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Threshold bound states

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Abstract. Relationships between the coupling constant and the binding energy of threshold bound states are obtained in a simple manner from an iterative algorithm for solving the eigenvalue problem. The absence of threshold bound states in higher dimensions can be easily understood.

PACS. 21.10.Dr Binding energies and masses – 03.65.Ge Solutions of wave equations: bound states – 02.60.Lj Ordinary and partial differential equations; boundary value problems

Recently there has been considerable interest in weakly bound states in atomic [1–3] as well as in nuclear [4–11] (and hypernuclear [12]) systems. Exotic nuclei, far from the stable regions in the periodic table, are now routinely produced with present-day heavy-ion accelerators and some, for example Li^{11}, are barely bound [13]. Such nuclei, particularly those close to the drip lines, are important in astrophysical processes and are therefore of great interest, both experimentally and theoretically [14]. In the following paper we wish to point out that under certain circumstances, at least in one and two dimensions, bound states can occur for arbitrarily small values of the potential. Simple expressions for the binding energy of these threshold bound states as a function of the interaction strength can be obtained. Unfortunately this is not the case in higher dimensions and we discuss in a simple manner the reasons for this.

In a mathematically elegant paper, Simon studied the one- and two-dimensional Schrodinger operators $-\partial^2/\partial x^2 + \lambda V(x)$ and $-\Delta + \lambda V(\mathbf{x})$ where, in this work, either $\lambda V(x)$ or $\lambda V(\mathbf{x})$ is described as the potential and the parameter λ (> 0) is termed the strength of the potential. Simon provided necessary and sufficient conditions for the existence of a bound state when λ is small [15]. In one dimension a threshold bound state (*i.e.*, one just bound) exists for many finite short-range potentials and its binding energy is an analytic function of λ [16,17]. Furthermore, using the theory of trace class determinants [18, 19], a simple expansion for the binding energy of the threshold bound state has been obtained (see ref. [15]). More recently, Gat and Rosenstein have pointed out that perturbative methods provide a suitable means for calculating the binding energy of this state [20,21]. This is somewhat peculiar since a convergent expansion for the binding energy in λ exists, but no apparent poles appear in the expansion of the S-matrix to any finite order in perturbation theory. Rather than use perturbation theory, we wish to point out that the expression for the binding energy of the threshold bound state obtained by Simon in one and two dimensions can easily be obtained from a simple non-perturbative iterative algorithm [22] and we provide an intuitive explanation of the form of the expansion in different dimensions.

In the algorithmic approach, eigenvalues, and the associated eigenfunctions, are determined as functions of the strength of the potential, λ. To illustrate the method, we consider the one-dimensional eigenvalue equation [22]

$$[-\partial_x^2 - \lambda V(x)]u(x) = -\epsilon u(x), \tag{1}$$

subject to

$$\lim_{|x|->\infty} u(x) = 0. \tag{2}$$

Here $\partial_x = \partial/\partial x$, $\lambda > 0$ and $\int V(x)\mathrm{d}x \geq 0$. We shall always assume $V(x) \to 0$ as $|x| \to \infty$. The energy eigenvalue, $-\epsilon$ (with $\epsilon > 0$), is negative and corresponds to a bound state. We can combine eqs. (1) and (2) in a single equation, namely

$$u(x) = \lambda \int_{-\infty}^{\infty} G_\epsilon(x - x')V(x')u(x')\mathrm{d}x'. \tag{3}$$

Here $G_\epsilon(x)$ is a Green's function that satisfies

$$[-\partial_x^2 + \epsilon]G_\epsilon(x) = \delta(x) \tag{4}$$

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and has the asymptotic behaviour appropriate to bound states:

$$\lim_{|x|->\infty} G_\epsilon(x) = 0. \tag{5}$$

We normalise $u(x)$ at an arbitrary reference point, x_{ref}:

$$u(x_{ref}) = 1 \tag{6}$$

and using eq. (3), this allows λ to be written as

$$\lambda = \frac{1}{\int_{-\infty}^{\infty} G_\epsilon(x_{ref} - x')V(x')u(x')\mathrm{d}x'}\,. \tag{7}$$

This equation can then be used to eliminate λ from eq. (3), with the result

$$u(x) = \frac{\int_{-\infty}^{\infty} G_\epsilon(x - x')V(x')u(x')\mathrm{d}x'}{\int_{-\infty}^{\infty} G_\epsilon(x_{ref} - x')V(x')u(x')\mathrm{d}x'}\,. \tag{8}$$

Equations (7) and (8), allow the bound-state eigenvalue, ϵ, to be determined as a function of the strength of the potential, λ. For simplicity, we assume that $V(x)$ has a finite range and, for a particular choice of ϵ, determine the solution of eq. (8), via iteration. That is, from a starting point $u_0(x)$, we iterate

$$u_{n+1}(x) = \frac{\int_{-\infty}^{\infty} G_\epsilon(x - x')V(x')u_n(x')\mathrm{d}x'}{\int_{-\infty}^{\infty} G_\epsilon(x_{ref} - x')V(x')u_n(x')\mathrm{d}x'} \tag{9}$$

to convergence. The conditions on $u_0(x)$ are fairly mild; this function must be non-negative and normalisable, and have some overlap with $V(x)$. Given this, $u_1(x)$, and all subsequent $u_n(x)$, will have inherited the property of the Green's function of extending over all x, and $u_0(x)$ need only be sufficient to "get the iteration going".

Once the converged solution, $u(x) \equiv u_\infty(x)$, is found, it is used in eq. (7) to determine λ and an (ϵ, λ) pair is found. From a practical point of view, $u(x)$ is only required (and hence only has to be found) for those x where $V(x)$ is non-zero, since $u(x)$ only appears, above, in the combination $V(x)u(x)$.

Repeating the iterative procedure for a different value of ϵ yields the corresponding value of the strength of the potential, λ. When a number of (ϵ, λ) pairs have been determined, a simple interpolation procedure can be used to determine the dependence of ϵ on λ. Furthermore, for larger values of ϵ a simple relationship between λ and ϵ can be obtained for non-singular symmetric potentials which vanish asymptotically, which can be used to make the algorithm more efficient [23].

For small values of ϵ, corresponding to states close to the threshold of being bound, the analytical dependence of ϵ on λ may be obtained by approximating the Green's function (which satisfies eq. (4)). We have

$$G_\epsilon(x) = \frac{e^{-\sqrt{\epsilon}|x|}}{2\sqrt{\epsilon}} \tag{10}$$

and expanding in ϵ yields

$$G_\epsilon(x) = \frac{1}{2\sqrt{\epsilon}} + \ldots \tag{11}$$

Substituting this result into eq. (8) gives

$$u(x) = 1 + \ldots \tag{12}$$

to leading order in ϵ. From eq. (7) one therefore easily obtains the following approximate relationship between the strength of the potential, λ, and ϵ:

$$\lambda = \frac{2\sqrt{\epsilon}}{\int_{-\infty}^{\infty} V(x)\mathrm{d}x}\,. \tag{13}$$

This is valid for small values of ϵ. Indeed for small coupling it provides an analytical approximation for the lowest bound state for a large class of potentials in one dimension provided $\int_{-\infty}^{\infty} V(x)\mathrm{d}x \geq 0$ [15]. Furthermore, had we included the standard factor of $1/2$ in the first term of the eigenvalue equation, eq. (1), then we would have obtained

$$\epsilon = \frac{1}{2}\lambda^2 \left(\int_{-\infty}^{\infty} V(x)\mathrm{d}x\right)^2, \tag{14}$$

which is precisely the result obtained by Simon, to $O(\lambda^2)$. For a finite square-well potential of depth λ and $x < |a|$, $\epsilon \approx \lambda^2$ for the ground-state eigenvalue [24] which agrees well with eq. (13), for small values of λ.

An important feature of eq. (3) is that it has a solution for ϵ, for arbitrarily small λ. This follows from the property of the Green's function, eq. (10), that it is unbounded from above, as $\epsilon \to 0$:

$$\lim_{\epsilon \to 0_+} G_\epsilon(x) = +\infty. \tag{15}$$

Hence for very small values of λ, the value of ϵ can always be adjusted until the product $\lambda G_\epsilon(x)$, which appears in eq. (3), is non-negligible, and hence there is a solution for ϵ.

We note these results can be generalized to higher dimensions, since it can easily be seen that eqs. (3) and (8) become

$$u(\mathbf{x}) = \lambda \int_{all\ \ space} G_\epsilon(\mathbf{x} - \mathbf{x}')V(\mathbf{x}')u(\mathbf{x}')\mathrm{d}^n x' \tag{16}$$

and

$$u(\mathbf{x}) = \frac{\int_{all\ \ space} G_\epsilon(\mathbf{x} - \mathbf{x}')V(\mathbf{x}')u(\mathbf{x}')\mathrm{d}^n x'}{\int_{all\ \ space} G_\epsilon(\mathbf{x}_{ref} - \mathbf{x}')V(\mathbf{x}')u(\mathbf{x}')\mathrm{d}^n x'}\,. \tag{17}$$

The essential difference arises only from the different form the Green's function takes in different dimensions.

In two dimensions

$$G_\epsilon(\mathbf{x}) = \frac{1}{2\pi} K_0(\sqrt{\epsilon}|\mathbf{x}|), \tag{18}$$

where $K_0(\cdot)$ is a Bessel function of the second kind of order zero [25]. Expanding $K_0(\sqrt{\epsilon}|\mathbf{x}|)$ for small ϵ yields

$$K_0(\sqrt{\epsilon}|\mathbf{x}|) = \ln(1/\sqrt{\epsilon}) + \ln\left(2e^{-\gamma}/|\mathbf{x}|\right) + O(\epsilon^2), \tag{19}$$

where $\gamma = 0.57721\ldots$ is Euler's constant. Thus from eq. (17) we obtain, for sufficiently small ϵ,

$$u(\mathbf{x}) = 1 + \ldots \tag{20}$$

and using eq. (16) we obtain $\lambda \ln(\frac{1}{\sqrt{\epsilon}})\frac{1}{2\pi}\int V(\mathbf{x})\mathrm{d}^2x \simeq 1$. That is

$$\ln\epsilon = -\frac{4\pi}{\lambda\int V(\mathbf{x})\mathrm{d}^2x} + O(\lambda^0). \tag{21}$$

As in one dimension, a threshold bound state exists for arbitrarily small λ, provided $\int V(\mathbf{x})\mathrm{d}^2x \geq 0$. More precise conditions on the existence of threshold bound states require $\int |V(\mathbf{x})|^{1+\beta}\mathrm{d}^2x < \infty$ (for some $\beta > 0$) and $\int(1+x^2)^{\beta}|V(\mathbf{x})|\mathrm{d}^2x < \infty$ [15].

To illustrate the above, consider a finite spherically symmetric potential well

$$-\lambda V(\mathbf{x}) = \begin{cases} -\lambda, & \|\mathbf{x}\| < a, \\ 0, & \|\mathbf{x}\| > a. \end{cases} \tag{22}$$

Equation (21) yields

$$\ln\epsilon \simeq -\frac{4}{\lambda a^2}\,. \tag{23}$$

The ground-state eigenvalue, $-\epsilon$, in the above potential well can be shown to be the solution of

$$\sqrt{\lambda-\epsilon}\frac{J_1(a\sqrt{\lambda-\epsilon})}{J_0(a\sqrt{\lambda-\epsilon})} = \sqrt{\epsilon}\frac{K_1(a\sqrt{\epsilon})}{K_0(a\sqrt{\epsilon})}\,, \tag{24}$$

where $J_n(\cdot)$ is a Bessel function of the first kind, of order n. Expanding the left and right sides, assuming $\lambda\alpha^2$ and $\epsilon a^2 \ll 1$ yields $(\lambda-\varepsilon)a/2 + O((\lambda-\varepsilon)^2)\ldots = [-a\ln(2e^{-\gamma}/(\sqrt{\epsilon}a))]^{-1} + O(\epsilon)$. This leads to a result for $\ln\epsilon$ that coincides with eq. (23), to the same level of accuracy.

We are thus able to make the observation that again it is the divergence of the Green's function, at fixed spatial argument, when $\epsilon \to 0$, that results in a threshold bound state at arbitrarily small λ.

On the other hand, in three dimensions the Green's function is

$$G_\epsilon(\mathbf{x}) = \frac{\exp(-\sqrt{\epsilon}|\mathbf{x}|)}{4\pi|\mathbf{x}|}\,. \tag{25}$$

At fixed $|\mathbf{x}|$, this does not diverge as $\epsilon \to 0$. This is suggestive of the known fact that in three and higher dimensions an arbitrarily weak attractive potential does not possess a bound state [15]; there has to be a certain strength of the potential before it can support a bound state. We note that the leading term in an expansion of ϵ of the Green's function, in $n = 3$ and higher dimensions, is not independent of $\mathbf{x}$. This is in contrast to the corresponding behaviour of the Green's functions when $n = 1$ and $n = 2$ and suggests that $n = 1$ and $n = 2$ which may be thought of as being atypical of all other dimensions.

To understand the property of an arbitrarily weak attractive potential to bind a particle in $n = 1$ and $n = 2$ two dimensions but not in three or more dimensions, we can relate it to an apparently different problem of how much time a random walk in n dimensions spends in the vicinity of its starting position. To see this, we use Dirac notation in the general n-dimensional case where $\hat{\mathbf{p}}$ is the momentum operator and $|\mathbf{x}\rangle$ ($\langle\mathbf{x}|$) is an eigenket (eigenbra) of the coordinate operator. We then can write the Green's function as

$$G_\epsilon(\mathbf{x}) = \langle\mathbf{x}|(\hat{\mathbf{p}}^2+\epsilon)^{-1}|\mathbf{0}\rangle = \int_0^\infty \mathrm{d}t\langle\mathbf{x}|e^{-(\hat{\mathbf{p}}^2+\epsilon)t}|\mathbf{0}\rangle \tag{26}$$

and

$$\lim_{\epsilon\to 0} G_\epsilon(\mathbf{x}) = \int_0^\infty \mathrm{d}t\langle\mathbf{x}|e^{-\hat{\mathbf{p}}^2 t}|\mathbf{0}\rangle = \int_0^\infty \frac{e^{-|\mathbf{x}|^2/(4t)}}{(4\pi t)^{n/2}}\mathrm{d}t. \tag{27}$$

In a random walk in discrete space and discrete time, let $P(\mathbf{x}_1,t_1;\mathbf{x}_0,t_0)$ denote the probability that the random walker is at position $\mathbf{x}$ at time t, given it was at position $\mathbf{x}_0$ at time t_0. Then the mean time spent at position $\mathbf{x}$ is $\sum_{t=0}^{\infty} P(\mathbf{x},t;\mathbf{0},0)$ [26]. The distribution $P(\mathbf{x},t;\mathbf{0},0)$ is the discrete analogue of the continuous time and space diffusion density $(4\pi t)^{-n/2}\exp(-|\mathbf{x}|^2/(4t))$ which appears in eq. (27). We thus see that $\lim_{\epsilon\to 0} G_\epsilon(\mathbf{x})$ has the interpretation as the mean time a random walker spends in the vicinity of a site at position $\mathbf{x}$, given it was at position $\mathbf{0}$ at time $t = 0$. In $n = 1$ and $n = 2$ dimensions, it follows from eq. (27) that $\lim_{\epsilon\to 0} G_\epsilon(\mathbf{x})$ is infinite, implying an infinite amount of time is spent in the vicinity of any position, $\mathbf{x}$. By contrast, when $n \geq 3$, $G_0(\mathbf{x})$ is finite. In the quantum-mechanical problem considered here, it is precisely the finiteness (or lack of finiteness) of $\lim_{\epsilon\to 0} G_\epsilon(\mathbf{x})$ that determines the dimensionalities where an arbitrarily weak potential can possess a threshold bound state. Thus there is the intimate relation between the mean time spent by random walks and the existence of bound states of arbitrarily weak potentials.

At first glance our results seem to be in disagreement with recent three-dimensional mean field calculations [27–33] in exotic nuclei which suggest that threshold bound states exist. However we wish to point that this need not necessarily be so as mean-field calculations are not simple eigenvalue problems. They are, intrinsically, nonlinear problems for which the analysis we have presented is not directly appropriate. Secondly, because mean-field calculations yield mean values for the ground-state energies, quantum fluctuations should not be ignored. Hence, if there are no threshold bound states in three dimensions, mean field predictions may not be able to ascertain this because of the presence of quantum fluctuations.

We conclude by pointing out that at least for small values of λ, good approximate analytical relationships between ϵ and λ exist in one and two dimensions which may be used to improve the convergence rate of the afore-mentioned iterative algorithm [22]. Such simple relationships do not occur in higher dimensions as threshold bound states cannot occur. For example, for a square well in 3 dimensions there is no s-wave eigenstate unless $V_0a^2 > \frac{\pi^2\hbar^2}{8m}$, where a is the radius of the well and V_0 its depth and there is one bound state if $\frac{\pi^2\hbar^2}{8m} < V_0a^2 \leq \frac{9\pi^2\hbar^2}{8m}$ [24].

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