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Potentials and Bound States

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Abstract

We discuss several quantum mechanical potential problems, focusing on those which highlight commonly held misconceptions about the existence of bound states. We present a proof, based on the variational principle, that certain one dimensional potentials always support at least one bound state, regardless of the potential's strength. We examine arguments concerning the existence of bound states based on the uncertainty principle and demonstrate, by explicit calculations, that such arguments must be viewed with skepticism.

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I Introduction

One of the first types of problems encountered by students beginning a study of quantum mechanics is that of finding the eigenstates of a potential. Such problems form the basis of understanding for a great many physical systems, and so are important not just as pedagogical exercises, but also as real world models in solid state, nuclear, atomic and molecular physics. In addition, simple one and two dimensional potentials form the basis of our understanding of low dimensional structures such as quantum well devices.[1]

There is a substantial folklore concerning these simple potential problems. In surveying a variety of standard introductory (or even advanced) quantum mechanics texts, one finds various fragments of this folklore but rarely are they presented in a comprehensive fashion which would allow the reader to apply them to more general problems or, for that matter, to understand their physical and mathematical origin. This situation is made worse by the fact that some of these so called standard results are wrong. Our purpose here is to present an organized view of a selection of this folklore, expunging the erroneous results along the way.

Before proceeding, the reader is asked to apply his or her knowledge of this folklore to the following questions: How would you modify the statement "Every potential has at least one bound state." in order to make it true? (Not comprehensive, only correct.) How would you prove it? Can the condition for the existence of at least one bound state in a spherical step well be related to the Heisenberg uncertainty relation? If so, does such a relation also apply to the one dimensional step well? How does $\Delta x \Delta p$ behave as a potential well is made deeper and additional eigenstates appear?

To focus the discussion of the issues raised above, we consider the spherically symmetric step well:

$$V(r) = \begin{cases} -V_0 & r \leq a; \\ 0 & r > a, \end{cases} \tag{1}$$

which supports a bound state only for

$$V_0 > \frac{\hbar^2 \pi^2}{8ma^2} . \tag{2}$$

This is a generic feature of three dimensional central potentials. Numerous authors[2,3] have attempted to give a physical explanation of this by means of the uncertainty principle. The essence of the argument is as follows: Assuming $\Delta x \sim a$, from the uncertainty relation one obtains

$$\Delta p \sim \frac{\hbar}{2a}\,. \tag{3}$$

For the states under consideration it is reasonable to assume

$$p_{\max} \sim 2\Delta p\,. \tag{4}$$

Since the particle is bound,

$$V_0 > \frac{p_{\max}^2}{2m} = \frac{\hbar^2}{2ma^2}\,, \tag{5}$$

which is not all that different from the correct threshold value. So it appears that one can understand the bound state behavior of the spherical step well in terms of the uncertainty principle — As the well becomes narrower, it must also become deeper to "contain" the particle which has ever increasing momentum uncertainty.

The above argument is not specific to three dimensions and thus should be equally applicable to one and two dimensional potentials. As we shall demonstrate below, this leads to a contradiction, indicating a flaw in the reasoning that led to (5).

II One Dimensional Potentials

As a starting point for our detailed analysis we consider a general one dimensional potential, $V(x)$, subject only to the condition that, as $x \to \pm\infty$, $V \to 0$ sufficiently fast that all required integrals exist. Further consider the Hamiltonian

$$H = \frac{p^2}{2m} + V(x)\,. \tag{6}$$

We can obtain an upper bound on the energy of the ground state of this potential using the variational principle: for any normalized function ψ, $E_{\min} \le (\psi\,, H\psi)$ (see Schiff[4]). To this end take for our trial wavefunction, Ψ, a normalized gaussian,

$$\psi_\alpha(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}\,,\ \alpha > 0\,, \tag{7}$$

and evaluate

$$E(\alpha) \equiv (\psi_\alpha\,, H\psi_\alpha)\,. \tag{8}$$

Using the Hamiltonian (6), integrating by parts in the first term gives

$$E(\alpha) = \frac{\hbar^2}{2m}(\psi'_\alpha, \psi'_\alpha) + (\psi_\alpha, V\psi_\alpha) . \tag{9}$$

Notice that the first term in (9) is positive definite. Evaluating the integrals, we find

$$E(\alpha) = \frac{\hbar^2 \alpha}{4m} + \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} V(x) e^{-\alpha x^2} dx . \tag{10}$$

We now examine the sign of the quantity

$$\frac{E(\alpha)}{\sqrt{\alpha}} = \frac{\hbar^2}{4m}\sqrt{\alpha} + I(\alpha) , \tag{11}$$

where

$$I(\alpha) \equiv \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} V(x) e^{-\alpha x^2} dx \tag{12}$$

is a continuous function of α. As $\alpha \to 0$, $E(\alpha)/\sqrt{\alpha} \to I(0)$. Therefore, if $I(0) < 0$, then $\exists\, \epsilon > 0$ such that $I(\alpha) < 0$ for $\alpha \in [0, \epsilon)$. That is, for a sufficiently small value of α, $E(\alpha)/\sqrt{\alpha} < 0$ and hence the energy of the ground state is negative. The sole additional condition on V for at least one bound state to exist is then

$$\int_{-\infty}^{\infty} V(x) dx < 0 , \tag{13}$$

which depends on the shape of the potential, not its strength. That is, if (13) is satisfied, then ϵV will support a bound state for all positive ϵ. (It is then obvious that all purely attractive potential in one dimension always supports a bound state regardless of how weak and/or localized the potential.) We summarize our results thus far in

> PROPOSITION I: *For all one dimensional potentials such that*
>
> $$\int_{-\infty}^{\infty} V(x) dx < 0 ,$$
>
> ϵV *supports at least one bound state for all* $\epsilon > 0$.

Proposition I is a statement of *sufficiency* for a class of potentials to have bound states; it is not a statement of *necessity* for a given potential to have a bound state. In particular, *it is **not** true that if* $\int V(x)dx > 0$, *the potential has no bound state.* As an example, consider the potential

$$V = V^-(x) + V^+\delta(x - X)\,, \tag{14}$$

where $V^-(x) \leq 0$ for $|x| \leq a$, $V^-(x) = 0$ for $|x| > a$ and

$$V^+ > \left|\int V^- dx\right|. \tag{15}$$

Clearly (13) is not satisfied, but this potential may still support a bound state. Equation (11) now reads

$$\frac{E(\alpha)}{\sqrt{\alpha}} = \frac{\hbar^2}{4m}\sqrt{\alpha} + \frac{1}{\sqrt{\pi}}V^+ e^{-\alpha X^2} + \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} V^-(x)e^{-\alpha x^2}dx\,. \tag{16}$$

Since V^- satisfies (13) it supports at least one bound state, thus the sum of the first and third terms in (16) can be made negative for small enough α. Further, for large enough X, the second term can be made sufficiently small that $E(\alpha) < 0$. Intuitively this result makes sense, since it is reasonable to presume that regardless of the strength of the δ-function spike, it may always be moved far enough from the well so that it has a negligible effect on the bound states. It is also easy to see that this result is not dependent on the use of a δ-function for $V^+(x)$; we can just as easily replace it with a localized bump of the necessary height and width, and the argument goes through as before. The significance of the fact that we have violated condition (13) in constructing V is that we can always find an $\epsilon > 0$ such that ϵV has no bound state, *not* that any potential violating (13) has no bound states. (In fact, Simon[5] has shown that if $\int_{-\infty}^{\infty}(1 + x^2)\,|V(x)|\,dx < \infty$ then ϵV has a bound state for all small positive ϵ *if and only if* $\int_{-\infty}^{\infty} V(x)dx \leq 0$.)

While on the surface, one might suppose that Proposition I generalizes to two and three dimensions, this is not so. The variational proof of the existence of at least one bound state is firmly rooted in one dimension. The result is true in two dimensions[5] (with some additional conditions on V) but appears to be unobtainable with a variational argument. As we have seen above, in three dimensions the situation is even worse; a potential well need not support any bound states at all.

III Discussion

This apparent contradiction can be understood by considering the one dimensional square well. (See Schiff[4] for a particularly lucid treatment.) This is the relevant example since the ground state of the spherical step well corresponds to the first excited state of the symmetric one dimensional step well which, of course, need not exist. (Recall that the requirement that the wavefunction be finite at the origin[6] implies that states of the spherical well correspond to the odd parity states of the one dimensional well.)

The flaw in the argument that led to (5) lies in the presumption that the width of the potential is indicative of the value of Δx. In reality, as the depth of the well approaches zero, the ground state wavefunction becomes infinitely broad. The importance of this result extends beyond this example: *Without solving for the wavefunction, one can* ***not*** *determine the value of* Δx. *In particular, there is no justification for assuming that* Δx *will be comparable to some "characteristic" size of the potential.*

While this explains why arguments based on the uncertainty relations fail when applied to one dimension, it does not explain these same arguments give a reasonable estimate for the value of V_0 necessary for the spherical well to have a bound state. One might suspect that the ground state of the spherical well for $V_0 \gtrsim \hbar^2\pi^2/8ma^2$ is a minimum uncertainty state, thereby explaining the successful prediction of the threshold well depth. In turns out, however, that rather than being of minimum uncertainty, the ground state of the spherical well at threshold has infinitely large $\Delta x \Delta p$.

Plotted in figure 1 is $\Delta x \Delta p/\hbar$ as a function of $ma^2V_0/\hbar^2$, for the first four states of the one dimensional square well:

$$V(x) = \begin{cases} -V_0 & |x| \leq a; \\ 0 & |x| > a, \end{cases} \tag{17}$$

For the ground state, $\Delta x \Delta p$ always has a finite value, even for zero well depth, while for the excited states this becomes infinite as the well depth approaches the corresponding threshold value. At the threshold for a given state the energy of that state is zero. This results in an infinitely broad wavefunction and thus infinite position uncertainty. For all states, the momentum uncertainty goes to zero as the energy of the state vanishes. However, the asymptotic behavior of Δp is different for the ground state than for the excited states. This can be seen explicitly by taking the appropriate limits of the expressions for Δx

and Δp. For V_0 near the threshold for the n-th state,

$$(\Delta x)^2 \approx \frac{ma^4}{4\hbar^2}\frac{1}{e_n}, \tag{18}$$

and

$$(\Delta p)^2 \approx \begin{cases} \dfrac{\hbar^4}{ma^4} e_0\,, & \text{for } n = 0, \\ \dfrac{n^2\hbar^2\pi^2}{2\sqrt{2}a^2}\sqrt{e_n}\,, & \text{otherwise.} \end{cases} \tag{19}$$

The additional factor of $\sqrt{e_0}$ in the ground state expression for Δp is responsible for the finite limit of $\Delta x \Delta p$ as $e \to 0$ compared to the excited states where this limit is infinite.

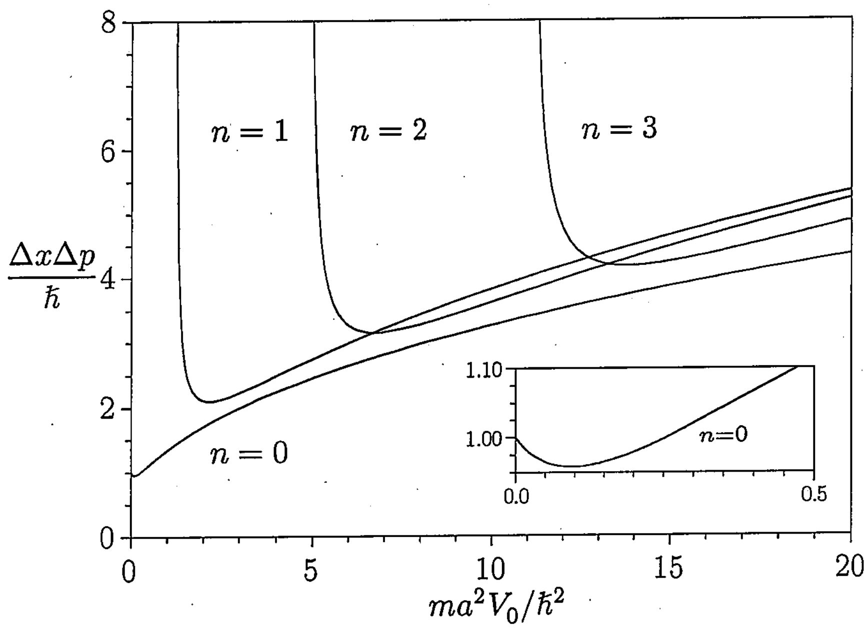

Figure 1: $\Delta x \Delta p/\hbar$ for several states of the one dimensional square well.

IV Conclusion

Summarizing, we have seen that in one dimension a potential will always support a bound state provided $\int dx\, V(x) < 0$. However, in three (and higher) dimensions a potential may not support a bound state even when $\int d^n\boldsymbol{x}\, V(\boldsymbol{x}) < 0$. Arguments that attempt to explain this by means of the uncertainty relation are fundamentally flawed; we have seen that as V_0 approaches threshold for the spherical well, the product of the uncertainties becomes infinite, thereby eliminating any hope of explaining the threshold for the existence a state in the spherical well by invoking the uncertainty principle. The main point here is that *a priori* one cannot reliably estimate the position uncertainty. To obtain a value for Δx, one must have the solution of Schrödinger's equation. We feel that this point cannot be overstressed: *The characteristic size of the wavefunction, Δx, need not in any way be comparable to the characteristic size of the potential.*

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[6] Strictly speaking, we require that no *expectation value* be infinite. In the case of the spherical well, the state corresponding to the ground state of the one dimensional problem would have infinite momentum.