Bound states in the continuum for separable nonlocal potentials

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As an addendum to the recent work of Stillinger and Herrick, we have constructed a separable nonlocal potential which generates a bound state in the continuum.

In 1929, von Neumann and Wigner[1] showed that the single-particle Schrödinger equation could have a bound-state wave function corresponding to a positive-energy eigenvalue. Starting from amplitude-modulated plane wave as a localized (i.e. integrable) wave function, they constructed a local potential which produces this wave function. This construction was recently revived by Stillinger and Herrick[2] in view of the growing suspicion that some atomic and molecular systems might exhibit bound states in the relevant continua.[3-5] In this note we extend their method of constructing the potential to the case of separable nonlocal potentials. We shall do it for the S wave only; the extension to higher angular momenta is straightforward.

The partial-wave Schrödinger equation for a separable nonlocal potential of the form[6]

$$\langle \vec{r}|V|\vec{r}'\rangle = \sum_{l,m} \epsilon g_l(r) g_l(r') Y^*_{lm}(\hat{r}) Y_{lm}(\hat{r}'), \tag{1}$$

(where $\epsilon = 1$ for repulsive and -1 for attractive potentials), is

$$\epsilon g_l(r) \int_0^\infty g_l(r')\psi_l(k,r')r'^2\,dr' = \left[E + \frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) - \frac{l(l+1)\hbar^2}{2mr^2}\right]\psi_l(k,r),$$

in which $\psi_l(k,r)$ is the radial part of the wave function and $\hbar k$ is the momentum. Since the value of the integral on left-hand side is a function of k only, we may write,

$$g_l(r) = \chi_l(r)/\phi_l(k), \tag{2}$$

where

$$\chi_l(r) = \left[E + \frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{l(l+1)\hbar^2}{2mr^2}\right]\psi_l(k,r), \tag{3}$$

and

$$\phi_l(k) = \epsilon \int_0^\infty g_l(r')\psi_l(k,r')r'^2\,dr'. \tag{4}$$

From Eqs. (2) and (4) it can be easily shown that

$$\phi_l(k) = \left(\epsilon \int_0^\infty \chi_l(r)\psi_l(k,r)r^2\,dr\right)^{1/2}. \tag{5}$$

Thus once a suitable wave function is chosen, $\chi_l(r)$ and $\phi_l(k)$ may be obtained from Eqs. (3) and (5) and the form factor $g_l(r)$ is then given by Eq. (2). It may be noted that the function $\phi_l(k)$ may be either real or pure imaginary. However, the nonlocal separable potential for the lth partial wave, $V_l(r,r') = \epsilon g_l(r) g_l(r')$, obtained by using Eq. (2) will still be real and Hermitian. This should indeed be so since the potential given by (1) for $\epsilon = \pm 1$ is a Hermitian interaction and manipulations that we carried out based on it cannot generate a non-Hermitian interaction. Let us now take the case of $l=0$ and construct $g_0(r)$. The wave function will be assumed to be a modulated plane wave,

$$\psi_0(k,r) = \sin(kr)\, f(r)/kr, \tag{6}$$

where $f(r)$ is such that $\psi_0(k,r)$ is square integrable, so that it corresponds to a localized or bound state. Substitution of Eq. (6) in Eq. (3) gives

$$\chi_0(r) = \frac{\hbar^2}{2m}\left[\left(\frac{2mE}{\hbar^2} - k^2\right)\frac{\sin(kr)}{kr} f(r) + \frac{2\cos(kr)}{r} f'(r) + \frac{\sin(kr)}{kr} f''(r)\right].$$

This has a simple pole at $r=0$. In order to eliminate this so that the potential is bounded, we must have $f'(0)=0$. A simple choice of such a modulating function is

$$f(r) = [A^2 + (kr)^2]^{-1}, \tag{7}$$

where A is a dimensionless parameter. For this choice, $\chi_0(r)$ is given by

$$\chi_0(r) = \frac{\hbar^2}{2m}\left[\left(\frac{2mE}{\hbar^2} - k^2\right)\frac{\sin(kr)}{(kr)(A^2+k^2r^2)} - \frac{1}{(A^2+k^2r^2)^2}\left(\frac{2k\sin(kr)}{r} + 4k^2\cos(kr)\right) + \frac{8k^3 r\sin(kr)}{(A^2+k^2r^2)^3}\right], \tag{8}$$

and $\phi_0(k)$ is given by

$$\phi_0(k)=\epsilon^{1/2}\Big[\frac{(2mE/\hbar^2-k^2)\pi}{8k^3A^3}(1-(1+2A)e^{-2A})+\frac{\pi}{16kA^5}[e^{-2A}(3+6A+4A^2)-3]$$
$$-\frac{\pi}{4kA^3}(1+2A)e^{-2A}+\frac{\pi}{24kA^5}[3-e^{-2A}(8A^3-6A-3)]\Big]^{1/2}. \tag{9}$$

Since the plane-wave part of the wave function corresponds to energy eigenvalue $\hbar^2k^2/2m$, let us assume $E=\hbar^2k^2/2m$. The first terms in both Eqs. (8) and (9) then vanish. The form factor $g_0(r)$ is then obtained from Eqs. (2), (8) and (9). The behavior of $g_0(r)$ for large and small values of r is given by

$$g_0(r)\xrightarrow[r\to 0]{}\frac{6k^2/A^4}{\phi_0(k)}, \tag{10}$$

and

$$g_0(r)\xrightarrow[r\to\infty]{}\frac{4\cos(kr)/k^2r^4}{\phi_0(k)}. \tag{11}$$

In this note we have shown that one can construct a separable nonlocal potential for which there is bound state for positive energy. We believe this construction will be useful in the generalization of Stillinger and Herrick theory developed for atomic physics to related problems in nuclear physics.

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