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Von Neumann–Wigner-type potentials and the wavefunctions' asymptotics for discrete levels in continuum

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Abstract. One-to-one correspondence between the decay law of von Neumann–Wigner-type potentials and the asymptotic behaviour of the wavefunctions representing 'bound states' in the continuum is established.

Many years ago von Neumann and Wigner [1] discovered a class of potentials that gives isolated quantum mechanical levels embedded in the continuum of positive energy states. The underlying strategy of these authors was used in [2] to produce additional examples. The main features of these potentials are the oscillations together with a relatively slow decrease at the spatial infinity. Several authors have contributed to the solid mathematical substantiation of this extraordinary phenomenon and most of the results are collected in the excellent books of Reed and Simon [3]. Recently, interest in this problem was excited anew due to possible applications in the physics of atoms and molecules. In spite of a large number of publications 'there is not as yet a fully systematic approach', as it was noted in a recent review [4]. In [4] the isospectral technique was applied to generate this kind of potentials.

One of the most fundamental conclusions of all previous investigations is that, for the modulating functions used there, the normalizable (square integrable) wavefunctions have only a power-like decay at large distances while the potentials vanish in the same limit. Hence, these wavefunctions can hardly be called bound states in the usual sense, because in general they do not guarantee finiteness even of the square radius of the state.

Below we present a slightly modified, but in our opinion more convenient method, that allows one to observe a one-to-one correspondence between the decay law of the potentials and the wavefunction corresponding to the bound states in continuum. Moreover, we will demonstrate that there exist potentials which lead to wavefunctions with a decay more rapid than the power-like decrease.

We will consider S-waves only. The corresponding Schrödinger equation for the radial function χ has the form

$$\chi''(r) + \frac{2m}{\hbar^2}\,[E - U(r)]\,\chi(r) = 0. \tag{1}$$

Denoting

$$\frac{2mE}{\hbar^2} = k^2 \qquad \frac{2mU(r)}{\hbar^2} = V(r) \tag{2}$$

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we find from equation (1) that

$$V(r) = k^2 + \frac{\chi''}{\chi}. \tag{3}$$

Following [1, 2] we take

$$\chi(r) = \chi_0(r) f(r) \tag{4}$$

where $\chi_0(r)$ is a solution of some solvable Schrödinger equation and $f(r)$ is a modulating function. As a rule, the free or Coulomb solutions are used for χ_0 [1, 2, 4] which satisfy the boundary condition at the origin: $\chi(0) = 0$. As an example let us take the free particle solution

$$\chi_0(r) = \frac{1}{k}\sin(kr). \tag{5}$$

After substituting (4) and (5) into equation (3) one obtains [2]

$$V(r) = \frac{f''}{f} + 2k\frac{f'}{f}\operatorname{ctg}(kr). \tag{6}$$

We must choose the function $f(r)$ such as to provide cancellation of the poles of $\operatorname{ctg}(kr)$, i.e. the zeros of $\sin(kr)$. Usually this is achieved by taking $f(r)$ to be a differentiable function of the variable [1, 2]

$$s(r) = k\int_0^r \sin^2(kr')\,\mathrm{d}r' = \tfrac{1}{2}kr - \tfrac{1}{4}\sin(2kr). \tag{7}$$

Instead of setting the function $f(r)$, we will set its logarithmic derivative:

$$\mathcal{C}(r) \equiv \frac{f'}{f}. \tag{8}$$

Then, from (6),

$$V(r) = \mathcal{C}^2(r) + \mathcal{C}'(r) + 2k\operatorname{ctg}(kr)\mathcal{C}(r) \tag{9}$$

and the modulating function $f(r)$ can be constructed by solving equation (8):

$$f(r) = A\exp\left\{\int_0^r \mathcal{C}(z)\,\mathrm{d}z\right\}. \tag{10}$$

First of all we must take care of the above-mentioned cancellation of the poles. We can take

$$\mathcal{C}(r) = \phi(r)\sin^2(kr) \tag{11}$$

where $\phi(r)$ is a smooth but arbitrary function. Then the potential becomes

$$V(r) = \phi^2(r)\sin^4(kr) + \phi'(r)\sin^2(kr) + 2k\phi(r)\sin(2kr). \tag{12}$$

Next, to obtain a potential that vanishes at infinity we try

$$\phi(r) = \frac{a}{r^\beta} \qquad a = \text{constant} \qquad \beta > 0. \tag{13}$$

So the potential takes the form

$$V(r) = \frac{a^2\sin^4(kr)}{r^{2\beta}} - \frac{a\beta\sin^2(kr)}{r^{1+\beta}} + \frac{2ak\sin(2kr)}{r^\beta} \tag{14}$$

and the corresponding modulating function is

$$f(r) = A\exp\left\{a\int_0^r \frac{\sin^2(kz)}{z^\beta}\,\mathrm{d}z\right\}. \tag{15}$$

Evidently, if $\beta > 0$ the last term in (14) will dominate as $r \to \infty$. According to theorem XIII.58 from [3] if the potential vanishes at infinity like $r^{-\beta}$ with $\beta > 1$ there are no normalizable wavefunctions for positive eigenvalues. Validity of this theorem in our case can be checked explicitly by studying the behaviour of the wavefunction corresponding to (15). Therefore only the case $\beta \leqslant 1$ is of interest. Let us take $\beta = 1 - \epsilon$ with $\epsilon > 0$ (the case $\epsilon = 0$ must be considered separately). We have

$$\int_0^r \frac{\sin^2(kz)}{z^{1-\epsilon}}\,\mathrm{d}z \approx \frac{r^\epsilon}{2\epsilon} \qquad r \gg 1 \tag{16}$$

and if we take the coefficient a in (15) to be negative, then $f(r)$ would have quasi-exponentially decreasing asymptotics leading to square integrable wavefunctions. Moreover, the modulating function $f(r)$ tends to a constant as r approaches the origin and does not destroy the correct boundary behaviour of the wavefunction χ.

Collecting all the above results we conclude that if the potential has dominating asymptotics like

$$V(r) \sim -\frac{2|a|k}{r^\beta}\sin(2kr) \qquad 0 < \beta < 1 \tag{17}$$

then the wavefunction χ behaves as

$$\chi(r) \sim \sin(kr)\exp\left\{-\frac{|a|r^{1-\beta}}{2(1-\beta)}\right\} \qquad r \gg 1 \tag{18}$$

and so decreases fast enough to be normalizable.

Let us now consider the limiting case $\beta = 1$ and define

$$I = \lim_{\sigma\to 0}\int_\sigma^r \frac{\sin^2(kz)}{z}\,\mathrm{d}z = \tfrac{1}{2}\left(\ln(kr) - \mathrm{Ci}(2kr) + \gamma + \ln 2\right) \tag{19}$$

where γ is the Euler constant and $\mathrm{Ci}(u)$ is the integral cosine, which has the following asymptotics [5]:

$$\begin{aligned} &\mathrm{Ci}(u) \approx \gamma + \ln(u) - \frac{u^2}{4} + \mathrm{O}\left(u^4\right) && u \ll 1 \\ &\mathrm{Ci}(u) \approx \sin(u) + \mathrm{O}\left(u^{-1}\right) && u \gg 1. \end{aligned} \tag{20}$$

Therefore

$$\begin{aligned} &I \longrightarrow \tfrac{1}{2}(kr)^2 && kr \ll 1 \\ &I \longrightarrow \tfrac{1}{2}\ln(kr) && kr \gg 1. \end{aligned} \tag{21}$$

Making use of (20) and (21) in (19) and then in (15), we see that

$$\begin{aligned} &f(r) \longrightarrow \text{constant} && kr \ll 1 \\ &f(r) \longrightarrow (kr)^{a/2} && kr \gg 1 \end{aligned} \tag{22}$$

and therefore

$$\chi(r) \longrightarrow r^{-|a|/2}\sin(kr) \qquad kr \gg 1. \tag{23}$$

This unifies correctly all known results derived for the $r^{-1}\sin(2kr)$ asymptotic behaviour of the potential and agrees with Atkinson's theorem [3].

As a conclusion we can say that there is a one-to-one correspondence between the asymptotic behaviour of potentials decreasing with oscillations and that of the wavefunctions belonging to bound states in the continuum. A minor modification of the point of view (see equations (8)–(12)) allowed us to obtain generalized von Neumann–Wigner-type potentials with a more arbitrary power decrease, $\beta \neq 1$. Only $\beta \leqslant 1$ gives bound states in the continuum. Of course the correspondence found above between the asymptotics does not depend on the method of construction—it is general because its validity depends only on the asymptotic behaviour of the potential under consideration. The last comment we want to make is that the purely exponential decrease $\exp(-|a|r/2)$ of the wavefunction corresponds to potentials that do not vanish at infinity, but merely oscillate (the case $\beta = 0$). The finiteness of any characteristic dimensions of the bound state (such as square radius or any higher moments of r) makes the principal difference between the new solutions (for $\beta \neq 1$) and the known ones ($\beta = 1$), namely the former are localized like ordinary bound states, while the latter are not.

References

[1] von Neumann J and Wigner E 1929 *Z. Phys.* **30** 465
[2] Stillinger F H and Herrik D R 1975 *Phys. Rev.* A **11** 446
[3] Reed M and Simon B 1975 *Methods of Modern Mathematical Physics* vols 3–4 (New York: Academic)
[4] Cooper F, Khare A and Sukhatme U 1995 *Phys. Rep.* **251**
[5] Bateman H and Erdelyi A 1953 *Higher Transcendental Functions* vol 2 (New York)