dimensional and three-dimensional quantum wells

If the spatial dependences of the fields differ from $1/r$, it is not possible to diagonalise the Hamiltonian and other methods have to be adopted. For example, in the case of a rectangular cylindrical well of radius a the function $f(\rho)$ is

$$f(\rho)=(\mu+1)\theta(\rho-a)-1\,, \tag{4.4}$$

where the parameter μ governs the well depth. In this case the relevant equation (5.10) can be solved separately in each region bearing in mind that at the interface the derivative of the wave function $\hat{\chi}_\mp(\rho)$ has a discontinuity:

$$\left.\frac{d\hat{\chi}_\mp}{d\rho}\right|_{\rho=a^+}-\left.\frac{d\hat{\chi}_\mp}{d\rho}\right|_{\rho=a^-}=\mp(\mu+1)\left[\Delta_0^2-g_0^2\right]^{1/2}\hat{\sigma}_1\hat{\chi}_\mp(a). \tag{4.5}$$

The result is the following dispersion equation [22]:

$$\frac{q_eq_i}{(\mu+1)^2(\Delta_0^2-g_0^2)-q_e^2-q_i^2}=\frac{I_m(q_ia)I_{m+1}(q_ia)K_m(q_ea)K_{m+1}(q_ea)}{I_{m+1}^2(q_ia)K_m^2(q_ea)+I_m^2(q_ia)K_{m+1}^2(q_ea)}\,, \tag{4.6}$$

where $q_i^2=(\Delta_0-\Delta_1)^2-(E+g_0)^2+p_z^2$, $q_e^2=(\mu\Delta_0+\Delta_1)^2-(E-\mu g_0)^2+p_z^2$ and $m=(M-1/2)$; $I_m(q_ia)$, $K_m(q_ea)$ are modified Bessel functions of the first and second kinds.

For simplicity, we shall consider the case when $\Delta_1=g_0=0$ and $q_e^2=q_i^2+(\mu^2-1)\Delta_0^2$. It should be pointed out that the real values of q_i correspond to the levels localised on the boundary of a cylinder, that the imaginary values of q_i in combination with the real q_e represent size-quantisation levels inside the cylinder, and the imaginary values of $q_{i,e}$ indicate delocalised states in the continuous spectrum. For real values of q_i, the right-hand side of Eqn (4.6) is positive. However, the left-hand side, which is then $\{q_i[q_i^2+(\mu^2-1)\Delta_0^2]^{1/2}/2\}[(\mu+1)\Delta_0^2-q_i^2]$, is positive only if $\mu>0$. Hence, it follows that the interface states appear in a cylindrical quantum well only if the bands of the semiconductors are mutually inverted in and outside the well.

In the simplest case of a 'symmetric' well ($\mu = 1$, $q_i = q_e = q$), the dispersion equation (4.6) becomes

$$\frac{q^2}{4\Delta_0^2} = \frac{I_m(qa)I_{m+1}(qa)K_m(qa)K_{m+1}(qa)}{\left[I_{m+1}(qa)K_m(qa) + I_m(qa)K_{m+1}(qa)\right]^2} . \tag{4.7}$$

In the limit $a \to \infty$ the solution of (4.7) is $q = \Delta_0$ and $E = \mp p_z$, i.e. the problem becomes equivalent to that of a one-dimensional inverted contact [23] and the zeroth mode is characterised by degeneracy of infinite multiplicity in terms of the projections of the total angular momentum M on the z axis. A reduction of the radius of this well lifts the degeneracy of m, corresponding to different absolute values of M, and the doubly degenerate spectrum of localised states becomes the gap spectrum

$$E = \pm\left[\Delta_0^2 + p_z^2 - q^2\right]^{1/2} . \tag{4.8}$$

The number of levels inside the band gap is governed by the maximum value of the angular momentum, which is

$$2|M|_{\max} = \left[1 + 4\Delta_0^2 a^2\right]^{1/2} . \tag{4.9}$$

The levels with high values of M are within the continuous spectrum. Obviously, there is a critical value of the radius $a_c = 1/\sqrt{8}\,\Delta_0$, for which all the levels inside the band gap are expelled from it to the continuous spectrum and there are no localised states.

A small change in the shape of the well, for example, a change from the circular to the elliptic shape of a cylinder, shifts only slightly the energy levels. This is confirmed by calculations carried out on the basis of perturbation theory in which the ellipse eccentricity is a small parameter. All the levels remain, as before, doubly degenerate. If the area of a circle 'deformed' into an ellipse is conserved, there is no shift of the levels.

In the case of a three-dimensional spherically symmetric quantum well the dispersion equation is analysed exactly as described above. For a well with a finite radius the spectrum of states localised at an interface is a set of discrete levels whose degeneracy multiplicity is $2N$, where N is the number of different projections of the total angular momentum along the z axis. As in the preceding case, there is a certain critical value of the radius at which all the localised levels are expelled into the continuous spectrum.

5. Appendix. Factorisation and supersymmetry methods for solving the Dirac equation

5.1 One-dimensional case

We shall use the methods of factorisation [24] and supersymmetry [10] to solve the Dirac equation in the presence of one-dimensional scalar $\Delta(z)$, axial $u(z)$ and vector $A^\mu = [0,0,0,G(z)]$ potentials:

$$\hat{H}\hat{\Psi} = \left\{v\gamma^0\boldsymbol{\gamma}\cdot\hat{\boldsymbol{p}} + \gamma^0\Delta(z) + \mathrm{i}\gamma^3 u(z) + G(z)\right\}\hat{\Psi} = E\hat{\Psi} . \tag{5.1}$$

The wave function $\hat{\Psi}$ can be selected in the form $\hat{\Psi} = \hat{\Psi}(z)\exp(\mathrm{i}\boldsymbol{k}_\perp\cdot\boldsymbol{r})$, where $\boldsymbol{k}_\perp = (k_x, k_y, 0)$. Then, in place of Eqn (5.1), we obtain

$$\hat{H}\hat{\Psi} = \left\{v\gamma^0\gamma^3\hat{p}_z + v\gamma^0(\boldsymbol{\gamma}\cdot\boldsymbol{k}_\perp) + \gamma^0\Delta(z) + \mathrm{i}\gamma^3 u(z) + G(z)\right\}\hat{\Psi} = E\hat{\Psi} . \tag{5.2}$$

We can show that the Hamiltonian $\hat{H}$ commutes with the pseudoparity operator $\hat{P}$ [14]

$$\hat{P} = \gamma^5(\boldsymbol{\gamma}\cdot\boldsymbol{l}) = \frac{\mathrm{i}\gamma^0\gamma^3(\boldsymbol{\gamma}\cdot\boldsymbol{k}_\perp)}{k_\perp} , \tag{5.3}$$

where $\boldsymbol{l}$ is a unit vector which lies in the (x, y) plane and is perpendicular to the wave vector $\boldsymbol{k}_\perp$: $\boldsymbol{l} = [\boldsymbol{n}\times\boldsymbol{k}_\perp]/|\boldsymbol{k}_\perp|$ ($\boldsymbol{n}$ is a unit vector along the z axis). The eigenvalues of the operator $\hat{P}$ are ± 1. The operator $\hat{P}$ is associated with the operator of spin projection along the direction of $\boldsymbol{l}$:

$$\hat{\Sigma}_l = |\hat{\boldsymbol{\Sigma}}\times\boldsymbol{l}| = \gamma^0\hat{P} . \tag{5.4}$$

It follows that the wave functions of the Hamiltonian (5.2) can be the eigenfunctions of the operator $\hat{P}$, so that

$$\hat{P}\hat{\Psi}_\lambda(z) = \lambda\hat{\Psi}_\lambda(z) , \tag{5.5}$$

and the equation for $\hat{\Psi}_\lambda$ becomes

$$\left\{\gamma^0\left[\gamma^3\hat{p}_z + \Delta(z)\right] + \mathrm{i}\gamma^3\left[u(z) - \lambda k_\perp\right] + G(z) - E\right\}\hat{\Psi}_\lambda = 0 . \tag{5.6}$$

The process of finding the quadrature of this equation gives

$$\left\{\hat{p}_z^2 + \Delta^2(z) + \left[u(z) - \lambda k_\perp\right]^2 - \left[E - G(z)\right]^2 + \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}z}\left[\gamma^3\Delta(z) - \gamma^0\gamma^3 G(z) + \mathrm{i}\gamma^0 u(z)\right]\right\}\hat{\Psi}\lambda = 0 . \tag{5.7}$$

The matrix part of this equation can be diagonalised only if the spatial dependences Δ, G, and u are given by the same function $f(z)$

$$\Delta(z) = \Delta_1 + \Delta_0 f(z) ,$$
$$u(z) = u_1 + u_0 f(z) , \tag{5.8}$$
$$G(z) = g_0 f(z) .$$

Such diagonalisation is performed by the canonical transformation $\hat{\Psi} = \hat{S}\hat{\chi}$, where

$$\hat{S} = \exp\left(\frac{\alpha\gamma^0}{2}\right)\exp\left(\frac{\mathrm{i}\beta\gamma^0\gamma^3}{2}\right) ,$$
$$\tanh(\alpha) = \frac{g_0}{\Delta_0} , \tag{5.9}$$
$$\tan(\beta) = \frac{u_0}{\sqrt{\Delta_0^2 - g_0^2}} .$$

Consequently, Eqn (5.7) becomes

$$\hat{H}_s\hat{\chi}_\lambda = \left[\hat{p}_z^2 + W_\lambda^2 - \mathrm{i}\gamma^3\frac{\mathrm{d}W_\lambda}{\mathrm{d}z}\right]\hat{\chi}_\lambda = E^2\hat{\chi}_\lambda \equiv E_s\hat{\chi}_\lambda , \tag{5.10}$$

where

$$W_\lambda(z) = w_\lambda + \varkappa f(z) , \tag{5.11}$$

$$E_s = \varepsilon^2 = E^2 - \Delta_1^2 - (u_1 - \lambda k_\perp)^2 + w_\lambda^2 , \tag{5.12}$$

and

$$w_\lambda = [\Delta_1\Delta_0 + (u_1 - \lambda k_\perp)u_0 + Eg_0]/\varkappa,$$
$$\varkappa = \sqrt{\Delta_0^2 + u_0^2 - g_0^2}.$$

The Hamiltonian (5.10) has a specific symmetry due to the special nature of the potential energy, representing the

sum of the square and of the derivative of the same function $W_\lambda(z)$. This becomes obvious if $\hat{H}_s$ is represented in the form

$$\hat{H}_s = Q_+Q_- + Q_-Q_+ , \tag{5.13}$$

where

$$Q_+ = B^-S^+ , \quad Q_- = B^+S^- ,$$
$$B^\pm = (\mp i\hat{p}_z + W_\lambda) , \quad S^\pm = \tfrac{1}{2}\begin{pmatrix} \sigma^\pm & 0 \\ 0 & \sigma^\pm \end{pmatrix} , \tag{5.14}$$
$$\sigma^\pm = \sigma_1 \pm i\sigma_2 .$$

Here, $B^\pm$ are the Bose operators which generally describe 'interacting bosons' [10] and the operators $S^\pm$ obey the Fermi transposition relationships and have the nilpotent property $(S^\pm)^2 = 0$. Consequently, we can demonstrate that the operators $Q_\pm$ commute with the Hamiltonian: $[\hat{H}_s, Q_\pm] = 0$. This is evidence of invariance of the Hamiltonian $\hat{H}_s$ under the transformations performed by the operators $Q_\pm$, i.e. the transformations involving the replacement of a boson by a fermion and vice versa. Consequently, the Hamiltonian $\hat{H}_s$ is the Hamiltonian of Witten's supersymmetric mechanics [25].

We shall consider the problem of the ground state of $\hat{H}_s$ by representing this Hamiltonian in the matrix form:

$$\hat{H}_s = \begin{bmatrix} H_+ & & & 0 \\ & H_- & & \\ & & H_- & \\ 0 & & & H_+ \end{bmatrix} , \tag{5.15}$$

where

$$H_+ = B^-B^+ = \hat{p}_z^2 + U_+(z) ,$$
$$H_- = B^+B^- = \hat{p}_z^2 + U_-(z) , \tag{5.16}$$
$$U_\pm = W^2(z) + W'(z) .$$

The Hamiltonians $H_\pm$ act in the space of one-component wave functions and each of these Hamiltonians is factorised, i.e. it is a product of two conjugate first-order differential operators. Consequently, the problem of finding zero-energy states reduces to that of solving the equations $B^+\hat{\chi}^+ = 0$ or $B^-\hat{\chi}^- = 0$.

Expression (5.14) for the operators $B^\pm$, makes it possible to write the system of equations $B^\pm\hat{\chi}^\pm = 0$ in the form

$$\left[\frac{d}{dz} \pm W(z)\right]\hat{\chi}^\pm = 0 . \tag{5.17}$$

The solutions of these equations are

$$\hat{\chi}^\pm = c\exp\left[\pm\int_0^z W(x)\,dx\right] . \tag{5.18}$$

However, since $\chi^\pm$ are the eigenfunctions of the Hamiltonian $\hat{H}_s$, they should be quadratically integrable. According to expression (5.18), this is possible if the following conditions are satisfied:

$$\int_0^z W(x)\,dx \to \mp\infty \quad \text{for} \quad |z| \to \infty , \tag{5.19}$$

where the minus and plus signs on the right of integral (5.19) correspond to the functions $\hat{\chi}^+$ and $\hat{\chi}^-$.

The conditions (5.19) are incompatible, so that only one of the functions $\hat{\chi}^\pm$ can be normalised. Therefore, if the state with the energy $E_s = 0$ ('zeroth mode') does exist, it is nondegenerate and this state corresponds to that of the functions $\hat{\chi}^\pm$ which is normalisable [i.e. the spinor part of the wave function corresponding to the zeroth mode has a structure either (1 0 0 1), or (0 1 i 0)]. However, it may prove that none of the functions is normalisable.

It should be noted that the Hamiltonian $\hat{H}_s$ can be represented in the form of the square of the Hermitian operators Q_1 and Q_2:

$$Q_1 = Q_+ + Q_- , \quad Q_2 = -i(Q_+ - Q_-) . \tag{5.20}$$

The operators Q_1, Q_2, and $\hat{H}_s$ obey the following algebra:

$$\{Q_i, Q_k\} = 2\delta_{ik}\hat{H}_s , \quad [Q_i, \hat{H}_s] = 0 , \quad i,k = 1,2 , \tag{5.21}$$

which includes both the commutation and anticommutation relationships (this is known as the Lie superalgebra). Consequently, the spectrum of the Hamiltonian $\hat{H}_s$ is nonnegative and the levels with $E_s \neq 0$ are doubly degenerate. It follows that the Hamiltonians $\hat{H}_\pm$ have almost the same spectrum for arbitrary functions $W(z)$. The only difference is that one of the Hamiltonians $H_\pm$ has the lowest level whose energy is zero and the other Hamiltonian does not have such a level [26, 27]. It then follows from formula (5.12) that in this case we have the ground-state solution for the Hamiltonian of Eqn (5.1).

Following Refs [28, 29], we can find the complete spectrum by making use of two properties of supersymmetric theories: the degeneracy of the spectrum and zero energy of the ground state.

Let us consider the specific case when the Hamiltonian H_- has the zero level. If the potentials $U_\pm$ differ only in respect of the parameters (including an additive constant) which occur in them, the complete spectrum of $H_\pm$ and, consequently, of the supersymmetric Hamiltonian $\hat{H}_s$ can easily be found. In fact, let us assume that

$$U_+(\alpha, z) = U_-(\alpha_1, z) + Q(\alpha_1) , \tag{5.22}$$

where α is the set of all the parameters and α_1 is some function of α [$\alpha_1 = f(\alpha)$], the form of which is governed by the potentials. Let us now derive a series of Hamiltonians H_n, where $n = 0, 1, 2, \ldots$:

$$H_n = \hat{p}_z^2 + U_-(\alpha_n, z) + \sum_{k=1}^{n} Q(\alpha_k) , \tag{5.23}$$

where α_n is the result of the n-fold application of the function f, and let us compare the spectra H_n and H_{n+1}. It follows from relationship (5.22) that

$$H_{n+1} = \hat{p}_z^2 + U_+(\alpha_n, z) + \sum_{k=1}^{n} Q(\alpha_k) . \tag{5.24}$$

As pointed out above, H_n and H_{n+1} have the same spectra with the exception of the lowest level H_n [with energy $\sum_{k=1}^{n} Q(\alpha_k)$]. Going over from H_n to H_{n-1} and so on, we obtain the initial Hamiltonian H_- with the lowest level of zero energy and all the other levels coincide with the lowest levels of the Hamiltonians H_n. Therefore, the complete spectrum of H_- is given by $\tilde{E}_n = \sum_{k=1}^{n} Q(\alpha_k)$. Consequently, the spectrum of the Hamiltonian with the potential $U(\alpha, z) = U_-(\alpha, z) + Q_0(\alpha)$ is [28]

$$E_s^n = \tilde{E}_n + Q_0(\alpha) = \sum_{k=1}^{n} Q(\alpha_k) + Q_0(\alpha) . \tag{5.25}$$

For the potentials $U_\pm$ obeying condition (5.22) the corresponding function $W(\alpha, z)$ satisfies the functional differential equation

$$W^2(\alpha, z) + \frac{\mathrm{d}}{\mathrm{d}z} W(\alpha, z) = W^2(\alpha_1, z) - \frac{\mathrm{d}}{\mathrm{d}z} W(\alpha_1, z) + 2Q(\alpha_1) \,. \tag{5.26}$$

Therefore, the spectra of the Hamiltonians $H_\pm$ and, therefore, the spectrum of $\hat{H}_s$ can easily be found by solving Eqn (5.26) and are given by formula (5.25).

Application of the supersymmetry method to the complete spectrum of the Hamiltonian (5.6) will now be considered for the specific case of the following spatial dependence on the fields described by expressions (5.8):

$$f(z) = \tanh\left(\frac{z}{l}\right) . \tag{5.27}$$

Substitution of dependence (5.27) into expressions (5.8), (5.11), and (5.16) gives

$$U_\pm = \frac{1}{l^2}\, a(a \pm 1) \tanh^2\left(\frac{z}{l}\right) + 2ab \tanh\left(\frac{z}{l}\right) + l^2 b^2 \pm \frac{a^2}{l^2} \,, \tag{5.28}$$

where $a = \varkappa/l = l/l_0$, $b = [\Delta_1 \Delta_0 + (u_1 - \lambda k_\perp)u_0 + Eg_0](l_0/l)$, and $l_0 = 1/\varkappa$ is the wave-function localisation length. Successive application of formulas (5.22)–(5.25) gives [$a_1 = a - 1$, $a_n = a - n$, $b_n = ab/a_n$, $Q_k = l^2(b_{k-1}^2 - b_k^2) + (2a + 1 - 2k)/l^2$, $Q_0(a) \equiv 0$].

$$E_s^n = \sum_{k=1}^{n} Q_k = l^2(b^2 - b_n^2) + \frac{n(2a - n)}{l^2} \,. \tag{5.29}$$

Finally, substitution of expression (5.29) into formula (5.12) yields the complete spectrum of localised states of the Hamiltonian (5.1) (representing the doubly degenerate 'Dirac' branch of the spectrum)

$$\begin{aligned} E^\pm = {} & \frac{1}{g_0^2 l^2 + (n - l/l_0)} \\ & \times \left\{ -g_0 l^2 \left[\Delta_1 \Delta_0 + (u_1 - \lambda k_\perp)u_0 \pm \left(-n + \frac{l}{l_0}\right) \right] \right. \\ & \times \left[g_0^2 l^2 + \left(n - \frac{l}{l_0}\right)^2 \left(\Delta_1^2 + (u_1 - \lambda k_\perp)^2 - \frac{n(n - 2l/l_0)}{l^2} \right) \right. \\ & \left. \left. - \left(\Delta_1 \Delta_0 + (u_1 - \lambda k_\perp)u_0\right)^2 \right]^{1/2} \right\} , \end{aligned} \tag{5.30}$$

where $n = m + (1 + \lambda)/2$ and $m = 0, 1, 2, \ldots$.

5.2. Multidimensional case

Application of the supersymmetry method to the spectrum of the Hamiltonian (5.1) can be generalised to the multidimensional case. When the potentials occurring in the Hamiltonian depend only on the vector $\boldsymbol{\rho} = (x, y, 0)$, the wave function can be selected in the form $\hat{\Psi} = \hat{\Psi}(\boldsymbol{\rho}) \exp(\mathrm{i}p_z z)$ and then Eqn (5.1) (with $u = 0$), written down in a cylindrical coordinate system, becomes

$$[\tilde{\gamma}^0(\tilde{\boldsymbol{\gamma}} \cdot \tilde{\boldsymbol{p}}) + \tilde{\gamma}^0 \Delta(\boldsymbol{\rho}) + G(\boldsymbol{\rho})]\hat{\Psi}(\boldsymbol{\rho}) = E\hat{\Psi}(\boldsymbol{\rho}) \,, \tag{5.31}$$

where

$$\tilde{\gamma}^\mu = h_\nu^\mu \gamma^\nu \,, \qquad h = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\varphi) & \sin(\varphi) & 0 \\ 0 & -\sin(\varphi) & \cos(\varphi) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{5.32}$$

and $\tilde{\boldsymbol{p}} = (-\mathrm{i}\partial_\rho, -\mathrm{i}\partial_\varphi/\rho, p_z)$. Next, if Δ and G depend only on $|\rho|$ (cylindrical symmetry), we can simplify Eqn (5.31) by eliminating the angular variables with the aid of the nonunitary transformation $\hat{\Psi}(\rho) = \hat{S}\hat{\Phi}(\rho) = \sqrt{\rho}\exp(\gamma^0\gamma^1\varphi/2)\hat{\Phi}(\rho)$. The equation for $\hat{\Phi}(\rho)$ then becomes

$$\left[\gamma^0\gamma^1\hat{p}_\rho + \gamma^0\gamma^2\frac{M}{\rho} + \gamma^0\gamma^3 p_z + \gamma^0\Delta(\rho) + G(\rho)\right]\hat{\Phi}(\rho) = E\hat{\Phi}(\rho) \,. \tag{5.33}$$

where $\hat{\Phi} = \Phi(\rho)\exp(\mathrm{i}M\varphi)$ and $M = \pm(1/2), \pm(3/2), \ldots$ because of the condition $\hat{\Psi}(\varphi + 2) = \hat{\Psi}(\varphi)$. If the coordinate dependences of Δ and G are described by the same function $f(\rho)$, namely

$$\Delta(\rho) = \Delta_0 f(\rho) + \Delta_1 \,, \qquad G(\rho) = g_0 f(\rho) \,, \tag{5.34}$$

the canonical transformation $\hat{\Phi} = \hat{S}_0\hat{\chi} = \exp(\gamma^0\omega/2)\hat{\chi}$, where $\tan(\omega) = -g_0/\Delta_0$, can be used to transform Eqn (5.33) to

$$\{\gamma^0[\gamma^1\hat{p}_\rho + w(\rho)] + \gamma^0\gamma^2\frac{M}{\rho} + \gamma^0\gamma^3 p_z\}\hat{\chi}(\rho) = \tilde{E}\hat{\chi}(\rho) \,, \tag{5.35}$$

where

$$w(\rho) = \sqrt{\Delta_0^2 - g_0^2}\, f(\rho) + \frac{\Delta_0\Delta_1 + Eg_0}{\sqrt{\Delta_0^2 - g_0^2}} \,, \qquad \tilde{E} = \frac{g_0\Delta_1 + E\Delta_0}{\sqrt{\Delta_0^2 - g_0^2}} \,. \tag{5.36}$$

Taking quadratures of Eqn (5.35), we obtain ($\hat{\chi}$ is a column of spinors χ_- and χ_+):

$$\hat{H}_1\hat{\chi}_\pm(\rho) \equiv \left\{\hat{p}_\rho^2 + \frac{M^2}{\rho^2} - \sigma_3\frac{M}{\rho^2} + w^2(\rho) \mp \sigma_1\frac{\mathrm{d}w}{\mathrm{d}\rho}\right\}\hat{\chi}_\mp = (\tilde{E}^2 - p_z^2)\tilde{\chi}_\mp \,. \tag{5.37}$$

Here, $\hat{H}_1$ is the Hamiltonian of supersymmetric quantum mechanics

$$\hat{H}\hat{\chi} = \left[\partial_\rho^2 + \hat{V}^2 + \frac{\mathrm{d}\hat{V}}{\mathrm{d}\rho}\right]\hat{\chi} = (E^2 - p_z^2)\hat{\chi} = E_s\hat{\chi} \tag{5.38}$$

and its matrix potential is

$$\hat{V}(\rho) = \Sigma_3\frac{M}{\rho} + \mathrm{i}\gamma^2 w(\rho) \,. \tag{5.39}$$

Then the 'supercharges' $\hat{Q}^\pm$ are

$$\hat{Q}^\pm \equiv [\mp\partial_\rho + \hat{V}(\rho)] \,. \tag{5.40}$$

It can easily be shown that the Hamiltonian (5.38) can be diagonalised only if $f(\rho) = 1/\rho$. The transformation $\hat{\chi}(\rho) = \exp(\gamma^2\omega_2/2)\eta(\rho)$, where $\tan(\omega_2) = (\Delta_0^2 - g_0^2)^{1/2}/M$, can reduce the Hamiltonian (5.38) to the following form

$$\hat{H}_s^{\mathrm{eff}}\eta(\rho) = [\hat{p}_\rho^2 + W^2(\rho) - \hat{\Sigma}_3 W'(\rho)]\eta(\rho) = \tilde{E}_s^2\eta(\rho) \,, \tag{5.41}$$

where

$$W(\rho)=\frac{\sqrt{M^2+\Delta_0^2-g_0^2}}{\rho}+\frac{\Delta_0\Delta_1+Eg_0}{\sqrt{M^2+\Delta_0^2-g_0^2}}\equiv\frac{c}{\rho}-d\,,$$

$$\tilde{E}_s^2=E^2+\frac{(\Delta_0\Delta_1+Eg_0)^2}{M^2+\Delta_1^2-g_0^2}-\Delta_1^2-p_z^2= \tag{5.43}$$

$$=E^2-\Delta_1^2-p_z^2+d^2\,,$$

and $\hat{\Sigma}_3$ is the third component of the spin operator. It then follows from general theorems of supersymmetric mechanics [10] that the zeroth mode of the Hamiltonian (5.41) exists if

$$\Delta_0\Delta_1+Eg_0<0\,. \tag{5.44}$$

The ground state energy (5.33) is found from the equation $\tilde{E}_s=0$. It should also be noted that the Hamiltonian (5.41) is identical in form with the SchroSdinger equation of supersymmetric quantum mechanics for the motion of a particle in a Coulomb field [29], where the role of the orbital momentum l is played by the quantity $(M^2+\Delta_0^2-g_0^2)^{1/2}$ with a known spectrum. The results of the preceding subsection [Eqns (5.22)–(5.25)] can be used to write down the general spectrum of localised [near $\rho_n=(c+n)^2/cd$, where $n=0,1,2,\ldots$] states of the Hamiltonian (5.33):

$$E_n^{\pm}=\frac{g_0\Delta_0\Delta_1}{(c+n)^2+g_0^2}\left[-1\pm\frac{c+n}{g_0\Delta_1\Delta_0}\right. \tag{5.45}$$

$$\left.\times\sqrt{\left[g_0^2+(c+n)^2\right](\Delta_1^2+p_z^2)-\Delta_1^2\Delta_0^2}\right]\,.$$

It should be noted that if $p_z=0$ and $\Delta_0=0$, expression (5.45) yields the familiar spectrum of the Coulomb states of three-dimensional fields:

$$E_n^{\pm}=-\mathrm{sign}(g_0)\frac{(c+n)\Delta_1}{\sqrt{(c+n)^2+g_0^2}}\,,\quad c=\sqrt{k^2-q^2}\,. \tag{5.46}$$

Here, g_0 plays the role of the interaction constant. In fact, in the case of three-dimensional spherically symmetric potentials $\Delta(r)$ and $G(r)$, the Hamiltonian (5.1) commutes with the operator

$$\hat{K}=\gamma^0(\hat{\boldsymbol{\sigma}}\cdot\hat{\boldsymbol{L}}+1)\,, \tag{5.47}$$

the eigenvalues of which are $k=\mp(j+1/2)=\mp1,\mp2,\ldots$. Here, $\hat{\boldsymbol{L}}$ is the orbital momentum operator and j is the total angular momentum of the electron. Therefore, the wave functions of the Hamiltonian (5.1) can be the eigenfunctions of the operator $\hat{K}$, such that $\hat{K}\hat{\Psi}(r)=k\hat{\Psi}(r)$, where $\hat{\Psi}=(1/r)\hat{\Phi}(r)$, and the function $\hat{\Phi}(r)$ can be found from the equation

$$\left[\tau_2\hat{p}_r+\frac{k}{r}\tau_1+\tau_3\Delta(r)+G(r)\right]\hat{\Phi}(r)=E\hat{\Phi}(r)\,, \tag{5.48}$$

where $\hat{p}_r=-\mathrm{i}\partial_r$, and $\tau_1,\tau_2,$ and τ_3 are the Pauli matrices. Taking quadratures of Eqn (5.48), we obtain

$$\left\{\hat{p}_r^2+\frac{k^2}{r^2}+\tau_3\frac{k}{r^2}+\frac{\mathrm{d}}{\mathrm{d}r}\left[\tau_1\Delta(r)+\mathrm{i}\tau_2G(r)\right]\right. \tag{5.49}$$

$$\left.-\left[E-G(r)\right]^2\right\}\hat{\Phi}=0\,.$$

It is easy to show that for the same spatial dependences of Δ and G [given by expression (5.34) where ρ is replaced with r], the nonunitary transformation $\hat{\Phi}(r)=\exp(\tau_3\beta/2)\hat{\chi}(r)$, where $\tanh(\beta)=g_0/\Delta_0$, can reduce Eqn (5.49) to

$$\left\{\hat{p}_r^2+\frac{k^2}{r^2}+\tau_3\frac{k}{r^2}+w^2(\rho)\mp\tau_1\frac{\mathrm{d}w}{\mathrm{d}r}\right\}\hat{\chi}=\tilde{E}^2\hat{\chi}\,, \tag{5.50}$$

where the expressions for $w(r)$ and $\tilde{E}$ are exactly the same as those given by expressions (5.36), apart from the replacement of ρ with r. Comparison of Eqns (5.37) and (5.50) shows that all subsequent comments relating to the solutions of Eqn (5.37) apply also in the three-dimensional case if ρ is replaced with r, M with $-k$, and it is assumed that $p_z=0$.

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