Explicit results for the quantum-mechanical energy states basic to a finite square-well potential

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The theory of complex variables is used to establish explicit expressions for the discrete energy states relevant to a square-well potential.

INTRODUCTION

As one of the first examples of the principles of quantum mechanics, Schiff[1] solves the Schrödinger equation for a square-well potential,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}U(x)+V(x)U(x)=EU(x), \tag{1}$$

where

$$V(x)=0, \quad x\in(-a,a), \tag{2a}$$

and

$$V(x)=V_0, \quad |x|>a, \tag{2b}$$

to find the discrete energy levels. Thus, on establishing the solution to Eq. (1), subject to $U(x)$ and $U'(x)$ being continuous at $x=\pm a$, Schiff[1] finds that the bound states $(E<V_0)$ can be expressed as

$$E_j=\frac{\hbar^2}{2ma^2}\xi_j^2, \quad j=1,2,3,\ldots,n, \tag{3}$$

where ξ_j denotes one of the n positive solutions of

$$\xi\tan\xi=(A^2-\xi^2)^{1/2}, \quad j \text{ odd}, \tag{4a}$$

$$\xi\cot\xi=-(A^2-\xi^2)^{1/2}, \quad j \text{ even}, \tag{4b}$$

where $A\in(0,n\pi/2)$ is given by

$$A=\frac{a}{\hbar}\sqrt{2mV_0}. \tag{5}$$

Here we wish to report explicit solutions of Eqs. (4) that yield exact closed-form results for the discrete energy levels.

ANALYSIS

In order to relate the roots of Eqs. (4) to the zeros of a sectionally analytic function, we wish to consider

$$\Lambda_k(z)=-iAz+D(z)\left(k\pi i-\frac{1}{2}\int_{-1}^{1}\frac{d\mu}{\mu-z}\right), \tag{6}$$

where k is a constant and

$$D(z)=(z^2-1)^{1/2}. \tag{7}$$

Here we use a branch of the square root function such that $D(z)=-D(-z)$ is analytic in the complex plane cut from -1 to 1 along the real axis and $\arg D(z)\in(-\pi,\pi)$. We conclude that $\Lambda_k(z)$ is analytic in the complex plane cut from -1 to 1 along the real axis. Further, we can use the argument principle[2] to deduce that $\Lambda_k(z)$ has one zero in the finite cut plane for $k\in(-\frac{1}{2},\frac{1}{2})$, that $\Lambda_k(z)$ has two zeros for $k>\frac{1}{2}$ and that $\Lambda_k(z)$ has no zeros for $k<-\frac{1}{2}$.

We first consider $k=0$ and note[3] that

$$\frac{\Lambda_0(k)}{z-z_0}=K_0X_0(z), \tag{8}$$

where $X_0(z)$ is a canonical solution of the Riemann problem[4] defined by

$$X_0^+(\tau)=G_0(\tau)X_0^-(\tau), \quad \tau\in(-1,1). \tag{9}$$

Here K_0 is a constant to be determined and

$$G_0(\tau)=\frac{\Lambda_0^+(\tau)}{\Lambda_0^-(\tau)}, \tag{10}$$

where the $\pm$ superscripts are used to denote the limiting values as z approaches the branch cut $[-1,1]$ from above and below. The Riemann problem defined by Eq. (9) can be solved, as discussed by Muskhelishvili,[4] to yield

$$X_0(z)=\exp\left[\frac{1}{2\pi i}\int_{-1}^{1}\log G_0(\tau)\frac{d\tau}{\tau-z}\right], \tag{11}$$

where we use the log function such that $\arg\log G_0(\tau)$ varies continuously from 0 at $\tau=-1$. If we now investigate Eq. (8) as $|z|\to\infty$ we find that $K_0=-iA$ and that $z_0=-iy_0$, where

$$y_0=\frac{1}{A}-\frac{1}{2\pi}L_0, \tag{12}$$

with, in general,

$$L_k=\int_0^1 \ln(\{(\tfrac{1}{2}-k)^2\pi^2(1-t^2)+[(1-t^2)^{1/2}\tanh^{-1}(t)-At]^2\}/\{(\tfrac{1}{2}+k)^2\pi^2(1-t^2)+[(1-t^2)^{1/2}\tanh^{-1}(t)+At]^2\})\,dt. \tag{13}$$

It is now apparent that

$$\xi_1=\mathrm{Tan}^{-1}\left(\frac{1}{y_0}\right) \tag{14}$$

is the first of the desired solutions of Eqs. (4).

For $k>\frac{1}{2}$, we can readily generalize Eq. (8) to obtain

$$\frac{\Lambda_k(z)}{(z-z_{k,1})(z-z_{k,2})}=i(k\pi-A)X_k(z), \tag{15}$$

where $z_{k,1}$ and $z_{k,2}$ are the two zeros of $\Lambda_k(z)$. Here we write a canonical solution of the Riemann problem defined by the $k>\frac{1}{2}$ generalization of Eq. (9) as

$$X_k(z)=\frac{1}{z-1}\exp\left[\frac{1}{2\pi i}\int_{-1}^{1}\log G_k(\tau)\frac{d\tau}{\tau-z}\right]. \tag{16}$$

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Here

$$G_k(\tau)=\frac{\Lambda_k^+(\tau)}{\Lambda_k^-(\tau)}, \tag{17}$$

and again we use $\log G_k(\tau)$ such that $\arg \log G_k(\tau)$ varies continuously from 0 at $\tau=-1$. With $\log G_k(\tau)$ so defined, we deduce, for $k>\frac{1}{2}$, that $\log G_k(1)=2\pi i$; and thus, as discussed by Muskhelishvili,[4] the factor $(z-1)$ appears explicitly in Eq. (16) to insure that $X_k(z)$ does not vanish at $z=1$. We can now investigate Eq. (15) for large $|z|$ to deduce that $z_{k,1}=-iy_{k,1}$ and $z_{k,2}=-iy_{k,2}$, where

$$y_{k,1}=B_k+(B_k^2+W_k)^{1/2} \tag{18a}$$

and

$$y_{k,2}=B_k-(B_k^2+W_k)^{1/2}. \tag{18b}$$

Here

$$B_k=\frac{1}{2}\left(\frac{1}{A-k\pi}-\frac{1}{2\pi}L_k\right) \tag{19}$$

and

$$W_k=\left(\frac{1}{A-k\pi}\right)\left(\frac{1}{2\pi}L_k+\frac{k\pi}{2}\right)-\frac{1}{8\pi^2}L_k^2-1+M_k. \tag{20}$$

In addition,

$$M_k=\frac{1}{\pi}\int_0^1 t\Theta(t)\,dt, \tag{21}$$

where

$$\Theta(t)=\tan^{-1}([\pi(1-t^2)\tanh^{-1}(t)-2kAt\pi(1-t^2)^{1/2}]/\{(\tfrac{1}{4}-k^2)\pi^2(1-t^2)-(1-t^2)[\tanh^{-1}(t)]^2+A^2t^2\}), \tag{22}$$

with $\Theta(0)=\pi$. If we now let $j=2k+1$, then the last $n-2$ desired positive solutions of Eqs. (4) can be expressed as

$$\xi_j=k\pi+\mathrm{Tan}^{-1}\left(\frac{1}{y_{k,1}}\right),\quad j=3,4,5,\ldots,n. \tag{23}$$

The case $k=\frac{1}{2}$ requires special attention since the corresponding $G_k(\tau)$ vanishes on the cut. We thus find it convenient to introduce

$$\Omega(z)=\Lambda_{1/2}(z)\Lambda_{1/2}(-z) \tag{24}$$

and consider the Riemann problem defined by

$$Y^+(\tau)=\frac{\Omega^+(\tau)}{\Omega^-(\tau)}Y^-(\tau),\quad \tau\in(-1,1). \tag{25}$$

We find we can write a canonical solution here as

$$Y(z)=\frac{1}{z-1}\exp\left[\frac{1}{\pi}\int_{-1}^1\phi(t)\frac{dt}{t-z}\right], \tag{26}$$

where

$$\phi(t)=\tan^{-1}\left(\frac{\pi(1-t^2)^{1/2}}{-(1-t^2)^{1/2}\tanh^{-1}(t)-At}\right), \tag{27}$$

with $\phi(-1)=0$. Thus, since $\Omega(z)$ has a zero at the origin and two additional zeros, $\pm z_{1/2}$, we can write

$$\frac{\Omega(z)}{z(z^2-z_{1/2}^2)}=\left(\frac{\pi}{2}-A\right)^2Y(z), \tag{28}$$

and let $|z|\to\infty$ to deduce that $z_{1/2}=\pm iy_{1/2}$, where

$$y_{1/2}=\left(\frac{2(\pi-A)}{2A-\pi}+\frac{2}{\pi}\int_0^1 t\phi(t)\,dt+\frac{4}{(2A-\pi)^2}\right)^{1/2}. \tag{29}$$

The positive solution of Eqs. (4) corresponding to $j=2$ thus is given by

$$\xi_2=\frac{\pi}{2}+\mathrm{Tan}^{-1}\left(\frac{1}{y_{1/2}}\right). \tag{30}$$

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