Bound states in the continuum

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Introduction

In 1929, von Neumann and Wigner claimed [1] that the single-particle Schrödinger equation could possess isolated eigenvalues embedded in the continuum of positive energy states. They offered a constructive method based upon amplitude modulation of a free-particle wave function and leading to a localized (i.e., integrable) eigenfunction and a local potential which produces it. The potential was bounded and could be made to vanish at infinity. Diffractive interference was proposed as the reason such localized positive-energy states could exist.

Objectives

The aim of Stillinger and Herricks's paper [2] was to construct quantum-mechanical examples with local potentials that allow bound eigenstates embedded in the dense continuum of scattering states.

In the light of the Further Examples section, attention is focused on quantitative interpretation of real tunneling phenomena, and on the existence of continuum bound states in atoms and molecules.

Definitions

Bound state = a bound state is a special quantum state of a particle subject to a potential such that the particle has a tendency to remain localized in one or more regions of space.

Continuum = matter continuously distributed and fills the entire region of space it occupies. Here, continuum is considered to be wave functions with positive energies, compared to bound states with negative energies.

Node = a point along a standing wave where the wave has minimum (usually vanishing) amplitude.

Separability = the wave function can be written as a direct product of individual wave functions. Usually the case for non-interacting particles.

Von Neumann-Wigner Method

In natural units, the single-particle Schrödinger wave equation is to be solved in infinite three-space:

$$\left(-\frac{1}{2}\nabla^2 + V\right)\psi = E\psi \tag{1}$$

Momentarily, we consider only bounded potentials V, and which are local operators in position representation. Eqn. 1 can be reversed to obtain the potential,

$$V = E + \frac{1}{2}\left(\frac{\nabla^2\psi}{\psi}\right) \tag{2}$$

which implies that the nodes of the wave function ψ must be matched by vanishing of its Laplacian. For $V = 0$, the free particle S-wave,

$$\psi_0(r) = \sin(kr)/kr \tag{3}$$

satisfies the above with energy eigenvalue $E = k^2/2$. To obtain potentials yielding bounded states, consider an amplitude modulation $f(r)$ and $\psi(r) = \psi_0(r)f(r)$.

$$V(r) = E - \frac{1}{2}kr^2 + k\cot(kr)\frac{f'(r)}{f(r)} + \frac{1}{2}\frac{f''(r)}{f(r)} \tag{4}$$

Further constrains are needed for the envelop function $f(r)$ to keep the potential bounded. The specific choice suggested by von Neumann and Wigner [1] is:

$$f(r) = \{A^2 + [2kr - \sin 2kr]^2\}^{-1} \tag{5}$$

where A is an arbitrary nonzero constant. Thereby:

$$V(r) = -\frac{64k^2A^2\sin^4(kr)}{[A^2 + (2kr - \sin(2kr)^2]^2} + \frac{48k^2\sin^4 kr - 8k^2(2kr - \sin 2kr)}{A^2 + (2kr - \sin 2kr)^2} \tag{6}$$

Near the origin, the function reduces to:

$$V(r) = (80/3A^2 - 64)k^2(kr)^4 + O((kr)^6) \tag{7}$$

while its large r form is expressed as:

$$V(r) \sim -8k^2(\sin 2kr)/2kr \tag{8}$$

Graphical Results

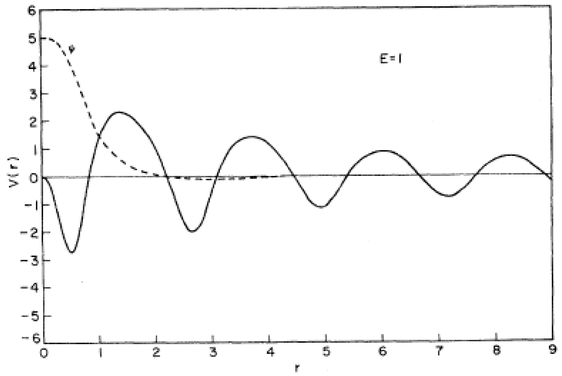

Figure 1: Potential-energy function for particle energy l. [2] Classically, the particle would have been trapped inside the potential barrier since its energy is lower than the barrier.

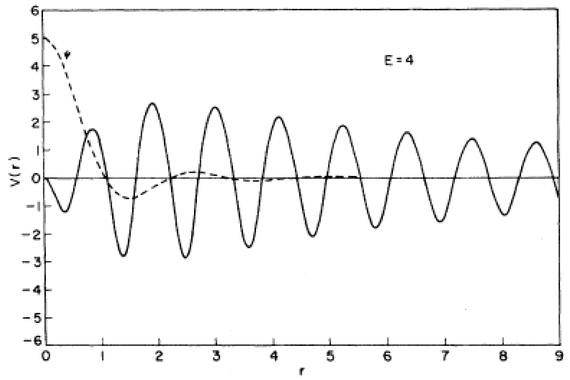

Figure 2: Potential-energy function with energy 4. [2] This energy exceeds the maximum value for the potential, so the particle could not be trapped even by classical mechanics.

Further Examples

These examples involve just single particles, furthermore, they can be reduced to one-dimensional form by virtue of separability:

A Higher angular momentum: for a free-particle state with total-angular-momentum quantum number l; $\psi^{(l)} = f_l(r)R_l(kr)Y_{lm}(\theta,\phi)$

B Variable dimensionality: ground state of the helium isoelectronic sequence for variable dimensionality.

C Coulomb interactions (only for repulsive potentials)

D Constant electric field (potential linear in displacement along the field)

The non-separable case is given by the Doubly Excited atom: a model "two-electron" atom which, with suitable interaction between the electrons, will have a doubly excited state with infinite lifetime (within the Schrödinger description).

Discussion

The eigenvalue for the preceding positive-energy bound state can be moved up or down within the continuum merely by varying the wave vector k. Equation 6 specifies the way in which $V(r)$ must deform to continue supporting its bound state nature.

The examples of continuum bound states constructed by Stillinger and Herrick [2] sent a warning against quantitative over-interpretation of the tunneling phenomena:

1. Cold emission of electrons from metals, under the influence of strong electric fields,
2. Alpha decay rates of radioactive nuclei,
3. Tunneling through films between adjacent solid phases.

If a given physical system were to possess a potential close to the subspace of potentials with continuum bound states, then its tunneling rate would be anomalously small.

Ongoing Research

The very existence of Bound States in Continuum defies conventional wisdom. Although first proposed in quantum mechanics, they are a general wave phenomenon and have since been identified in electromagnetic waves, acoustic waves in air, water waves and elastic waves in solids. These states have been studied in a wide range of material systems, such as piezoelectric materials, dielectric photonic crystals, optical waveguides and fibres, quantum dots, graphene and topological insulators.

References

[1] J. von Neumann and E. P. Wigner. *Über merkwürdige diskrete Eigenwerte*, pages 291–293. Springer Berlin Heidelberg, Berlin, Heidelberg, 1993.

[2] Frank H. Stillinger and David R. Herrick. Bound states in the continuum. *Phys. Rev. A*, 11:446–454, Feb 1975.