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LETTER TO THE EDITOR

Resonances in bent quantum wires

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Abstract. We studied the problem of the bound state in a slightly bent two-dimensional quantum wire with the confining potential being an arbitrary function. The problem is mapped to a particle Hamiltonian with a slowly varying centre of the confining potential. For the class of even analytic potentials we proved that an arbitrary small bend will always produce a resonant state, but a true bound state will be absent. The energy of the resonant state is calculated to the lowest order in perturbation theory, for the case of the harmonic oscillator confining potential.

In recent years, it has become possible to fabricate very narrow two-dimensional (2D) layers which serve as confining geometries for propagation of electrons [1]. If this kind of quantum wire is made sufficiently clean, the electron mean free path due to impurity scattering may become very long and the dominant scattering mechanism at low temperatures is interaction with surface imperfections and the edges of the sample. It has been shown that edges of these structures can bind electrons [2–4]. This represents a purely quantum effect and the formation of the bound state is not due to the existence of the classically forbidden region of electron motion. Recently Goldstone and Jaffe [5] obtained a general result: an infinite tube of constant and arbitrary large cross-section, will always have a bound electron state in any dimension, as long as its curvature is not constant. Since it is known that the presence of a bound state below the continuum spectrum strongly affects conductance properties of these systems, and because the effect is intuitively surprising, it is interesting to devise different ways to address the problem.

All the theoretical and experimental evidence [2–6] presented so far in favour of the existence of the bound states due to the edges assumed Dirichlet boundary conditions, i.e. wavefunctions are required to vanish at the edges of the wire. To complement this formalism and study effects of more realistic boundary conditions, in this paper we formulate a perturbation theory for the problem of a 2D wire with a small dent. It is demonstrated that, to the lowest order in perturbation theory, the variational argument of Goldstone *et al* [5] implies that the resonant state will exist at least for confining potential which is an even function of particle coordinate. We determined the electron propagator for the particular choice of harmonic oscillator confining potential and calculated the energy of the resonance to the lowest order. It is found that the energy measured from the bottom of the lowest band is proportional to the $-\delta^4$, where δ is the introduced small parameter. This behaviour is distinct from all other cases of binding in 1D or quasi-1D systems, and we argued that this is a general feature of bent wires. Then we found that the next-order term in the expansion of the Hamiltonian pushes all the states up in energy for the amount proportional to δ^2.

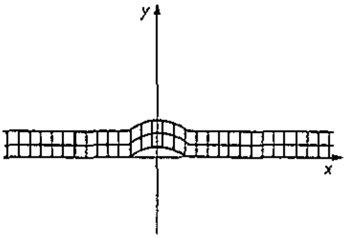

Figure 1. The 2D strip with a small dent. The shape of the edge determines the function $f(x)$.

This implies that there is no truly bound state in the problem for an arbitrary weak bend, in stark contrast to the case of hard-walls boundary conditions.

Consider a 2D strip of constant width, straight everywhere except in the bounded region with the 'dent' (figure 1). This is analogous to the case of a bent strip since the only perturbation of the electronic motion is again due to the change of curvature in some localized region of the strip. The idea is to describe the dent as a variation of the centre of the confining potential along the strip. We define the quantum mechanical problem with the Hamiltonian

$$H[f(x)] = -(\hbar^2/2m)(\partial_x^2 + \partial_y^2) + V(y + f(x)) \tag{1}$$

where $V(y)$ is a confining potential along y axis. The length scale implicit in $V(y)$ determines the width of the strip. Expanding the Hamiltonian in powers of $f(x)$, to the lowest order one gets

$$H[f(x)] \simeq H[0] + f(x)V'(y) \tag{2}$$

where $V'(y) = \mathrm{d}V(y)/\mathrm{d}y$. We first study this approximate Hamiltonian. Note that the problem of strip with a bulge can be treated in similar way, where one would represent the bulge as a variation of the length scale of the confining potential [7]. To the lowest order in this variation the bulge would correspond to an attractive channel-mixing 1D potential and always produce a bound state. The present case of dent is rather different, since the sign of $f(x)$ is left to our choice. Thus, it is not obvious that the simplified Hamiltonian defined by (2) would have a bound state for an arbitrary small perturbation $f(x)$.

To demonstrate the existence of the bound state in the spectrum of Hamiltonian (2) we use the variational argument of Goldstone and Jaffe [5]. We assume a smooth function $f(x)$ which vanishes for $|x| > a$. Take the variational ground state $\Psi(x, y) = \Phi_0(y) \exp -\lambda(|x| - x_0)$ for $|x| > a$ (regions I and III) and arbitrary for $|x| < a$ (region II), where $\lambda > 0$ is a variational parameter. State $\Phi_0(y)$ is the normalized ground state of the confining potential, i.e.

$$(-(\hbar^2/2m)\partial_y^2 + V(y))\Phi_0(y) = E_0\Phi_0(y).$$

We also assume Ψ to be continuous and smooth everywhere. One is interested in finding a state for which the energy expectation value is below the ground state energy for non-perturbed Hamiltonian:

$$E[\Psi] = (\langle\Psi|H|\Psi\rangle)/(\langle\Psi|\Psi\rangle) < E_0. \tag{3}$$

It is easy to calculate

$$\langle\Psi|\Psi\rangle = \frac{1}{\lambda} + \int_{\mathrm{II}} |\Psi|^2 \tag{4}$$

$$\langle\Psi|H|\Psi\rangle = \lambda + \frac{E_0}{\lambda} + \int_{\mathrm{II}} \Psi^* H \Psi. \tag{5}$$

The second equation holds for any even function $V(y)$ because

$$\int_{\mathrm{I+III}} V'(y)|\Phi_0(y)|^2 = 0$$

since $\Phi_0(y)$ has to be even and $V'(y)$ odd function. Thus the inequality (3) is equivalent to

$$I[\Psi] = \int_{\mathrm{II}} (E_0|\Psi|^2 - \Psi^* H \Psi) > \lambda. \tag{6}$$

We need to prove that a state exists for which $I[\Psi] > 0$; then one can choose the parameter λ such that $I[\Psi] > \lambda > 0$ and satisfy the inequality (3). For the case of even confining potential, by taking $\Psi_0(x, y) = \Phi_0(y)$ for $|x| < a$ we get $I[\Psi_0] = 0$. However, Ψ_0 is not a stationary point of $I[\Psi]$ since

$$H\Psi_0 = E_0\Psi_0 - f(x)V'(y)\Psi_0 \neq E_0\Psi_0 \tag{7}$$

and the continuity of functional $I[\Psi]$ implies that there exists a neighbourhood around Ψ_0 in functional space where $I[\Psi] > 0$.

The presented argument proves that there is a bound state in the problem defined by the Hamiltonian given in (2), but tells us very little about its energy. To address this question we take the simplest realization of the confining potential that is sure to produce a bound state: $V(y) = m\omega^2 y^2/2$. It is convenient to rewrite the Hamiltonian (2) in second-quantized form as

$$H = \sum_{k,n} (e_k + E_n) C^\dagger_{k,n} C_{k,n} + \sum_{k,q,n,m} f(q) V_{n,m} C^\dagger_{k+q,n} C_{k,m} \tag{8}$$

where $f(q)$ is a Fourier transform of $f(y)$, $e_k = \hbar^2 k^2/2m$ and $E_n = \hbar\omega(n + 1/2)$ $V_{n,m} = (\hbar\omega/l2^{1/2})(m^{1/2}\delta_{n,m-1} + (m+1)^{1/2}\delta_{n,m+1})$ for our choice of harmonic oscillator confining potential. The width of the strip is determined by the length $l = (\hbar/m\omega)^{1/2}$. The matrix equation for the particle's Green function is

$$G_{n,m}(p, p'; \epsilon) = G^0_n(p; \epsilon)\delta_{n,m}\delta(p - p') + G^0_n(p; \epsilon) \sum_{q,j} f(q - p) V_{n,j} G_{j,m}(q, p'; \epsilon) \tag{9}$$

where the free propagator is $G^0_n(p; \epsilon) = (\epsilon - (e_p + E_n) + i\eta)^{-1}$. To simplify calculations we assume an infinitely short-ranged perturbation $f(y) = f\delta(y)$. The momentum-diagonal part of the particle's Green function may then be expressed as

$$G_{n,m}(p; \epsilon) = G^0_n(p; \epsilon)\delta_{n,m} + G^0_n(p; \epsilon) T_{n,m}(\epsilon) G^0_m(p; \epsilon) \tag{10}$$

where the transfer matrix is given by $\hat{T} = (f/L)(1 - (f/L)\hat{A}(\epsilon))^{-1}\hat{V}$, $A_{n,j}(\epsilon) = V_{n,j} g_j(\epsilon)$, $g_j(\epsilon) = \sum_q G^0_j(q; \epsilon)$, and L is the length of the strip. The energy of the bound state is determined by the position of the pole of the transfer matrix, i.e.

$$\det[\hat{I} - (f/L)\hat{A}(\epsilon)] = 0. \tag{11}$$

Matrix $\hat{I} - (f/L)\hat{A}(\epsilon)$ is an infinite tridiagonal matrix and equation (11) is practically unsolvable. However, we recall that our method is consistent only to the lowest order in f, and the determinant in equation (11) may then be expanded as

$$\det(\hat{I} - (f/L)\hat{A}(\epsilon)) \simeq 1 - \frac{(f\hbar\omega)^2}{2(Ll)^2}\sum_{n=1}^{\infty} n g_{n-1}(\epsilon) g_n(\epsilon) \tag{12}$$

and

$$g_n(\epsilon) = -L(2m)^{1/2}/2\hbar(E_n - \epsilon)^{1/2}$$

for $\epsilon < E_0$. Since the bound state energy measured from the bottom of the lowest band is proportional to f, to obtain its leading order behaviour it suffices to keep only the first term in the sum in the last equation. Parameter f has a dimension of (length)^2 and we introduce a small number $\delta = f/2l^2$. The bound state energy can now be written to the lowest order in small δ as

$$\epsilon \simeq E_0 - \delta^4\hbar\omega. \tag{13}$$

The reader should note that the energy of the bound state of the first-order Hamiltonian (2) when measured from E_0 is proportional to δ^4 which tells us that the state is very weakly bound. This, for instance, should be contrasted with the case of a bulge in the strip, where one obtains the same energy to be $\epsilon \propto \delta^2$, which is the typical dependence of the bound state energy on combination (depth$\times$width) of the potential well in 1D. As a consequence, even if the expression (2) was the full Hamiltonian, the bound state would be localized on the length scale $\lambda \propto \delta^{-2}l$, which is long for small δ. For a finite range function $f(y)$ we believe that the leading δ^4 dependence of the bound state energy will persist. The only difference is that parameter f will be replaced by the product of lengths that determine width and depth of the dent.

This result is in qualitative agreement with the calculations for the slightly bent 2D strip of Goldstone *et al* [5]. The authors studied the limit when the angle of the bend $\alpha \to 0$ and the radius of the bend curvature $r \to \infty$, and obtained the energy $\epsilon \propto \alpha^2 r^{-2}$. Also the numerical calculations of Carini *et al* [6] show that the resonant state energy versus bend angle curve is very flat for small angles. Even though the geometry of their setup is different than in the case we studied (sharp edges at the place of the bend, Dirichlet boundary conditions) it seems that treating δ as a phenomenological parameter linearly related to the bend angle one can fit their numerical data. The choice of $\delta = 0.017\alpha$, where α is a bend angle measured in degrees, fits their curve well for $\alpha < 30°$. This is somewhat ambiguous, however, because the energies in question are small and hard to read from their graph. Still, this gives us reason to believe that our conclusions are not very sensitive to the exact geometry of the bend nor to the type of the confining potential.

Let us now include the next-order term in the expansion (2). For the potential $V(y) \propto Y^{2n}$ it is proportional to $y^{2n-2}f^2(x)$. Since it is positive and even in y it will increase the energies of all states for the amount proportional to δ^2. Hence, for an arbitrary small bend there will be no true bound state, but only a resonance. For a non-analytic potential $V(y)$ our argument fails, and indeed Goldstone and Jaffe [5] have proved the existence of a true bound state in the case of hard walls.

To summarize, we have proved the existence of a resonant state in 2D quantum wires due to a small dent, for the class of even analytic confining potentials. We calculated the energy of the resonance using perturbation theory for the case of harmonic oscillator confining potential. It has been shown that the resonant state energy lies above the bottom of the lowest non-perturbed band, for small bend. Thus there is no true bound state, in contrast to the case of Dirichlet boundary conditions.

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