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1986 J. Phys. A: Math. Gen. 19 3845

(http://iopscience.iop.org/0305-4470/19/18/029)

J. Phys. A: Math. Gen. 19 (1986) 3845-3848. Printed in Great Britain

A simple separable Hamiltonian having bound states in the continuum

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Received 4 February 1986, in final form 4 April 1986

Abstract. We discuss a simple separable two-freedom Hamiltonian H describing the motion of a point particle in a plane region ($V=0$) between two infinite parallel hard walls ($V=\infty$) and with a rectangular finite potential well ($V=-V_0$). The quantal spectrum of H is discrete below the continuum limit (ionisation energy) different from the classical escape energy ($E=0$) by the zero point energy of the transverse motion and has infinitely many bound states embedded in the continuum. We show that this spectrum is fragile against perturbations of H: if the hard walls are made diverging, the bound states in the continuum disappear, while if they are converging, the continuum disappears and the spectrum is pure point.

Von Neumann and Wigner (1929) were the first to realise that bound states can exist embedded in the continuum. They attempted to construct a local scalar potential such that there exists a bound state in the continuum (BIC state) for the one-particle Schrödinger equation. Their analysis has been examined by Stillinger and Herrick (1975) in the context of possible BIC states in atoms and molecules. It has been demonstrated by Newton (1982) that strong coupling between scattering channels can give rise to BIC states and this has been rediscussed for the coupled Coulombic channels by Friedrich and Wintgen (1985), who have also given the example of the hydrogen atom in a uniform magnetic field. In view of the importance of the phenomenon of the BIC states it seems useful to study as simple a Hamiltonian with BIC states as possible for this might lead us towards a deeper understanding of more general conditions under which BIC states occur. It has been overlooked by those who have discussed this phenomenon that such a system can be separable. One would like to answer questions such as, for example, how stable BIC states are under small perturbations of a Hamiltonian. To provide and analyse one such simple system is the subject of this paper.

Our Hamiltonian $\hat{H}$ with two freedoms is

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

where the potential $V(x,y)$ in the xy plane is defined as follows:

$$V(x,y)=\begin{cases}\infty & \text{if } y\notin[0,b]\\ 0 & \text{if } y\in[0,b] \text{ and } x\notin[0,a]\\ -V_0 & \text{if } y\in[0,b] \text{ and } x\in[0,a].\end{cases} \tag{2}$$

The Schrödinger equation can be separated by the ansatz

$$\psi=\sin(n\pi y/b)\phi(x) \qquad n=1,2,\ldots \tag{3}$$

which leads to

$$\frac{\hbar^2}{2m}\partial_x^2\phi+\left[E-\left(V+\frac{\hbar^2n^2\pi^2}{2mb^2}\right)\right]\phi=0. \tag{4}$$

By introducing ε

$$E=\varepsilon+\frac{\hbar^2n^2\pi^2}{2mb^2} \tag{5}$$

and

$$\begin{aligned}\varkappa^2&=-2m\varepsilon/\hbar^2\\ k^2&=2m(\varepsilon+V_0)/\hbar^2\end{aligned} \tag{6}$$

we obtain the discrete energy levels ε,

$$\cot ka=\frac{1}{2}\left(\frac{k}{\varkappa}-\frac{\varkappa}{k}\right). \tag{7}$$

There is no solution if $\varepsilon<-V_0$. In the range $\varepsilon\in[-V_0,0]$ there are N energy levels, approximately given by

$$N=a(2mV_0)^{1/2}/\pi\hbar \tag{8}$$

which is asymptotically exact as $N\to\infty$.

For $\varepsilon>0$ there are no bound states, so $\varepsilon=0$ is the continuum limit, i.e. the ionisation energy. We see that in terms of E the continuum limit is equal to

$$E_c=\hbar^2\pi^2/2mb^2 \tag{9}$$

which is the zero point ('ground state') energy of the transverse motion. Thus the quantal ionisation energy marking the onset of the continuum differs from the classical escape energy ($E=0$) by the zero point energy of the transverse motion. Let ε_l, $l=1,2,\ldots,N$, denote the eigenvalues determined by (7). Then the spectrum consists of a superposition of identical finite bands corresponding to different n and shifted in E by $\hbar^2n^2\pi^2/2mb^2$. The continuum exists for

$$E>E_c=\hbar^2\pi^2/2mb^2 \tag{10}$$

which is the threshold for the $n=1$ band. Some of the higher states of the $n=2$ band obviously lie in the continuum and similarly for $n=3$, etc. Eventually entire bands lie in the continuum. Hence we have infinitely many bound states in the continuum.

The reason why the quantum ionisation energy E_c is greater than the classical escape energy lies in the fact that the zero point energy of the transverse motion represents an extra (effective) potential as is clear from equation (4). For energies E in the interval $[0, E_c]$ the classical phase space volume enclosed by the constant energy surface is *infinite* and yet we do *not* have a continuous quantal spectrum there. This is thus yet another counterexample to the naive and wrong rule that an unbounded energy surface at energy E, enclosing an infinite volume in the classical phase space, implies, at least partially, a continuous quantal spectrum below that same energy E. (The converse is true: finite phase space volume implies discrete spectrum.) See Rozenbljum (1972, 1973), Simon (1983a, b) and Van den Berg (1984) for further details and other less elementary counterexamples.

From equation (4) we can learn about the behaviour of the spectrum under small perturbations of the Hamiltonian. Suppose we have (arbitrarily weakly) diverging channel rather than plane parallel geometry, so $b(x)\to\infty$ as $|x|\to\infty$. For slow variations of $b(x)$ we can heuristically resort to the adiabatic picture. Equation (4) tells us then that the extra effective potential vanishes asymptotically. Therefore we shall have $E_c=0$ and there will be no bound states in the continuum, but resonances instead: a particle at $E>0$ can penetrate the finite potential barrier and can become asymptotically free.

On the other hand, applying the same heuristic arguments, we find that the spectrum is purely discrete if the channel is converging (on both sides), i.e. if $b(x)\to 0$ as $|x|\to\infty$. Let us assume a power law as an example, so

$$b(x)=\beta|x|^{-\alpha} \qquad |x|\gg a,\ 0<a\ll 1. \tag{11}$$

Then equation (4) becomes

$$\frac{\hbar^2}{2m}\partial_x^2\phi+\left(E-\frac{\hbar^2 n^2\pi^2}{2m\beta^2}|x|^{2\alpha}\right)\phi=0 \qquad |x|\gg a. \tag{12}$$

In the asymptotic limit $|x|\to\infty$ the number of modes below E is dominated by longitudinal modes (quantum number l) and a simple scaling gives

$$l \underset{E\to\infty}{=} \text{constant}\times E^{(1+1/\alpha)/2} \tag{13}$$

which agrees with Rozenbljum (1972, 1973) and Simon (1983a, b).

The 'adiabatic arguments' we used to explain the perturbational properties of the spectrum are particularly clear and give correct results, even though they are not rigorous. For the reader interested in a rigorous proof we refer to Molchanov (1953) and Mazya (1965), and also Rozenbljum (1972). There one finds the following necessary and sufficient condition for the discreteness of the spectrum of the Dirichlet Laplacian in a region D of the Euclidean space $\mathbb{R}^d$. For $d\leqslant 3$ the spectrum is discrete iff the region D does *not* contain an infinite sequence of disjoint but equal cubes. In our case D is a plane region, $d=2$ and the cubes are squares. The condition is obviously satisfied if the channel is convergent (on both sides), as distinct from the divergent case.

Let us now try to extract more general understanding from the specific but not too special example considered in this paper. For the occurrence of BIC states it seems essential that the equipotential surfaces open in a non-uniform way by forming channels connecting to infinity, rather than by uniformly receding to infinity as, for example, in the Coulomb potential. The continuum exists only if at least one channel is not converging (escape channel) and sets in above the classical escape energy, the shift being equal to the asymptotic zero point energy for the transverse motion across the escape channel. So bound states in the continuum exist only if each escape channel is *on the average* and asymptotically (at large distances) *exactly parallel.* Separability or integrability of the Hamiltonian are irrelevant in this context, because the transverse excitations always exist and give rise to the phenomenon described. The example of the hydrogen atom in a magnetic field was discussed by Robnik (1981, 1982) and Friedrich and Wintgen (1985). A spectrum with BIC states is obviously a fragile structure: upon a small perturbation of the potential BIC states disappear and may become resonances or else the continuum disappears.

We can now generalise even further. Think of a Hamiltonian with a given potential V. The continuum in the spectrum exists if above a certain threshold there are travelling waves that propagate to infinity. Bound states in the continuum exist if there exist special travelling waves which do not propagate to infinity but become totally reflected. One possibility for this to happen was described above. But there is another possibility in the case where the potential is modulated at the wavelength of the wave in such a way that total reflection of outgoing waves (interference effect) takes place and gives rise to the BIC states. The potential can even be spherically symmetric (no channels), such as the von Neumann–Wigner (1929) example discussed further by Stillinger and Herrick (1975). Its oscillatory nature implies total back-reflection of certain outgoing S waves (interference effect). In this way the localised standing waves corresponding to the bound states in the continuum emerge.

We conclude that the bound states in the continuum are as exceptional (non-generic) as the oscillatory potential barriers that transmit (at least partially) all waves except for certain discrete wavelengths for which total reflection occurs due to the interference effects. A necessary condition for the total reflection of plane waves is that the total variation of the logarithm of the refractive index is infinite, as was shown by Robnik (1979), where an upper bound to the reflectance was obtained. It is clear that such states cannot persist under small perturbations of the Hamiltonian.

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