Annals of the Academy of Romanian Scientists
Series on Physics and Chemistry Sciences
ISSN 2559-1061 Volume 3, Number 1/2018

PHYSICAL INTERPRETATION OF QUANTITIES IN THE COMPLEX ENERGY PLANE

R.J. Liotta*

Abstract

Since the first application of the probability interpretation of quantum mechanics by Gamow nearly nine decades ago the use of complex physical quantities, which are outside the framework of quantum mechanics, have been very useful in the description of processes occurring in the continuum part of quantum spectra. In this talk I will introduce and clarify the meaning of those complex quantities. This will bring my talk to discusions on dubious interpretations of some aspects of quantum mechanics itself.

*liotta@kth.se;Royal Institute of Technology (KTH), Alba Nova University Center, SE-10691 Stockholm, Sweden

One is often unaware of the bizarre properties that quantities provided by Quantum Mechanics may carry. To see this I will consider the most simple example of a potential that bounds a particle. That is, the one-dimension Hamiltonian corresponding to the square well potential shown in Fig. 1 with the condition $V(x) = \infty$ for $x \leqslant 0$. I will solve the Schrödinger equation corresponding to this case in detail, although it can be found in any elementary quantum mechanics text book. I will do this to avoid confusions and to make be clear about what quantum mechanics provides.

The Schrödinger equation is,

$$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right]\Phi_n(x) = E_n\Phi_n(x) \tag{1}$$

To solve the eigenvalue problem given by Eq. (1) we notice that there are two regions:

Region (1): $0 < x < a$; $V(x) = -V_0$
Region (2): $x \geqslant a$; $V(x) = 0$

There are also two possibilities for the state: Continuum ($E = E_c > 0$) and Bound ($E = -E_b < 0$)

$$\begin{aligned} \text{Region (1):} \qquad \left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - V_0\right]\Phi_n^{(1)}(x) &= E_n\Phi_n^{(1)}(x) \\ \text{Region (2):} \qquad \left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right]\Phi_n^{(2)}(x) &= E_n\Phi_n^{(2)}(x) \end{aligned}$$

with

$$q^2 = \frac{2\mu}{\hbar^2}(E_n + V_0); \quad k^2 = \frac{2\mu}{\hbar^2}E_n \tag{2}$$

Since Eq. (1) is a second order differential equation the general solution should be a combination of two independent particular solutions. Therefore the general eigenvectors of the eigenvalue problem are

$$\begin{cases} \Phi_n^{(1)}(x) = A_n\mathrm{e}^{\mathrm{i}qx} + B_n\mathrm{e}^{-\mathrm{i}qx} \\ \Phi_n^{(2)}(x) = C_n\mathrm{e}^{\mathrm{i}kx} + D_n\mathrm{e}^{-\mathrm{i}kx} \end{cases} \tag{3}$$

It is important for us to notice that the particular solutions $\mathrm{e}^{\mathrm{i}qx}$ and $\mathrm{e}^{-\mathrm{i}qx}$ are outgoing and incoming waves, respectively. To see this we apply the linear momentum operator $\mathbf{p}_x = \mathbf{e}_x\frac{\hbar}{i}\frac{d}{dx}$, where $\mathbf{e}_x$ is the unit vector, to get $\mathbf{p}_x\mathrm{e}^{\mathrm{i}qx} = \mathbf{e}_x\frac{\hbar}{i}\frac{d}{dx}\mathrm{e}^{\mathrm{i}qx}$ $= \mathbf{e}_x\hbar q\mathrm{e}^{\mathrm{i}qx}$ and $\mathbf{p}_x\mathrm{e}^{-\mathrm{i}qx} = -\mathbf{e}_x\hbar q\mathrm{e}^{-\mathrm{i}qx}$. As expected, $\mathrm{e}^{\pm\mathrm{i}qx}$ are eigenvectors of the linear momentum operator. The corresponding eigenvalues $\pm\mathbf{e}_x\hbar q$ indicate that the linear momentum (and therefore the velocity) correspondng to the wave $\mathrm{e}^{\mathrm{i}qx}$ goes in the direction of the unit operator, i.e. out from the origin of coordinates (outgoing) while $\mathrm{e}^{-\mathrm{i}qx}$ goes in the opposite direction (incoming).

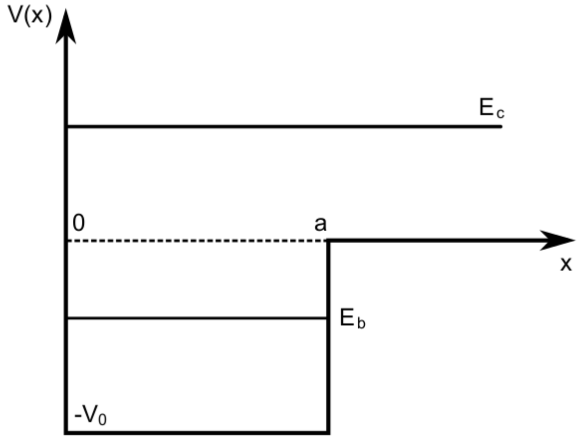

Figure 1: Square well potential in one-dimension. The range of the potential is a and the depth is $-V_0$. For $x < 0$ the potential is infinite and, therefore, the wave function vanishes at $x = 0$. We assume $E_b > 0$ and therefore $-E_b$ ($E_c > 0$) is the energy of a bound (continuum) state.

To determine the constant A_n, B_n, C_n and D_n, the boundary conditions for continuity of density and current have to be applied, i.e.

$$\begin{cases} \Phi_n^{(1)}(a) = \Phi_n^{(2)}(a) \\ \dfrac{\mathrm{d}}{\mathrm{d}x}\Phi_n^{(1)}(x)\Big|_{x=a} = \dfrac{\mathrm{d}}{\mathrm{d}x}\Phi_n^{(2)}(x)\Big|_{x=a} \end{cases}$$

I) Bound states

We assume $E_b > 0$ and, therefore, the energy of the bound state is $-E_b$.

$$q^2 = \frac{2\mu}{\hbar^2}(V_0 - E_b) > 0; \quad k^2 = -\frac{2\mu}{\hbar^2}E_b < 0$$

$$q = \sqrt{\frac{2\mu}{\hbar^2}(V_0 - E_b)}; \quad k = \mathrm{i}\chi, \quad \chi = \sqrt{\frac{2\mu E_b}{\hbar^2}}$$

and the wave function equations become,

$$\begin{cases} \Phi_n^{(1)}(x) = A_n \mathrm{e}^{\mathrm{i}qx} + B_n \mathrm{e}^{-\mathrm{i}qx} \\ \Phi_n^{(2)}(x) = C_n \mathrm{e}^{-\chi \mathrm{x}} + D_n \mathrm{e}^{\chi \mathrm{x}} \end{cases}$$

Since $V(x) = \infty$ for $x \leqslant 0$ it should be $\Phi_n^{(1)}(x)$=0, which implies $A_n = -B_n$ and

$$\Phi_n^{(1)}(x) = 2iA_n \sin qx$$

redefining A_n as $2\mathrm{i}A_n$ the continuity equations provide,

$$\begin{cases} A_n \sin qa = C_n \mathrm{e}^{-\chi \mathrm{a}} + D_n \mathrm{e}^{\chi \mathrm{a}} \\ qA_n \cos qa = \chi(-C_n \mathrm{e}^{-\chi \mathrm{a}} + D_n \mathrm{e}^{\chi \mathrm{a}}) \end{cases}$$

and the constants become

$$C_n = \frac{A_n \begin{vmatrix} \sin(qa) & e^{\chi a} \\ q\cos(qa) & \chi e^{\chi a} \end{vmatrix}}{Det}; D_n = \frac{A_n \begin{vmatrix} e^{-\chi a} & \sin(qa) \\ -\chi e^{-\chi a} & q\cos(qa) \end{vmatrix}}{Det}$$

where

$$Det = \begin{vmatrix} e^{-\chi a} & e^{\chi a} \\ -\chi e^{-\chi a} & \chi e^{\chi a} \end{vmatrix}$$

The constant A_n is determined by using the normalization condition $\int_0^\infty |\Phi_n(x)|^2 dx{=}1$. So far we have not given a prescription to evaluate the energy. Moreover, we (that is, quantum mechanics) have a serious problem because the wave function in region (2), i.e. $\Phi_n^{(2)}(x) = C_n \mathrm{e}^{-\chi x} + D_n \mathrm{e}^{\chi x}$ diverges as $x \to \infty$ since $\mathrm{e}^{\chi x}$ diverges. This is one of many instances in quantum mechanics where physical quantities diverge. In all cases one has found ways to overcome the problem with ingenious but somehow inconsistent solutions. In the present case the solution is just to impose the condition $D_n = 0$. This condition is fulfilled by values of E_b satisfying the equation $e^{-\chi a}(q\cos(qa) + \chi \sin(qa)) = 0$, or

$$\sqrt{V_0 - E_b} + \sqrt{E_b}\ tg\Big(\sqrt{\frac{2\mu}{\hbar^2}(V_0 - E_b)}a\Big) = 0 \tag{4}$$

In this equation one can take for a nucleon the mass $mc^2 \approx 939 MeV$ and $\hbar c \approx 200 MeV fm$, $\hbar \approx 6.6 \times 10^{-22} MeV sec$. Notice that it must be $E_b < V_0$, otherwise $\sqrt{V_0 - E_b}$ becomes a complex number.

The condition $D_n{=}0$ is called "outgoing boundary condition" because it implies, from Eq. (3), that only outgoing waves are allowed. This is an intriguing property since it breaks the mathematical necessity that both outgoing and incoming waves have to be present in the standing waves that our time-independent treatment assumes. To understand the extent of this assumption one can compare with classical mechanics. For instance, in the case of a projectile moving under the influence of the gravitational force, the second order Newton equation $\mathbf{F} = md^2/dt^2\mathbf{r}$ requires that there should be two constants which determine the trajectory of the projectile. Generally one imposes values of the coordinate $\mathbf{r}(t)$ and the velocity $\mathbf{v}(t)$ at a certain time, for instance $t{=}0$. If the quantum mechanics prescription would be imposed here, then one would reach the absurd conclusion that only orbits with $\mathbf{v}(t = 0) = 0$ are physically meaningful. Instead, in quantum mechanics this prescription determines the bound states. Only bound states satisfying the outgoing boundary condition are allowed, thus establishing the quantization of the states. This is in complete agreement with experimental data.

If this feature sounds bizarre, even more bizarre is what occurs with resonances and antibound states, as seen in the next Section.

As a summary of this Section, we found that a feature of bound states is that they are confined within a limited region in space. Outside this region the wave function vanishes. Thus, from Eq. (3) we see that the wave function at large distances is $\Phi_n(x) = C_n \mathrm{e}^{\mathrm{i}kx}$ with $k = \mathrm{i}\chi$, and $\Phi_n(x) \to 0$ as $x \to \infty$. An important point is that, for bound states, the wave number k is purely imaginary with positive real part. This shows an attribute of the wave number which makes it more important than the energy, which can be determined through k by the relation (2), i.e. $E_n = \hbar^2 k^2/(2\mu)$. But k also provides information on the wave function which cannot be extracted from the energy, for instance whether the state is bound, or whether a wave is incoming or outgoing. As we will see below, there are also states with negative energy but with the real part of k negative. Such states, called antibound states, diverge at large distance, but nevertheless they may have an important physical meaning.

An important point for us is that, from Eqs. (2) and (3), the wave function extends farther out from the point $x = a$ as the value of k becomes smaller, that is as E approaches the continuum threshold (i.e. the energy $E = 0$).

II) Continuum states

As shown in Fig. 1, the eigenvalues of the Hamiltonian in the positive-energy part of the spectrum are called E_c. The wave functions are still as in Eq. (3), but with q and k given by

$$q^2 = \frac{2\mu}{\hbar^2}(V_0 + E_c) > 0; \quad k^2 = \frac{2\mu}{\hbar^2} E_c > 0.$$

That is,

$$q = \sqrt{\frac{2\mu}{\hbar^2}(V_0 + E_c)}; \quad k = \sqrt{\frac{2\mu}{\hbar^2} E_c}$$

are real quantities.

As before, the wave function vanishes at $x = 0$ and therefore, replacing A_n by $2iA_n$, one gets

$$\begin{cases} \Phi_n^{(1)}(x) = A_n \sin(qx) \\ \Phi_n^{(2)}(x) = C_n \mathrm{e}^{\mathrm{i}kx} + D_n \mathrm{e}^{-\mathrm{i}kx} \end{cases}$$

Notice that all energies $E_c > 0$ are allowed in the continuum, but only a discrete number of energies $-E_b < 0$ are allowed as bound states. It may even be that there is no bound state if the potential is not attractive enough.

The constants C_n and D_n are evaluated as before by applying the conservation of density and current at the point $x = a$. But now there is no divergence of the wave function, since k is real. In the continuum, the wave functions at large distances consist of an incoming plus and outgoing wave, thus keeping the stationarity (i.e. the time independence) of the problem.

To evaluate the constant A_n, one often assumes that the system is confined in a finite region of length L, thus getting

$$0 < x < L \Longrightarrow \int_0^L |\Phi_n(x)|^2 \, \mathrm{d}x = 1.$$

In three dimensions, this region consists of a box of side L. In this choice of normalization of the wave function, one also assumes that the wave function vanishes at the walls of the box (but not at the origin of coordinates, as we do here). This condition plus the normalization of the wave function inside the box is called "box boundary condition".

Resonances and antibound states

We will proceed as above and study the simple case of a square potential, now with the shape shown in Fig. 2, which does not hold any bound state (except for the case $V_0 = \infty$). This potential is defined as

$V(x < 0) = \infty; V(0 < x < a) = 0; V(a < x < b) = V_0 > 0; V(x > b) = 0$

There are three regions now and, as before, we will apply the conservation laws of density and current at the borders of those regions. We thus have

Region **I**, $0 < x < a; V_I(x) = 0$

Schrödinger equation

$$H\varphi_I(k, x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx}\varphi_I(k, x) = E\varphi_I(k, x)$$

i.e., $(d^2/dx^2 + k^2)\varphi_I(k, x) = 0$, where $k = \sqrt{2mE}/\hbar$.

$\varphi_I(k, 0) = 0 \Longrightarrow \varphi_I(k, x) = A\sin(kx)$

Region **II**, $a < x < b; V_{II}(x) = V_0$

This region is forbidden in classical mechanics for energies $E < V_0$, as in the case of Fig. 2, since the kinetic energy $\frac{1}{2}mv^2 = E - V_0$ is negative, i.e. the velocity v is imaginary. Instead, quantum mechanics one has

$$H\varphi_{II}(k, x) = (-\frac{\hbar^2}{2m}\frac{d^2}{dx} + V_0)\varphi_{II}(k, x) = E\varphi_{II}(k, x)$$

i.e. $(d^2/dx^2 - \kappa^2)\varphi_{II}(\kappa, x) = 0$, where $\kappa^2 = 2m(V_0 - E)/\hbar^2 > 0$

$$\varphi_{II}(\kappa, x) = A_1 e^{\kappa x} + A_2 e^{-\kappa x} \tag{5}$$

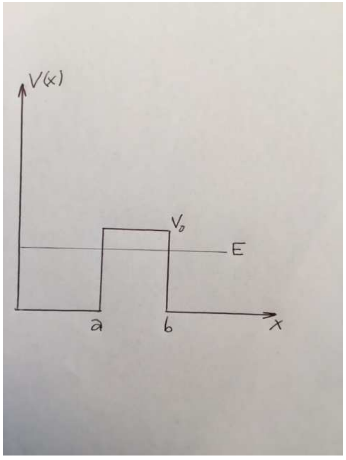

Figure 2: Positive energy square well potential in one-dimension. A particle moving under the influence of this potential at energy E may be trapped in the region $x < a$, inducing a resonance. The time during which the particle stays inside this region defines the mean life time of the resonance. For $x < 0$ the potential is infinite and, therefore, the wave function vanishes at $x = 0$.

Region **III**, $x > b; V_{III}(x) = 0$

$$\varphi_{III}(k,x) = B_o e^{ikx} + B_i e^{-ikx} \tag{6}$$

Boundary conditions

1) At x=a

$$A\sin(ka) = A_1 e^{\kappa a} + A_2 e^{-\kappa a}$$
$$Ak\cos(ka) = \kappa(A_1 e^{\kappa a} - A_2 e^{-\kappa a})$$

Which gives,

$A_1 = A\Delta_1/\Delta$, $A_2 = A\Delta_2/\Delta$, where

$$\Delta_1 = \begin{vmatrix} \sin(ka) & e^{-\kappa a} \\ k\cos(ka) & -\kappa e^{-\kappa a} \end{vmatrix} = -e^{-\kappa a}(\kappa\sin(ka) + k\cos(ka))$$

$$\Delta_2 = \begin{vmatrix} e^{\kappa a} & \sin(ka) \\ \kappa e^{\kappa a} & k\cos(ka) \end{vmatrix} = e^{\kappa a}(k\cos(ka) - \kappa\sin(ka))$$

$$\Delta = \begin{vmatrix} e^{\kappa a} & e^{-\kappa a} \\ \kappa e^{\kappa a} & -\kappa e^{-\kappa a} \end{vmatrix} = -2\kappa$$

2) At x=b

$$A_1 e^{\kappa b} + A_2 e^{-\kappa b} = B_o e^{ikb} + B_i e^{-ikb}$$

$$\kappa A_1 e^{\kappa b} - \kappa A_2 e^{-\kappa b} = ikB_o e^{ikb} - ikB_i e^{-ikb}$$

i.e.

$B_o = \Delta_3/\Delta_0$, $B_i = \Delta_4/\Delta_0$, where

$$\Delta_3 = \begin{vmatrix} A_1 e^{\kappa b} + A_2 e^{-\kappa b} & e^{-ikb} \\ \kappa A_1 e^{\kappa b} - \kappa A_2 e^{-\kappa b} & -ike^{-ikb} \end{vmatrix}$$

$$\Delta_4 = \begin{vmatrix} e^{ikb} & A_1 e^{\kappa b} + A_2 e^{-\kappa b} \\ ike^{ikb} & \kappa A_1 e^{\kappa b} - \kappa A_2 e^{-\kappa b} \end{vmatrix}$$

$$\Delta_0 = \begin{vmatrix} e^{ikb} & e^{-ikb} \\ ike^{ikb} & -ike^{-ikb} \end{vmatrix} = -2ik$$

If $V_0 = \infty$, then there should be bound states in the region $0 < x < a$, because the wave function vanishes for $x > a$. We may thus guess that by imposing outgoing boundary conditions here, one should get some sort of bound states even if V_0 is finite. A particle moving in a bound state lives in that state forever if no external perturbation takes place. One may thus expect that, if V_0 is very large, the particle would stay in a state equivalent to bound states during a long time. To explore this point we first notice that the imposing of outging boundary conditions breaks the assumption of time independence (remember, one needs outgoing and incoming waves to preserve stationarity). And indeed, for positive energies (states in the continuum, not bound states) the energies are complex. In our case, an outgoing boundary condition corresponds to $B_i = 0$, i.e. $\Delta_4 = 0$. One then has

$$\Delta_4 = e^{ikb}(\kappa A_1 e^{\kappa b} - \kappa A_2 e^{-\kappa b}) - ike^{ikb}(A_1 e^{\kappa b} + A_2 e^{-\kappa b}) = 0$$

Replacing A_1 and A_2 for the expressions given above results in

$$\Delta_4 = e^{ikb}\frac{\kappa A}{\Delta}(\Delta_1 e^{\kappa b} - \Delta_2 e^{-\kappa b}) - ike^{ikb}\frac{\kappa A}{\Delta}(\Delta_1 e^{\kappa b} + \Delta_2 e^{-\kappa b}) = 0,$$

or

$$\Delta_1 e^{\kappa b}(\kappa - ib) - \Delta_2 e^{-\kappa b}(\kappa + ib) = 0. \tag{7}$$

A complex solution of this equation has always a negative imaginary part, i.e. it is of the form $\mathcal{E}_n = E_n - i\Gamma/2$. This complex energy would be the equivalent of a bound state energy. The imaginary part $\Gamma/2$ diminishes as V_0 increases, and eventually it should vanish when V_0 becomes infinite, since the bound state energies are real. To see the physical meaning of the complex energy, we consider the time dependence of a stationary state, i.e.

$$\Psi(x,t) = e^{-i\mathcal{E}_n t/\hbar}\psi(x).$$

The probabilistic interpretation of this wave function is that $|\Psi(x,t)|^2$ represents the number of particles at the point x at time t. Calling N(t) that number of particles, one has

$$N(t) = |\Psi(x,t)|^2 = e^{-\Gamma t/\hbar}|\psi(x)|^2. \tag{8}$$

It is clear that $N(t)$ decreases as the time t increases. The physical meaning of this feature is that particles are ejected from the potential or, using the language of nuclear physics, the nuclei decay by emitting particles, for example α-particles. If one waits long enough, all particles will be emitted. In all cases, whether the particles are emitted quickly or slowly, one has $N(t=\infty)$=0. That is, at last the system becomes void of particles. One can says that it has "died". One defines as the mean life of the system the time T for which $N(T) = N(0)/e$. From Eq. (8), one sees that it is $T = \hbar/\Gamma$ or

$$T\Gamma = \hbar. \tag{9}$$

For bound states $T = \infty$ and therefore $\Gamma = 0$. Since for bound states the energy is exactly determined, it appears as a line in the spectrum. However, in the continuum there are no bound states, although the particle can be trapped within a barrier, as it happens in Fig. 2 in the region $0 < x < a$. In this case, no lines are seen in the spectrum.

The x-dependence of the outgoing part of the resonance wave function is e^{ikx} with $k = \sqrt{2m(E_0 - i\Gamma/2)/\hbar}$ (see Eq. (6)), which can be written as $k = Re(k) - i\ Im(k)$, where $Re(k)$ and $Im(k)$ are real quantities. Therefore, at large distances the resonance wave function diverges. If the resonance is narrow (i.e. if Γ is small), then even the imaginary part of the wave function is small. This is a necessary condition for the resonance to be meaningful, since a small imaginary part implies that it behaves like a bound state. Such a meaningful resonance wave function, which reaches far out in space, is a very important feature in the building of halo nuclei, as we will see below.

The time-energy relation (9) is often wrongly interpreted, since it is said to be one of the relations arisen from the Heisenberg uncertainty principle, and, therefore it is written as $T\Gamma \geq \hbar$. This cannot be the case, because the dynamical variables entering the uncertainty principle have to be conjugates of each other, like distance and linear angular momentum, or angle and orbital angular momentum. In quantum mechanics (i.e. the non-relativistic quantum mechanics that we deal with), time is not a dynamical variable, but a parameter. There are other approaches that arrive to the time-energy relation. In particular Sakurai, who also criticises the uncertainty interpretation of Eq. (9), arrives to it in his very good book "Modern quantum mechanics" by studying correlations between quantum states.

Antibound states

Besides complex energies, Eq. (7) has also real solutions E_a which, as for bound states, are negative. The difference from the case of bound states is that, for antibound states, the wave number is $k = -i\sqrt{2m|E_a|/\hbar}$. Therefore, the outgoing part of the wave function at large distances behaves as $e^{ikx} = e^{|k|x}$, thus diverging. This wave function extends far in space. In cases where $|E_a|$ is small, the antibound state may have physical meaning and it can be an important component in halo nuclei.

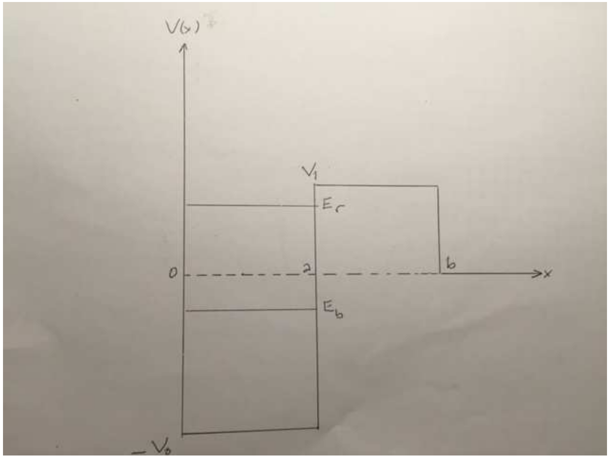

Figure 3: Square well potential in one-dimension containing an attractive part in the region $0 < x < a$ and a barrier in the region $a < x < b$. For $x < 0$ the potential is infinite and, therefore, the wave function vanishes at $x = 0$. The level at energy E_b represents a bound state and the one at E_b reresents the real energy of a resonance.

Halo nuclei

All states studied here, i.e. bound states, resonances and antibound states, can be obtained by using a potential which is attractive within a certain region and has a barrier in another region. The attractive part would induce bound states and the barrier would trap particles in the continuum to induce resonances and antibound states. Such a potential is shown in Fig. 3. Using outgoing boundary conditions one will get the bound state energy E_b and the resonance energy E_r. Antibound states do not appear in the spectrum. Yet their influence is felt through their wave functions.

The dynamics of a nucleus is determined by a few nucleons moving on the nuclear surface. These are called "valence nucleons", while the majority of nucleons in the nucleus, form what is called "the core". If the valence nucleons occupy states as the ones described here, then they will move far out from the nuclear surface. These few nucleons contribute little to the nuclear density, which is mostly determined by the core. The result is that the nucleus is abnormally large, consisting of a dense core and a faint and long outer part, like a halo. This is the origin of the name of such nuclei. An example of halo nuclei is ^{11}Li, which has the same size as the much heavier ^{48}Ca.