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Physics

Remarks on the Bound States in Continuum

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Abstract. An alternative example of a discrete state embedded in the continuum for positive energies is introduced. It has been shown that many such potentials can arise from relativistic three-dimensional quasipotential equations. The key feature of such construction lies in the energy dependence of quasi-potential. For this reason, the potential proposed by Von Neuman and Wigner should not be regarded as an anomaly. © *2025 Bull. Natl. Acad. Sci. Georg.*

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Bound states play an important role in nature – everything around us is composed of a smaller bound objects. What exactly does the term “bound state“ mean? It has a different meaning in classical and quantum physics. Let us start with an example from classical physics.

For simplicity, consider a two-particle case interacting through a distance-dependent (central) force. The total energy of such a system is the sum of kinetic and potential energies:

$$E = \frac{m_1 V_1^2}{2} + \frac{m_2 V_2^2}{2} + V\left(\left|r_1 - r_2\right|\right) = const. \tag{1}$$

Let us consider the case when $V \to 0$ if the distance $\left|r_1 - r_2\right| \to \infty$. It is well known that if the particles attract each other, then $V < 0$, and if the total energy $E > 0$, nothing prevents the particles to move in infinite distance from each other. However, if $E < 0$, particles cannot move into infinite distance from each other, because the potential approaches zero at this time leaving only two positive kinetic energy terms in (1) but their sum cannot be negative. This is a well known fact in classical mechanics: the motion can be either infinite or finite as well. In case of finite motion, the body is moving on the close trajectory. In quantum mechanics (QM), the notion of a “trajectory” loses its meaning because of the uncertainty principle (Heisenberg, 1927). Therefore, how can we describe finite and infinite motions in this case?

As is well known, the motion in quantum mechanics is described by the Schrodinger equation

$$H\varphi(r) = E\varphi(r), \tag{2}$$

$$H = \frac{\hat{\boldsymbol{p}}_1^2}{2m_1} + \frac{\hat{\boldsymbol{p}}_2^2}{2m_2} + V\left(\left|\boldsymbol{r}_1 - \boldsymbol{r}_2\right|\right) \to \frac{\hat{\boldsymbol{p}}^2}{2\mu} + V(\boldsymbol{r}). \tag{3}$$

The quantity $|\varphi|^2$ is a probability density to find a particle at a point with a coordinate $\boldsymbol{r}$. Now, it is easy to see what finite motion is. For the motion to be finite, the probability of finding the particles at finite distance from each other must be zero. Therefore, the wave function, describing finite motion must tend to zero very rapidly at infinite distance. This rapid fall ensures that the probability cannot be more than one. Thus, a bound state in QM corresponds to a normalized wave function at a given energy. Potentials, falling at infinity lead to a bound state with negative energy. A good example is the so-called effective potential:

$$V_{eff} = \frac{l(l+1)}{2\mu r^2} + V(r) \Rightarrow \frac{\hat{L}^2}{2\mu r^2} + V(r). \tag{4}$$

The first term represents the centrifugal energy, which gives us repulsion and prevents the particle from falling to the center. The total energy can be expressed as a sum of radial kinetic energy $\frac{p_r^2}{2\mu}$ and V_{eff}. If the total energy is negative, the motion will be finite. The points, where $E = V_{eff}$ and $p_r = 0$, are called the turning points.

We can pose the following question: Can a system possess a bound state with positive total energy when the potential energy tends to zero?

In classical physics, yes – this is possible if the potential has a barrier.

In quantum mechanics: we'll have tunneled (as in the case of α – particle decay).

Now, imagine that after the first tunneling, there are subsequent hills, which our particle must also tunneling, and so on. After scattering from a large number of hills, the intensity of the wave function falls to zero and we won't have outgoing wave after an infinite number of barriers.

Von Neuman and Wigner (1929) built an example, which was considered a mathematical curiosity for a long time. These authors have shown that it is possible, for example, if the potential has the form at infinity

$$V \to \gamma \frac{\sin(2kr)}{r}. \tag{5}$$

In this case, we obtain bound states for positive energies (in continuum) and it might be possible that the sign of the potential does not make any difference. Read and Simons (1978) present the following theorem proved by Atkinson (1954):

Theorem: If potential has a following form

$$V(r) = \sum_{j=1}^{N} \gamma_j \frac{\sin(\sigma_j r)}{r} + Q(r), \tag{6}$$

where $\left|Q(r)\right|_{r \gg 1}$ falls faster than r^{-1} and $k^2 = (\sigma_j / 2)^2$ for some j, the Schrodinger equation has a solution of the following form:

$$u = \begin{cases} r^{-\gamma_j/2\sigma_j}\left(\cos\frac{\sigma_j r}{2} + 0(1)\right), & \gamma_j/\sigma_j > 0 \\ r^{+\gamma_j/2\sigma_j}\left(\sin\frac{\sigma_j r}{2} + 0(1)\right), & \gamma_j/\sigma_j < 0. \end{cases} \tag{7}$$

Thus, the sign of the potential is not important (this happens, because the potential oscillates very fast at infinity) and the bound state in the continuum is possible even we have a repulsion instead of attraction. The question arises whether such a potential has any physical meaning. Some authors state that they can "make" any kind of potential. Capasso et al. (1992) observed experimentally bound states in continuum in some potentials they made by themselves using "bandgap engineering" in ultra-thin semiconductor layered structures grown by molecular beam epitaxy.

Despite this, it is still interesting to know, whether those kinds of states have a deeper source rather than mechanically made crystals.

Let us consider the following relativistic quasipotential Logunov-Tavkhelidze equation (1963)

$$\left(E-2\sqrt{p^2+m^2}\right)\psi(\boldsymbol{p})=\frac{1}{(2\pi)^3}\int d^3q V(E;\boldsymbol{p},\boldsymbol{q})\psi(\boldsymbol{q}). \tag{8}$$

In general, the quasipotential $V(E;\boldsymbol{p},\boldsymbol{q})$ is not local and depends upon the energy. But there are exclusions, the simplest example in QED is (Faustov, 1970)

$$V(E;\boldsymbol{p},\boldsymbol{q})=\frac{e^2}{|\boldsymbol{p}-\boldsymbol{q}|\left(E-\sqrt{p^2+m^2}-\sqrt{q^2+m^2}-|\boldsymbol{p}-\boldsymbol{q}|\right)}. \tag{9}$$

It is known that in the Born approximation the scattering amplitude coincides with quasipotential on a mass-shell

$$E=2\sqrt{p^2+m^2}=2\sqrt{q^2+m^2}. \tag{10}$$

In this case, it is clear that

$$V(E;\boldsymbol{p},q)=-\frac{e^2}{|\boldsymbol{p}-\boldsymbol{q}|^2} \;\rightarrow\; -\frac{\alpha}{r},\; \left(\alpha=e^2/4\pi\right). \tag{11}$$

When $M<2m,$ then V has a definite sign, it has following properties: it depends on energy and can change sign, when $M>2m$. That's why, we can think that this potential might oscillate. In order to see that, consider small momenta (non-relativistic reduction). We arrive to the following equation

$$\left(E-\frac{p^2}{m}\right)\psi(\boldsymbol{p})=\frac{\alpha}{2\pi^2}\int d^3q\frac{\psi(\boldsymbol{q})}{|\boldsymbol{p}-\boldsymbol{q}|\left(E-|\boldsymbol{p}-\boldsymbol{q}|\right)}, \tag{12}$$

which in coordinate space gives us an ordinary Schrodinger equation with local potential having the following asymptotic at infinity:

$$V(r)\rightarrow-\frac{2\alpha}{r}\cos(Er). \tag{13}$$

Therefore, it seems that the von Neuman-Wigner potential is not a curiousity, but it appears to be a direct consequence of relativity. Its existence can be proved in relativity and also it can be "made" by hands in condensed matter physics.

ფიზიკა

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