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K. R. Brownstein

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Calculation of a bound state wavefunction using free state wavefunctions only

K. R. Brownstein
Department of Physics
University of Maine
Orono, Maine 04475
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A pedagogical example is presented in which the completeness of the free state wavefunctions of a Hamiltonian can be explicitly checked. For certain values of the potential strength the free states prove to be complete. For other values of the potential strength the free states are shown to be incomplete and the extent of this incompleteness is shown to consist of precisely one function. Using the fact that the totality of all energy eigenfunctions must be complete, this single bound state wavefunction is calculated using the free state wavefunctions only.

INTRODUCTION

The eigenfunctions of a Hamiltonian H, when properly normalized, form a complete orthonormal set of functions. Thus the quantum mechanical system possesses bound states if and only if the free states form an incomplete set. In particular it may be that the free states lack completeness by only one function. Using the fact that the totality of *all* energy eigenfunctions (both free and bound) is complete, it should then be possible to calculate the one bound state wavefunction from a knowledge of the free state wavefunctions only. The purpose of this article is to present a concrete pedagogical example of such a calculation.

ORTHONORMALITY AND COMPLETENESS

Consider a one dimensional Hamiltonian of the form

$$H = -\tfrac{1}{2}(d^2/dx^2) + V(x) \tag{1}$$

where the potential $V(x)$ is assumed to vanish for $x \to \pm\infty$. The energy eigenfunctions $\psi(x)$ satisfy $H\psi = E\psi$ and fall into two categories:

$$\text{bound states} \quad \psi_E{}^i(x) \text{ with } E < 0; \tag{2a}$$

$$\text{free states} \quad \psi_k{}^i(x) \text{ with } k = (2E)^{1/2} > 0. \tag{2b}$$

Here the index i is used to distinguish between possible degenerate eigenfunctions. For the particular Hamiltonian (1) it turns out that the bound states are all nondegenerate (hence the index i is really unnecessary) while the free states are all doubly degenerate. Use of the label k rather than E for the free states is merely a matter of convenience.

The orthonormality relation for the eigenfunctions (2) is

$$\int_{-\infty}^{\infty} \overline{\psi}_{E'}{}^{i'}(x)\, dx = \delta_{ii'}\delta_{EE'} \quad \text{for bound states} \tag{3a}$$

$$\int_{-\infty}^{\infty} \overline{\psi}_k{}^i(x)\psi_{k'}{}^{i'}(x)\, dx = \delta_{ii'}\delta(k-k') \quad \text{for free states,} \tag{3b}$$

where the overbar indicates complex conjugation. As usual, one uses the Kronecker delta for discrete indices and the Dirac delta for continuous indices. The completeness relation for the eigenfunctions (2) is

$$\sum_i \sum_{E<0} \overline{\psi}_E{}^i(x)\,\psi_E{}^i(x') + \sum_i \int_0^{\infty} \overline{\psi}_k{}^i(x)\,\psi_k{}^i(x')\, dk = \delta(x-x'). \tag{4}$$

Now consider the case in which the system possesses only one bound state. Assuming that the integrations in Eq. (4) involving the free states can actually be carried out (!), one can solve Eq. (4) for the normalized bound-state wave function (uniquely to within a phase factor of magnitude one). This is the calculation that will be illustrated in the example below.

FREE STATE WAVE FUNCTIONS

The potential chosen for this example is that of a Dirac delta function located at $x = 0$,

$$V(x) = V_0\delta(x) \tag{5}$$

where the strength V_0 may be positive or negative. As is well known the effect of such a potential is to make ψ satisfy

$$-\tfrac{1}{2}(d^2\psi/dx^2) = E\psi \text{ for } x \neq 0 \tag{6a}$$

and to impose the following matching conditions at $x = 0$:

$$\psi(x) \text{ is continuous} \tag{6b}$$

$$\left.\frac{d\psi}{dx}\right|_{0+} - \left.\frac{d\psi}{dx}\right|_{0-} = 2V_0\,\psi(0). \tag{6c}$$

The discontinuity (6c) in the slope of ψ at $x = 0$ is obtained by integrating $H\psi = E\psi$ in a small neighborhood of $x = 0$.

Rather than using the standard scattering boundary conditions (i.e., waves incident from either $x = -\infty$ or $x = +\infty$), it is more convenient to demand that the energy eigenfunctions have definite *parity*. This is possible since the potential $V(x)$ is an even function of x. These simultaneous eigenfunctions of energy and parity are

$$\psi_k{}^o(x) = \pi^{-1} \sin kx \tag{7a}$$

$$\psi_k{}^e(x) = V_0 \pi^{-1/2}(k^2 + V_0{}^2)^{-1/2} \times [\sin k|x| + (k/V_0) \sin k|x|] \tag{7b}$$

where $k = (2E)^{1/2}$. Here the index i of Eq. (2b) takes on the values $i = o$ (odd parity state) and $i = e$ (even parity state). Direct substitution shows that these obey the requirements (6). Further, these eigenfunctions (7) have been scaled in order to satisfy the normalization condition (3b). See the Appendix for some details concerning integrals used in normalizing these functions.

It is interesting to note that the odd parity wave functions (7a) are not affected at all by the presence of the potential. As for the even parity states (7b), for $V_0 \to 0$ one obtains $\pi^{-1/2} \cos k|x|$ while for $V_0 \to \pm\infty$ the result is $\pi^{-1/2} \sin k|x|$; both these limiting cases are seen to be similar to the odd parity wave function (7a) with regard to the normalization constant.

COMPLETENESS INTEGRALS

In this section the contribution

$$\sum_{i=o,e} \int_0^\infty \bar{\psi}_k{}^i(x)\psi_k{}^i(x')\, dk \tag{8}$$

of the free states to the completeness relation (4) will be calculated. The odd-parity free states contribute the following to (8):

$$\int_0^\infty \bar{\psi}_k{}^o(x)\psi_k{}^o(x')\, dk = \frac{1}{\pi}\int_0^\infty \sin kx \sin kx'\, dk = \tfrac{1}{2}\delta(x - x') - \tfrac{1}{2}\delta(x + x'). \tag{9}$$

(In passing it may be noted that when operating on an arbitrary *odd* function of x, Eq. (9) reduces to $\delta(x - x')$. Thus the odd-parity free states are complete insofar as odd-parity functions are concerned; consequently, there can be no odd-parity bound states. Since the bound states must alternate in parity with the lowest energy state being even, one can conclude at this point that the number of bound states must simply be either zero or one.)

The contribution of the even-parity free states to (8) is

$$\int_0^\infty \bar{\psi}_k{}^e(x)\psi_k{}^e(x')\, dk = \frac{V_0{}^2}{\pi}\int_0^\infty \frac{1}{k^2 + V_0{}^2}\left(\sin k|x| + \frac{k}{V_0}\cos k|x|\right) \times \left(\sin k|x'| + \frac{k}{V_0}\cos k|x'|\right) dk. \tag{10}$$

Using some trigonometric identities Eq. (10) can be decomposed into the sum of the following three terms:

$$\frac{1}{\pi}\int_0^\infty \cos k|x| \cos k|x'|\, dk \tag{11a}$$

$$-\frac{V_0{}^2}{\pi}\int_0^\infty \frac{1}{k^2 + V_0{}^2}\cos[k(|x| + |x'|)]\, dk \tag{11b}$$

$$+\frac{V_0}{\pi}\int_0^\infty \frac{k}{k^2 + V_0{}^2}\sin[k(|x| + |x'|)]\, dk. \tag{11c}$$

The integral (11a) is $\frac{1}{2}\delta(|x| - |x'|) + \frac{1}{2}\delta(|x| + |x'|)$ which is the same as

$$\tfrac{1}{2}\delta(x - x') + \tfrac{1}{2}\delta(x + x') \tag{12a}$$

regardless of the signs of x and x' (including the case $x' = 0$). The remaining two integrals (11b,c) can be evaluated using conventional contour integration techniques in the complex k plane. Briefly the procedure is:

(a) replace $\int_0^\infty (\,)\, dk$ by $\frac{1}{2}\int_{-\infty}^\infty (\,)\, dk$ since the integrand is even in k;

(b) write sine or cosine in exponential form;

(c) complete the contour for each such term with a semi-circular path in the appropriate upper or lower half-plane.

Note that the poles of all the integrands are located at $k = \pm|V_0|i$. It is precisely at this point in the calculation that the *sign* of V_0 enters. This is important since it will turn out that a bound state exists only for positive V_0. The result for (11b) is

$$-\tfrac{1}{2}|V_0| \exp[-|V_0|(|x| + |x'|)] \tag{12b}$$

and similarly the result for (11c) is

$$+\tfrac{1}{2}V_0 \exp[-|V_0|(|x| + |x'|)]. \tag{12c}$$

Collecting the sum of (12a,b,c) the contribution of the free states to the completeness relation (8) becomes

$$\sum_{i=o,e}\int_0^\infty \bar{\psi}_k{}^i(x)\psi_k{}^i(x')\, dk = \delta(x - x') - \tfrac{1}{2}(|V_0| - V_0)\exp[-|V_0|(|x| + |x'|)]. \tag{13}$$

RESULTS

When the contribution of the free states (13) is substituted into the general completeness relation (4), one obtains for the contribution of the bound states:

$$\sum_i \sum_{E<0} \bar{\psi}_E{}^i(x)\,\psi_E{}^i(x') = \tfrac{1}{2}(|V_0| - V_0)\exp[-|V_0|(|x|+|x'|)] \qquad (14)$$

Inspection of (14) yields the following information:

(a) For $V_0 > 0$ the right hand side of (14) vanishes. Thus the completeness of the free-state eigenfunctions has been explicitly verified; there are *no bound states*.

(b) For $V_0 < 0$ Eq. (14) becomes

$$\sum_i \sum_{E<0} \bar{\psi}_E{}^i(x)\,\psi_E{}^i(x') = |V_0|\,\exp[-|V_0|(|x|+|x'|)]. \qquad (15)$$

Although perhaps it is obvious[1] that this can only be satisfied if there is precisely one bound state, an easy way to prove this is to set x' equal to x and then integrate both sides of Eq. (15) from $x=-\infty$ to $x=+\infty$. Because the $\psi_E{}^i(x)$ are normalized, the left hand side integrates to the number of bound states N_b; the right hand side integrates to unity. Thus $N_b = 1$, i.e., there is *one bound state*. Also, from (15) the one bound state must satisfy

$$\psi_E(x) = (|V_0|)^{1/2}\exp(-|V_0|\,|x|) \qquad (16)$$

uniquely to within a phase factor of magnitude one. Direct substitution shows that (16) satisfies not only the free particle equation for $x \neq 0$ (6a) but also the two matching conditions at $x \neq 0$ (6b,c) and that the bound state energy eigenvalue E_b is

$$E_b = -\tfrac{1}{2}V_0{}^2. \qquad (17)$$

Furthermore, the bound state wave function (16) appears *automatically* with the *correct normalization* (3a). With the inclusion of this one bound state, the completeness of *all* (free and bound) energy eigenfunctions has been explicitly demonstrated.

It is to be emphasized that the above results (a) and (b) were obtained from a knowledge of the free states *only*.

CONCLUSION

The question of the completeness of the set of energy eigenfunctions is a confusing one to many beginning students of quantum mechanics. Among the conceptual difficulties is the difference in the normalization used for the free (continuum) states versus that used for the bound (discrete) states. Usually, completeness is demonstrated at most only for a free particle or a particle in a box. It is hoped that the calculation presented in this article may be of use in several ways:

(a) If one includes all the energy eigenfunctions, it furnishes a nontrivial example of a situation in which completeness can be explicitly shown. Both the case of no bound states $(V_0 > 0)$ and of a single bound state $(V_0 < 0)$ can be treated.

(b) For the case $V_0 < 0$, it serves as an example in which the free states can be shown to be incomplete and the extent of this incompleteness can be shown to consist of precisely one function. This missing function (the bound state energy eigenfunction) can be uniquely determined by answering the question: "What single function must be added to the free-state energy eigenfunctions so as to obtain a complete orthonormal set of functions?"

(c) In the evaluation of some of the completeness integrals, one is led to use contour integration in the complex k plane. At this point the student might be introduced to the concept that the poles of the scattering amplitude are related to the bound state energy eigenvalues.

APPENDIX

In order to carry out the normalization of the free-state wave functions it is necessary to evaluate certain integrals that are improper in the ordinary sense. These are

$$I(k_1,k_2) \equiv \int_0^\infty \sin(k_1x)\sin(k_2x)\,dx = \frac{\pi}{2}\,\delta(k_1-k_2), \quad k_1,k_2>0; \qquad (A1)$$

$$J(k_1,k_2) \equiv \int_0^\infty \cos(k_1x)\cos(k_2x)\,dx = \frac{\pi}{2}\,\delta(k_1-k_2), \quad k_1,k_2>0; \qquad (A2)$$

$$K(k_1,k_2) \equiv \int_0^\infty [k_2\sin(k_1x)\cos(k_2x) + k_1\sin(k_2x)\cos(k_1x)]\,dx = 0 \qquad (A3)$$

In each case the meaning is that $\int_0^\infty (\ )\,dx$ is to be replaced by $\int_0^L (\ )\,dx$ and the limit as $L\to\infty$ is taken last. For example, the meaning of (A1) is that for any "good" function $f(k_1)$

$$\lim_{L\to\infty}\int_0^\infty f(k_1)\,dk_1\int_0^L \sin(k_1x)\sin(k_2x)\,dx = \tfrac{1}{2}\pi f(k_2) \qquad (A4)$$

provided $k_2 > 0$.

To verify (A1),

$$\int_0^\infty I(k_1,k_2)f(k_1)\,dk_1 = \tfrac{1}{2}\lim_{L\to\infty}\left[\int_0^\infty \frac{\sin(k_1-k_2)L}{k_1-k_2}f(k_1)\,dk_1 - \int_0^\infty \frac{\sin(k_1+k_2)L}{k_1+k_2}f(k_1)\,dk_1\right.$$

$$= \frac{1}{2} \lim_{L\to\infty} \int_{-k_2 L}^{\infty} \frac{\sin\xi}{\xi} f(k_2 + \xi/L)\, d\xi - \int_{k_2 L}^{\infty} \frac{\sin\eta}{\eta} f(-k_2 + \eta/L)\, d\eta$$

$$= \frac{1}{2}\ f(k_2) \int_0^{\infty} \frac{\sin\xi}{\xi}\, d\xi - 0 \ = \frac{\pi}{2} f(k_2) \qquad \text{(A5)}$$

provided $k_2 > 0$. Here the changes of variable $\xi = (k_1 - k_2)/L$ and $\eta = (k_1 + k_2)/L$ have been used. The integral (A2) is proved in much the same manner. As for (A3), when the upper limit is replaced by L the integral becomes $\sin(k_1 L)\sin(k_2 L)$. When this is multiplied by any "good" function $f(k_l)$ and integrated with respect to k_l the result is zero in the limit $L \to \infty$.

To evaluate the odd parity free state contribution to the completeness relation (9), one would use (A1) with the roles of x and k interchanged. In addition, one would have to allow the possibility of any sign of x and x'; hence two delta functions emerge. Similarly, the integral (11a) is based upon (A2) with the roles of x and k interchanged.

[1]Since the right hand side of Eq. (15) is explicitly a *single* product of a function of x multiplied by (the complex conjugate of) the *same* function of x'.

RUSTIC PHYSICS

For the past five years we have had a small weekend ranch in the coast ranges of northern California, four miles from power lines, and dependent on springs for water. Among the problems we faced, several seemed unusual to countrymen and to physicists on the campus. We found that:

(1) Water will not always attain its own level: a spring will not always supply an outlet at a substantially lower point even if all intermediate points are lower than the spring. How can this be? Our outlet is 70 ft lower than a spring 2200 ft away, connected by 3/4″ PE pipe.

(2) A tank fed by a feeble spring (10 gal/h) can water a garden daily, vigorously, automatically—with no moving parts or valves. It sprays 200 gal in 10 min. What is the principle of operation? This is the principle of the classical vase of Tantalus and of the fountains of ancient Corinth. Our vegetables love it.

(3) The cabin water is from a 160-gal pressure tank, and we draw down from 50 to 20 lbs. We get a larger drawdown (volume) with the tank at the cabin rather than 20 ft. lower at the pump, for equal pressures at the cabin. Further, we can greatly increase the drawdown by priming the tank with 20 lbs. of air before pumping in water. How do you explain these observations?

(4) Our wood stove, like most country stoves, has the stovepipe too close to the wall, with the risk that a lively fire in the stove will burn down the cabin. A *black* aluminum sheet mounted 1″ from the wall is a very good insulator for the stovepipe. A shiny sheet is better. An asbestos backing is unnecessary, as well as unhealthy. Can you account for these facts?

(5) A 2.5 kW generator (delivering 22 A maximum at 115 V is easily adequate for family requirements, used 2 h/day with an auxiliary 12 V dc battery for lights. But even a 1/2 hp electric motor may need as much as 45 A to start, although it will subsequently run at 7 A. The starting current load can be lightened by putting a passive element across the line. What circuit element and of what value?

None of the solutions is difficult.

—Charles Kittel