Bound States in a Two-Dimensional Short Range Potential Induced by the Spin-Orbit Interaction

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We have discovered an unexpected and surprising fact: a 2D axially symmetric short-range potential contains an *infinite* number of the levels of negative energy if one takes into account the spin-orbit (SO) interaction. For a shallow well ($m_e U_0 R^2/\hbar^2 \ll 1$, where m_e is the effective mass and U_0 and R are the depth and the radius of the well, respectively) and weak SO coupling ($|\alpha| m_e R/\hbar \ll 1$, where α is the SO coupling constant) exactly one twofold degenerate bound state exists for each value of the half-integer moment $j = m + 1/2$, and the corresponding binding energy E_m extremely rapidly decreases with increasing m.

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As is well known from any textbook on quantum mechanics, a very shallow potential well ($m_e U_0 R^2/\hbar^2 \ll 1$) cannot capture a particle with a mass m_e in the 3D case and does this in 2D and 1D situations provided the wells are symmetric: even potential in a 1D, axially symmetric well in two dimensions. In the latter case the only negative level corresponds to the s state ($m = 0$). These statements relate to spinless particles.

During the past few years various effects depending on the spin degree of freedom of electrons have been intensively discussed in literature in connection with a spin transistor, quantum computer, and some other applications. Therefore the problem of localized states of charge carriers accounting for spin-orbit (SO) interaction becomes quite topical. In the present Letter we show that the SO interaction in 2D electron gas drastically changes the picture of the bound states formation for a short-range axially symmetric potential well $U(r)$: in contrast with the spinless case mentioned above, the number of levels of negative energy becomes infinite.

Consider a 2D electron accounting for the SO interaction in the Bychkov-Rashba form [1]. The Hamiltonian reads

$$\hat{H} = \frac{\hat{p}^2}{2m_e} + \alpha(\boldsymbol{\sigma}[\hat{\mathbf{p}} \times \mathbf{n}]) + U(r), \tag{1}$$

where r and $\hat{\mathbf{p}}$ are the radius in cylindrical coordinates and the 2D electron momentum operator, respectively, $\boldsymbol{\sigma}$ are Pauli matrices, and $\mathbf{n}$ is normal to the plane of the 2D system.

It is convenient to write down the Schrödinger equation in the $\mathbf{p}$ representation:

$$\left[\frac{p^2}{2m_e} + \alpha(\boldsymbol{\sigma}[\mathbf{p} \times \mathbf{n}])\right]\Psi(\mathbf{p}) + \int \frac{d\mathbf{p}'}{4\pi^2} \mathcal{U}(\mathbf{p} - \mathbf{p}')\Psi(\mathbf{p}') = \mathcal{E}\Psi(\mathbf{p}). \tag{2}$$

Here $\mathcal{U}(\mathbf{p}) = \int d\mathbf{r} e^{-i\mathbf{p}\mathbf{r}} U(r) = 2\pi \int_0^\infty dr r U(r) J_0(pr)$ is the Fourier transform of the potential [$J_0(z)$ is the Bessel function]. Because of the axial symmetry of the problem, it is possible to separate the cylindrical harmonics of the spinor wave function and search for the solution in the form

$$\Psi^{(m)}(\mathbf{p}) = \begin{pmatrix} \psi_1^{(m)}(p) e^{im\varphi} \\ \psi_2^{(m)}(p) e^{i(m+1)\varphi} \end{pmatrix} \tag{3}$$

(φ is the azimuthal angle of the vector $\mathbf{p}$). Using the summation theorem [2]

$$J_0(|\mathbf{p} - \mathbf{p}'|r) = \sum_{k=-\infty}^{\infty} J_k(pr) J_k(p'r) \cos(k\theta)$$

(θ is the angle between the vectors $\mathbf{p}$ and $\mathbf{p}'$), one can rewrite Eq. (2) for each mth harmonic:

$$\left[\frac{p^2}{2m_e} - \mathcal{E}\right]\psi_{1,2}^{(m)}(p) \pm i\alpha p \psi_{2,1}^{(m)}(p) + \int_0^\infty dr' r' U(r') J_{m+(1\mp 1)/2}(pr') C_{1,2}^{(m)}(r') = 0. \tag{4}$$

Here the functions $C_{1,2}^{(m)}$ have been introduced:

$$C_1^{(m)}(r) = \int_0^\infty dp\, p J_m(pr) \psi_1^{(m)}(p), \qquad C_2^{(m)}(r) = \int_0^\infty dp\, p J_{m+1}(pr) \psi_2^{(m)}(p). \tag{5}$$

Resolving Eq. (4) with regards to $\psi_{1,2}$, we find

$$\begin{pmatrix} \psi_1^{(m)}(p) \\ \psi_2^{(m)}(p) \end{pmatrix} = -\frac{1}{\Delta(p;\mathcal{E})} \int_0^\infty dr r U(r) \begin{pmatrix} [p^2/2m_e - \mathcal{E}] J_m(pr) C_1^{(m)}(r) - i\alpha p J_{m+1}(pr) C_2^{(m)}(r) \\ i\alpha p J_m(pr) C_1^{(m)}(r) + [p^2/2m_e - \mathcal{E}] J_{m+1}(pr) C_2^{(m)}(r) \end{pmatrix}, \tag{6}$$

where $\Delta(p;\mathcal{E}) = (p^2/2m_e - \mathcal{E})^2 - 4\alpha^2 p^2$. Zeros of $\Delta(p;\mathcal{E})$ as functions of $\mathcal{E}$ give two branches of the dispersion relation for free electrons: $\mathcal{E}_\pm(p) = p^2/2m_e \pm \alpha p$.

Finally, from Eq. (6) using the definitions (5) we arrive at the equations for $C_{1,2}^{(m)}$:

$$C_i^{(m)}(r) = \int_0^\infty dr' r' U(r') A_{ij}^{(m)}(r, r') C_j^{(m)}(r') \quad (i, j = 1, 2). \tag{7}$$

Here the matrix $\hat{A}_{ij}^{(m)}$ has been introduced:

$$A_{ii}^{(m)}(r, r') = -\int_0^\infty \frac{dp\, p}{\Delta(p;\mathcal{E})}\left(\frac{p^2}{2m_e} - \mathcal{E}\right) \times J_{m+i-1}(pr) J_{m+i-1}(pr'), \tag{8}$$

$$A_{12}^{(m)}(r, r') = -i\alpha \int_0^\infty \frac{dp\, p^2}{\Delta(p;\mathcal{E})} J_m(pr) J_{m+1}(pr'), \quad A_{21}^{(m)}(r, r') = (A_{12}^{(m)}(r', r))^*. \tag{9}$$

The function $\Delta(p;\mathcal{E})$ can be presented in the form $\Delta(p;E) = [(p - p_0)^2/2m_e - E][(p + p_0)^2/2m_e - E]$, where $p_0 = m_e|\alpha|$ is the radius of the loop of extrema, E is the energy counted from the bottom of continuum, and $E = \mathcal{E} + m_e\alpha^2/2$. Now we search for levels of negative energy satisfying the condition $|E| \ll m_e\alpha^2$, and simultaneously we assume $2m_e U_0 R^2/\hbar^2 \equiv \xi \ll 1$ (U_0, R are the characteristic depth and radius of the well). Then integrals in Eqs. (8) and (9) can be calculated in the "pole" approximation: we put $p = p_0$ everywhere in the integrand except the first factor in $\Delta(p;E)$. As a result we have ($\hbar = 1$)

$$\begin{aligned} C_1^{(m)}(r) = &-\frac{\pi p_0\sqrt{m}}{\sqrt{2|E|}} \int_0^\infty dr' r' U(r') \\ &\times [J_m(p_0 r) J_m(p_0 r') C_1^{(m)}(r') \\ &- i\,\mathrm{sgn}(\alpha) J_m(p_0 r) J_{m+1}(p_0 r') C_2^{(m)}(r')], \\ C_2^{(m)}(r) = &-\frac{\pi p_0\sqrt{m_e}}{\sqrt{2|E|}} \int_0^\infty dr' r' U(r') \\ &\times [i\,\mathrm{sgn}(\alpha) J_{m+1}(p_0 r) J_m(p_0 r') C_1^{(m)}(r') \\ &+ J_{m+1}(p_0 r) J_{m+1}(p_0 r') C_2^{(m)}(r')]. \end{aligned} \tag{10}$$

Thus, we obtained the system of linear integral equations with degenerate kernels which can be easily solved. This system can be reduced to a pair of linear algebraic equations for the quantities $t_m \equiv \int_0^\infty dr r U(r) J_m(p_0 r)$ and t_{m+1} (defined similarly):

$$\begin{aligned} t_m &= \frac{\chi_m}{\sqrt{2|E|}}[t_m - i\,\mathrm{sgn}(\alpha) t_{m+1}], \\ t_{m+1} &= \frac{\chi_{m+1}}{\sqrt{2|E|}}[t_{m+1} + i\,\mathrm{sgn}(\alpha) t_m]. \end{aligned} \tag{11}$$

Here $\chi_m = -\pi p_0\sqrt{m_e}\int_0^\infty dr r U(r) J_m^2(p_0 r)$. From Eq. (11) one immediately gets

$$\begin{aligned} E_m &= -(\chi_m + \chi_{m+1})^2/2 \\ &= -\frac{\pi^2 p_0^2 m_e}{2}\left(\int_0^\infty dr r U(r)[J_m^2(p_0 r) + J_{m+1}^2(p_0 r)]\right)^2 \\ &= -\frac{\pi^2 p_0^2 m_e}{2} \\ &\quad \times \left(\int_0^\infty dr r U(r)[J_{j-1/2}^2(p_0 r) + J_{j+1/2}^2(p_0 r)]\right)^2, \end{aligned} \tag{12}$$

where $j = m + 1/2 = \pm 1/2, \pm 3/2, \ldots$, is the z projection of the total moment. As it is seen from Eq. (12) all levels are twofold degenerate: E_m is even function of j. If the SO interaction is now small ($p_0 R \ll 1$), we can get the asymptotic behavior of the binding energy by expanding the Bessel functions in Eq. (12). For a rectangular well $U(r) = -U_0\theta(R - r)$, we have $|E_m| \propto \alpha^{4|j|}/\{2^{4|j|}[(|j| - 1/2)!]^4(2|j| + 1)^2\}$. For an exponential well $U(r) = -U_0 \times \exp(-r/R)$, one can find $|E_m| \propto \alpha^{4|j|}[(2|j|)!]^2/\{2^{4|j|}[(|j| - 1/2)!]^4\}$.

Thus, we see that in an arbitrary axially symmetric short-range [the integral in Eq. (12) converges] potential well there exists at least one bound state for each cylindrical harmonic with the energy level below the bottom of continuum ($-m_e\alpha^2/2$). The energy of this state E counted from $-m_e\alpha^2/2$ in the regime $|E| \ll m_e\alpha^2$ is proportional to U_0^2, where U_0 is the characteristic depth of the well. Such a dependence is typical for a shallow level in a symmetric 1D potential well. The one-dimensional character of the motion results from the so called "loop of extrema" (see [3]). In a small vicinity of the bottom of the continuum, the dispersion law of 2D electrons has a form $\mathcal{E}(p) = -m_e\alpha^2/2 + (p - p_0)^2/2m_e$ and corresponds to a 1D particle at least in the sense of the density of states: one may formally consider the problem as the motion of a particle with anisotropic effective mass; in the **p** space the radial component of the mass equals m_e, while its azimuthal component is infinitely large (the dispersion law is independent of the angle in the **p** plane) [4].

We realize that our conclusion looks paradoxical: for a sufficiently large value of m the centrifugal barrier (CB) can make the effective potential energy $U(r) + U_{\mathrm{CB}}$ positive all over the space. How can a bound state with *negative* energy be formed in such a situation? Our arguments are as follows: for a particle with dispersion relation $(p - p_0)^2/2m_e$ there exists no CB; the azimuthal effective mass tends to infinity and the CB vanishes.

For numerical estimates, take inversion layers on p-type InAs [5]. In this system, $\alpha = 3 \times 10^{-11}$ eV m and the Rashba energy $m\alpha^2 = 0.34$ meV; then for $U_0 = 0.1$ eV and $R = 20$ A, we get that the binding energy of the s state without SO interaction is about 7×10^{-4} meV, and with SO interaction it is about 6×10^{-2} meV, i.e., effectively the 1D state lies 2 orders of magnitude deeper. Without SO interaction, the p level does not exist in such a potential well; accounting for SO interaction its energy is extremely small: $|E_1| \simeq 0.3 \times 10^{-8}$ meV. Note, however, that the Rashba constant α can be essentially enlarged (2–3 orders of magnitude) in the perpendicular electric field [6] while the p-state binding energy rapidly increases with α: $|E_1| \propto \alpha^6$.

To check our results, we have numerically analyzed the square well potential $U(r) = -U_0\theta(R - r)$, where θ is the Heaviside function. We seek a solution of the Schrödinger equation in the form

$$\Psi(r, \varphi) = \begin{pmatrix} \psi_1(r)e^{im\varphi} \\ \psi_2(r)e^{i(m+1)\phi} \end{pmatrix}, \tag{13}$$

where now φ is the azimuthal angle of the vector $\mathbf{r}$. Spinor components $\psi_{1,2}(r)$ are given by linear combinations of the Bessel functions $J_m(\tilde{\kappa}_\pm r)$ and $J_{m+1}(\tilde{\kappa}_\pm r)$ for $r < R$, or $K_m(\kappa_\pm r)$ and $K_{m+1}(\kappa_\pm r)$ for $r > R$, where

$$\tilde{\kappa}_\pm = \sqrt{2m_e(E + U_0)} \pm m_e\alpha, \qquad \kappa_\pm = \sqrt{2m_e|E|} \pm im_e\alpha. \tag{14}$$

Expressions (14) are valid when the condition $E < 0$ is satisfied. Now we have to meet the matching conditions for the wave function and its derivative at $r = R$. After rather cumbersome algebra we arrive at the determinants, zeros of which give the required spectrum of localized states. The energy levels have been estimated numerically for the s and p states ($m = 0, 1$). The results totally coincide with the ones given above for $|E| \ll m_e\alpha^2$. Figure 1 demonstrates this for the s state. The exited p state at zero SO interaction appears when U_0 exceeds a certain critical value $U_0^{(c)}$, namely, when $\xi > \xi_c = x_1^2$, where x_1 is the first root of the Bessel function $J_0(x)$. Taking SO interaction into account results in the splitting of the p level and lowering the critical value $U_0^{(c)}$ for the upper of spin-split sublevels. The lower sublevel exists at any value of the parameter ξ (see Fig. 2).

Our last remark relates to the Coulomb interaction with a charged impurity. If one tries to apply the general relation (12) to the Coulomb potential $-e^2/r$, the integral logarithmically diverges at the upper limit: $J_m^2(z \to \infty) \sim (2/\pi z) \times \cos^2(z - \pi m/4 - \pi/4)$ does not depend on m after averaging over oscillations and can be replaced by $1/\pi z$. Equation (12) gives for the energy the value independent of m:

$$E = -2m_e e^4 \ln^2(p_0 L), \tag{15}$$

where L is some cutoff length. Its exact value depends on the concrete situations: it may be the screening radius or the thickness of two-dimensional electron gas. We see that the energy spectrum does not depend on m (as it must be for the Coulomb field) and exactly coincides with that of a "1D hydrogen atom": the ground state binding energy equals $2Ry$ (rather than $Ry/2$ as in 3D case) multiplied by $\ln^2(\Lambda)$, where Λ is the cutoff parameter (see, for example, the problem of the hydrogen atom in an extremely high magnetic field [7]). This result also supports our interpretation: in the region $|E| \ll m_e\alpha^2$ the particle becomes effectively one dimensional.

It is interesting from the general physics point of view to find a similar situation for the 3D case. Batyev has kindly reminded us that the roton spectrum of liquid He-4 also contains a part of dispersion relation that reads $\Delta + (p - p_0)^2/2M$, possesses not a loop but a surface of extrema, and, correspondingly, should describe an effectively 1D

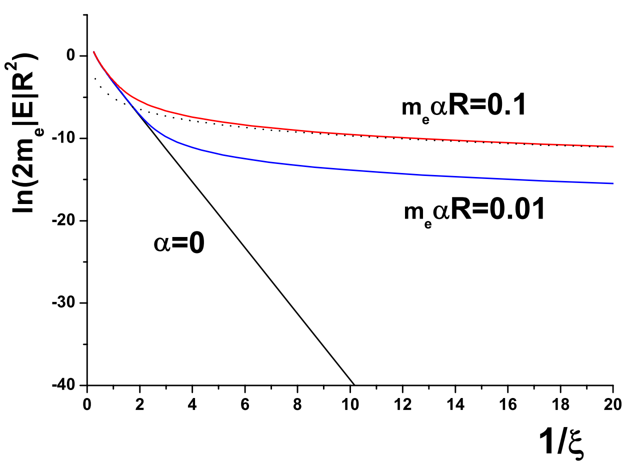

FIG. 1 (color online). The behavior of the s level versus the well depth. The curves demonstrate the transition between 2D and 1D regimes. At $\alpha = 0$ we have an exponentially shallow level (2D result), while for finite α at small enough $\xi \equiv 2m_eU_0R^2$ the binding energy parabolically depends on U_0 (1D regime). The dotted line represents the results of our pole approximation [Eq. (12)].

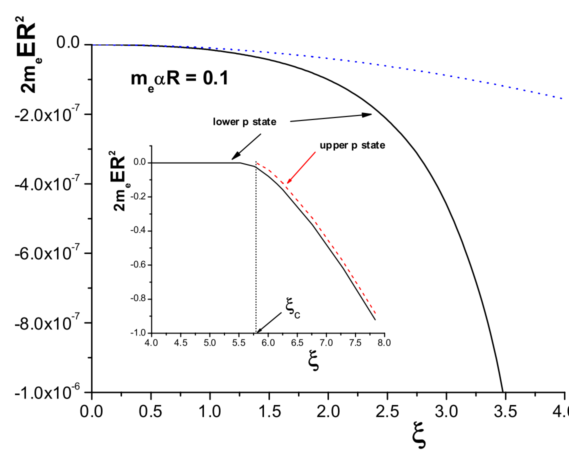

FIG. 2 (color online). p states. Comparison of the exact solution for the square well with Eq. (12) (dotted line). Inset: spin-split states of the p level: the upper curve terminates at $U_0 = U_0^{(c)}$—the level merges with continuum.

particle. We have made the proper calculation; in other words, we solved the Schrödinger equation in the momentum representation for the Hamiltonian $\Delta + (p - p_0)^2/2M + U(r)$ with $U(r)$ as an attractive spherically symmetric potential. We used the same method—expansion of the wave function over the spherical harmonics—and we got the same result: even in three dimensions, a shallow potential well contains one bound state for each moment l, and this state is $(2l + 1)$-fold degenerate:

$$E = -2\pi^2 p_0^2 M\left(\int_0^\infty dr r U(r) J_{l+1/2}^2(p_0 r)\right)^2. \quad (16)$$

For the Coulomb potential the last formula once again leads to the 1D result given by Eq. (15).

Until now we have been considering an axially symmetric potential $U(r)$. A question may arise as to what happens in the case of asymmetric short-range potentials. As is explained above, the essence of the effect under consideration is the loop of extrema that makes the problem effectively one dimensional. An asymmetric 1D potential well never has bound states, so we do not expect the infinite number of the negative energy levels in this case. Still we have to note that the problem of an asymmetric potential is much more difficult for the quantitative analysis due to nonseparability of the variables and it is beyond the scope of our present work.

In conclusion, we have shown that 2D electrons interact with impurities in a very special way if one takes into account SO coupling: because of the loop of extrema, the system behaves as a 1D one for negative energies close to the bottom of continuum. This results in the infinite number of bound states even for a short-range potential.

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