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The quantum-mechanical box effect

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Abstract. A particle moves in one spatial dimension in an attractive symmetric negative potential $vf(x)$, and obeys non-relativistic quantum mechanics. If the system is enclosed in a finite box $[-\ell, \ell]$, then, unlike the situation in $\mathbb{R}$, the ground-state energy E_0 is negative only when the coupling v is sufficiently large. General upper- and lower-bound formulae are derived for the critical coupling v_c which corresponds to $E_0 = 0$. Some generalizations are derived for potentials which change sign and for unsymmetric unimodal potentials.

1. Introduction

We consider the problem of a single particle in one dimension which moves in an attractive symmetric potential $vf(x)$. For convenience we assume that the potential is finite, that $f(x) \leqslant 0$, and that $\hbar = 2m = 1$. The term 'attractive' means that the potential shape $f(x)$ is monotone non-decreasing as we move away from $x = 0$. Thus the Hamiltonian H may be written

$$H = -\Delta + vf(x). \tag{1.1}$$

It is a well known elementary result of quantum mechanics in $\mathbb{R}$ that for every value of $v > 0$, H has a discrete eigenvalue $E_0 < 0$ at the bottom of the spectrum. This result can be proved in a particular case by applying a trial function ϕ, say a Gaussian, and minimizing the Rayleigh quotient $\langle H\rangle = (\phi, H\phi)/(\phi, \phi)$ with respect to a scale parameter: if the trial function is appropriate, then however small v is chosen, we can always find a value of the scale such that $\langle H\rangle < 0$. A more general result can be established by noting that for all $v > 0$ the potential lies entirely *below* a 'comparison' negative square well; and in one dimension such a square well always has at least one discrete eigenvalue [1]. A more abstract theorem to the same effect and only requiring that the potential (in $\mathbb{R}$ or $\mathbb{R}^2$) be non-positive is proved in [2]. If the system is enclosed in an impenetrable box, this result is no longer true: there now exists a critical value $v_c > 0$ of the coupling such that the discrete eigenvalue E_0 at the bottom of the spectrum is negative only if $v > v_c$.

Possible initial surprise at this claim is immediately lessened by the following three elementary considerations: (i) the variational characterization of the spectrum would lead us to expect that the spatial contraction from $\mathbb{R}$ to $[-\ell, \ell]$ is guaranteed to move the spectrum up; (ii) an argument based on Heisenberg's (uncertainty) inequality suggests that, as ℓ is reduced, the kinetic energy is increased, without a commensurate decrease in the potential energy, thus E_0 would eventually have to become positive; (iii) even when the potential is not constant, the spectrum of the particle in a box is entirely discrete and the value $E = 0$ is therefore no longer special. However, it is useful to have formulae for bounds on the

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critical coupling v_c which characterizes the 'box effect', the impact on the ground-state energy of solving the problem in the box $[-\ell, \ell]$ instead of in the real line $\mathbb{R}$. We would require these bounds to obey the natural correspondence limit $\lim_{\ell\to\infty}(v_c) = 0$.

The bounds we shall find are based on two earlier results: the exact solution of the square well in a box [3] and two recent comparison theorems [4], which allow us to predict spectral ordering of the ground-state energies even in cases where the graphs of the comparison potentials cross over each other. We suppose that the box $[-\ell, \ell]$ is fixed and we denote by $E = W(a, d)$ the negative eigenvalue at the bottom of the spectrum of the square-well problem

$$H = -\Delta + \mathrm{d}w(x) \tag{1.2}$$

where the potential shape $w(x)$ is given by

$$w(x) = \begin{cases} -1 & |x| \leqslant a \\ 0 & a < |x| \leqslant \ell. \end{cases} \tag{1.3}$$

Flügge [3] provides the following expression for this eigenvalue:

$$ka \tan ka = \chi a \coth \chi(\ell - a) \tag{1.4}$$

where

$$E = W(a, d) = -\chi^2 \qquad \text{and} \qquad k^2 = d - \chi^2.$$

The bottom of the spectrum of H is always a discrete eigenvalue E but, as it stands, (1.4) is presumptuous: we get a *negative* eigenvalue given by this formula only if the well depth d is sufficiently large. We can find the critical square-well coupling d_c by taking the limit of (1.4) as $\chi \to 0$. This yields the following transcendental formula for $d = d_c$:

$$\theta \tan\theta = \frac{a}{\ell - a} \qquad \text{where } \theta = d^{\frac{1}{2}} a < \frac{\pi}{2}. \tag{1.5}$$

A numerical example is given by

$$a = 1 \qquad \ell = 2 \qquad d_c \doteq 0.740\,17 \Rightarrow E = 0. \tag{1.6}$$

The tools we need to compare a given potential $vf(x)$ with the soluble potential $\mathrm{d}w(x)$ are the refined comparision theorems of [4]. For convenience we summarize the two results we need by reference to the example with $\ell = 2$ illustrated in figure 1. The figure shows the exponential potential with shape $f(x) = -\mathrm{e}^{-|x|}$ and coupling $v = 5$ together with two square wells, $w_1 \sim (a, v)$ and $w_2 \sim (b, d)$: the lower square well w_1 has the same area as does $vf(x)$, and the upper square well w_2 has the same area as that part of $vf(x)$ satisfying $|x| \leqslant b$. Clearly the upper square well is not uniquely specified (the 'best' one will be chosen later). However, by the theorems of [4]), the Schrödinger eigenvalues generated by these three potentials are ordered

$$W(a, v) < E(v) < W(b, d). \tag{1.7}$$

Thus the eigenvalue E corresponding to the given potential is bracketed by two known exact eigenvalues. Most of our results stem from these basic inequalities. The class of potential shapes we are able to treat by this elementary reasoning consists of those potentials which are 'like' the above exponential illustration in the following specific senses: (i) $f(x)$ is symmetric, (ii) $f(0) < 0$, (iii) $f(x)$ is monotone non-decreasing for $x > 0$, (iv) $\lim_{x\to\infty} f(x) = 0$, (v) $|f(x)|$ has (finite) area. The results are, of course, invariant with respect to vertical and horizontal shifts in space. Some other immediate generalizations are discussed in the conclusion.

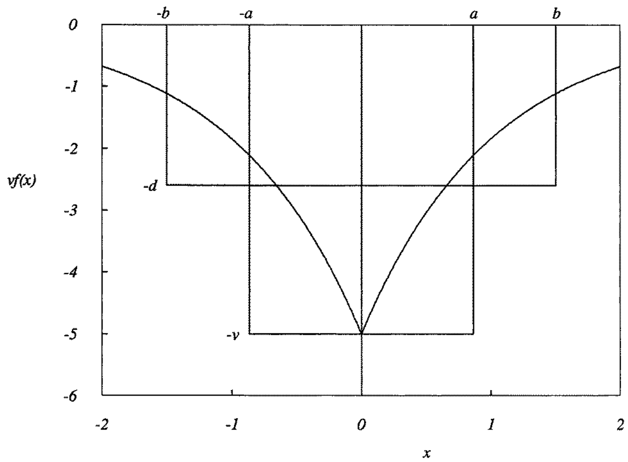

Figure 1. The exponential potential shape $f(x) = -e^{-|x|}$ with coupling $v = 5$ together with two square wells, $w_1 \sim (a, v)$ and $w_2 \sim (b, d)$ in the box $[-\ell, \ell] = [-2, 2]$: the lower square well has the same area as does $vf(x)$, and the upper square well has the same area as that part of $vf(x)$ satisfying $|x| \leqslant b$. According to the theorems in [4] the Schrödinger eigenvalues generated by these three potentials are ordered $W(a, v) < E(v) < W(b, d)$.

2. Sufficient conditions for $E_0 > 0$

If $W(a, v) = 0$ in (1.7), then $E(v) > 0$, which means that there are no negative eigenvalues. For the lower bound $W(a, v)$, the area of the square well is the same as the area of $vf(x)$. For convenience we shall work with positive areas and define A to be the area under the *shape* $f(x)$. Thus, since we require $vA = 2v|f(0)|a$, we have

$$A = A(\ell) = \int_{-\ell}^{\ell} |f(x)|\, dx = 2|f(0)|a \tag{2.1}$$

where the functional form of A has been defined for use in section 3. From (1.5) with $d = v|f(0)|$ and $\theta = d^{\frac{1}{2}}a$ we find

$$1 + \frac{\theta^2}{2} < \theta \cot\theta + \theta^2 = \frac{Av\ell}{2} \tag{2.2}$$

in which the equality is exact and the elementary inequality approximates, for our present purpose, in the 'right direction'. From (2.2) we deduce the following lower bound for the critical coupling associated with $f(x)$:

$$v_c \geqslant v_c^L = \frac{8|f(0)|}{A(4\ell|f(0)| - A)}. \tag{2.3}$$

Thus we have $v < v_c^L \Rightarrow E(v) > 0$. We note that $\lim_{\ell\to\infty}(v_c^L) = 0$. As a (self-referential) example, if we apply this general formula to the square well itself with $a = d = 1$ and $\ell = 2$, we obtain

$$\tfrac{2}{3} = v_c^L < v_c \doteq 0.740. \tag{2.4}$$

For the exponential potential exhibited in figure 1 we obtain, again from (2.3),

$$0.738 \doteq v_c^L < v_c \doteq 1.020. \tag{2.5}$$

in which the value of v_c was found by solving Schrödinger's equation numerically.

3. Sufficient conditions for $E_0 < 0$

We now find our best upper bound to the critical coupling v_c by setting to zero the minimum of $W(b,d)$ subject to the area constraint $vA(b) = 2bd$. From (1.5) we have with $W(b,d) = 0$ for the upper comparison square well and $\theta = d^{\frac{1}{2}}b$

$$\ell bd = \theta\cot\theta + \theta^2 < 1 + \frac{2\theta^2}{3} \tag{3.1}$$

where the inequality is elementary and, again, approximates in the 'right direction'. By this we mean that if v is chosen so that $\ell bd > 1 + 2\theta^2/3$, then it follows that $E(v) < W(b,d) < 0$, that is to say, the ground-state eigenvalue is negative. From (3.1) we deduce the upper bound to v_c

$$v_c < \frac{1}{A(b)(\frac{\ell}{2} - \frac{b}{3})}$$

or, since b is not determined, we may optimize with respect to b to obtain

$$v_c < v_c^U = \min_{b<\ell}\left\{\frac{1}{A(b)(\frac{\ell}{2} - \frac{b}{3})}\right\}. \tag{3.2}$$

We note that $\lim_{\ell\to\infty}(v_c^U) = 0$. We shall again apply our general formula to the square well and to the exponential potential. In the case of the square well itself with $a = d = 1$ and $\ell = 2$, we obtain

$$0.740 \doteq v_c < v_c^U = \tfrac{3}{4}. \tag{3.3}$$

For the exponential potential exhibited in figure 1 we obtain $A(b) = 2(1 - \mathrm{e}^{-b})$ and from (3.2)

$$v_c \doteq 1.020 < v_c^U \doteq 1.183 \tag{3.4}$$

where the critical value of b is $\hat{b} \doteq 1.074$.

4. Conclusion

If a bound system with negative energy is put in a box, then the energy increases and will become positive unless the coupling v is sufficiently large. We have provided general upper and lower estimates for the critical coupling v_c defined by this situation. The general formulae are easy to apply to any given problem. As another example, if the potential shape corresponds to the Gauss potential $g(x) = -\mathrm{e}^{-x^2}$, and $\ell = 2$, then we find from (2.3), (3.2), and numerical integration of Schrödinger's equation (for v_c)

$$0.727 \doteq v_c^L < v_c \doteq 0.887 < v_c^U \doteq 1.004. \tag{4.1}$$

Both of the bounds we have found can immediately be generalized. In the case of v_c^L we may allow the potential shape $f(x)$ to be positive for, say, $|x| \geqslant q < \ell$. By replacing $f(x)$ by another *lower* comparison potential which agrees with $f(x)$ for $|x| < q$ but is zero for $|x| \geqslant q$, and by redefining A to be equal to (the absolute value of) only the negative part of the area of $f(x)$, we see that the bound (2.3) stands for this more general class of symmetric unimodal potentials.

For the upper bound v_c^U we now retain the original assumption that the potential is negative but we allow it to be unsymmetrical in a controlled manner. That is to say, we assume that the potential has a finite minimum value $f(0)$ and that in directions away from

$x = 0$ the potential is non-decreasing (and not altogether constant). We then decompose the potential into its fundamental even and odd components:

$$f(x) = \tfrac{1}{2}(f(x) + f(-x)) + \tfrac{1}{2}(f(x) - f(-x)) = f_+(x) + f_-(x). \tag{4.2}$$

We denote the bottom of the spectrum of the Hamiltonian $H_+ = -\Delta + vf_+(x)$ by $E_+(v)$ and let the exact normalized ground state for this problem be the (symmetric) function $\psi_+(x)$. It then follows from the Rayleigh–Ritz principle that

$$E(v) \leqslant (\psi_+, H\psi_+) = (\psi_+, H_+\psi_+) = E_+(v). \tag{4.3}$$

The first equality on the right-hand side of (4.2) follows since, by symmetry, $(\psi_+, f_-\psi_+) = 0$. Thus the symmetrized problem provides an upper comparison problem to which the inequality (3.2) applies. Moreover, and again by symmetry, $A(b) = A_+(b)$. Hence the bound (3.2) applies to this more general problem without further change.

The main purpose of this paper is to point out the box effect and to characterize it quantitatively for a class of potentials that is sufficiently general to be useful and also sufficiently well defined that the bounds can be simply expressed. Although very specific detailed questions concerning problems of this sort can be swiftly resolved today with the aid of a computer, it is always useful to have general formulae.

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