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Normalization of WKB-Type Approximations

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A method is developed for normalizing WKB-type approximations to wave functions for a simple potential well type of problem. The procedure closely resembles Furry's method of finding the normalization for the usual WKB approximations.

I. INTRODUCTION

IN a recent paper[1] a WKB-type approximation for the solutions of the one-dimensional Schrödinger equation was described. The method was illustrated in that paper by using, as an example, the problem of a potential well with two classical turning points of the motion. In addition, for this example, an approximate method for normalizing the wave function was given. In the present paper an alternate method for obtaining the normalization is discussed. This treatment closely resembles one given by Furry[2] for the normalization of the usual WKB approximate wave functions in the case of a potential well problem with two turning points.

The function ψ for which an approximation is found by Miller and Good[1] satisfies the one-dimensional Schrödinger equation,[3]

$$d^2\psi(x)/dx^2+p^2(x)\psi(x)=0, \tag{1}$$

where

$$p^2(x)=W-V(x). \tag{2}$$

Here W is $2m$ times the total energy of a particle of mass m moving in a potential $V(x)/2m$. The function $V(x)$ will be limited to the general form shown in Fig. 1, a potential well giving two turning points x_1 and x_2 with $x_1<x_2$. The approximation is based on the function $\phi(S)$ which satisfies a Schrödinger equation,

$$d^2\phi(S)/dS^2-P^2(S)\phi(S)=0, \tag{3}$$

for some function

$$P^2(S)=E-U(S), \tag{4}$$

in which the parameter E is independent of S. The function $U(S)$ will here be taken qualitatively similar to $V(x)$, a potential well giving two turning points s_1 and s_2 with $s_1<s_2$. Moreover, it will be assumed that the normalizing constants of the bound states $\phi_n(S)$ are known. The approximate wave function is

$$\psi\cong S'^{-\frac{1}{2}}\phi(S), \tag{5}$$

where S is given as a function of x by

$$\int_{s_1}^{S} P(\sigma)d\sigma=\int_{x_1}^{x} p(\xi)d\xi. \tag{6}$$

Also the equation

$$\int_{s_1}^{s_2} P(\sigma)d\sigma=\int_{x_1}^{x_2} p(\xi)d\xi \tag{7}$$

gives the functional relationship between W and E. If E_n is the eigenvalue for the nth bound state of $U(S)$, the corresponding $W=W_n$ given by Eq. (7) is the approximate eigenvalue for the nth bound state of $V(x)$.

II. NORMALIZATION

In this discussion $\psi_\alpha(x)$ corresponding to any W will denote a solution of Eq. (1) which goes to zero as x approaches minus infinity but which does not necessarily go to zero as x approaches plus infinity. Likewise $\psi_\beta(x)$ is a solution which goes to zero as x approaches plus infinity but not necessarily as x approaches minus infinity. Furthermore the relative amplitudes of these two functions will be chosen so that when W is an eigenvalue W_n for the nth bound state, the functions ψ_α and ψ_β are both the same function ψ_n. This function goes to zero as x approaches either plus or minus infinity. Each of the functions ψ_α and ψ_β satisfies Eq. (1)

$$\psi_\alpha''(x)+(W-V)\psi_\alpha(x)=0, \tag{8}$$

$$\psi_\beta''(x)+(W-V)\psi_\beta(x)=0. \tag{9}$$

Likewise, the complex conjugate of ψ_n satisfies

$$\psi_n^{*\prime\prime}(x)+(W_n-V)\psi_n^*(x)=0. \tag{10}$$

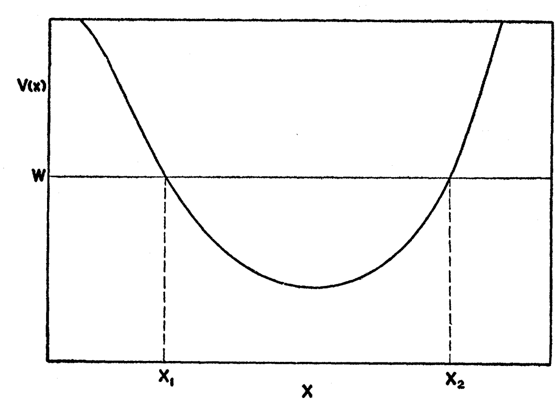

FIG. 1. Type of potential considered.

[1] S. C. Miller, Jr. and R. H. Good, Jr., Phys. Rev. **91**, 174 (1953).
[2] W. H. Furry, Phys. Rev. **71**, 360 (1947).
[3] Units have been chosen so that $\hbar=1$.

Upon multiplying Eq. (8) by $\frac{1}{2}\psi_n{}^*$ and Eq. (10) by $\frac{1}{2}\psi_\alpha$, subtracting one equation from the other, and integrating from $-\infty$ to a point a, one obtains

$$\tfrac{1}{2}\int_{-\infty}^{a}\psi_n{}^*\psi_\alpha dx=-\tfrac{1}{2}(W-W_n)^{-1}\times(\psi_n{}^*\psi_\alpha{}'-\psi_n{}^{*\prime}\psi_\alpha)_{x=a},\quad(11)$$

since the term in parentheses on the right is zero at $x=-\infty$. If Eq. (11) is added to its complex conjugate, the result is

$$\tfrac{1}{2}\int_{-\infty}^{a}(\psi_n{}^*\psi_\alpha+\psi_n\psi_\alpha{}^*)dx=-\tfrac{1}{2}(W-W_n)^{-1}\times[\psi_n{}^*(\psi_\alpha{}'-\psi_n{}')-\psi_n{}'(\psi_\alpha{}^*-\psi_n{}^*)+\text{c.c.}]_{x=a},\quad(12)$$

where terms have been added and subtracted on the right and c.c. means complex conjugate. Similarly using Eqs. (9) and (10), one obtains

$$\tfrac{1}{2}\int_{a}^{\infty}(\psi_n{}^*\psi_\beta+\psi_n\psi_\beta{}^*)dx=\tfrac{1}{2}(W-W_n)^{-1}\times[\psi_n{}^*(\psi_\beta{}'-\psi_n{}')-\psi_n{}'(\psi_\beta{}^*-\psi_n{}^*)+\text{c.c.}]_{x=a}.\quad(13)$$

In the limit as W approaches W_n, a term such as $(\psi_\alpha{}'-\psi_n{}')/(W-W_n)$ becomes $\partial\psi_\alpha{}'/\partial W$. Therefore, the sum of Eqs. (12) and (13) in this limit is

$$\int_{-\infty}^{\infty}|\psi_n|^2dx=-\tfrac{1}{2}[\psi_n{}^*\partial(\psi_\alpha{}'-\psi_\beta{}')/\partial W-\psi_n{}'\partial(\psi_\alpha{}^*-\psi_\beta{}^*)/\partial W+\text{c.c.}]_{x=a},\quad(14)$$

evaluted at $W=W_n$.

A similar expression holds for the integral of $|\phi_n|^2$ over S in terms of ϕ_α and ϕ_β and their derivatives with respect to S and E, evaluated at $S(a)$ and E_n. The functions ϕ_α and ϕ_β are to have the same properties for large S as ψ_α and ψ_β have for large x.

An approximate expression for the integral in Eq. (14) is obtained by substituting for ψ from Eq. (5) in the right side of Eq. (14) and changing variables from x to S and W to E. Since, from Eqs. (6) and (7), S' is here real and positive, this approximate expression simplifies to

$$\int_{-\infty}^{\infty}|\psi_n|^2dx=-\tfrac{1}{2}(dE/dW)[\phi_n{}^*\partial(d\phi_\alpha/dS-d\phi_\beta/dS)/\partial E-(d\phi_n/dS)\partial(\phi_\alpha{}^*-\phi_\beta{}^*)/\partial E+\text{c.c.}]_{S=S(a)}=(dE/dW)\int_{-\infty}^{\infty}|\phi_n|^2dS,\quad(15)$$

where each of the expressions is evaluated at $E=E_n$. With the definitions of p^2 and P^2 in Eqs. (2) and (4), differentiation of Eq. (7) leads to

$$dE/dW=\int_{x1}^{x2}[p(\xi)]^{-1}d\xi\Big/\int_{s1}^{s2}[P(\sigma)]^{-1}d\sigma.\quad(16)$$

If, then, A_n is the approximate normalizing constant of ψ_n and $A_n{}'$ is the normalizing constant of ϕ_n, Eq. (15) can be written as

$$A_n{}^2/A_n{}'^2=\int_{s1}^{s2}[P(\sigma)]^{-1}d\sigma\Big/\int_{x1}^{x2}[p(\xi)]^{-1}d\xi.\quad(17)$$

This is the desired approximate expression giving the normalizing constant A_n.

For the particular $P(S)$ used in reference 1 for which $U(S)=S^2$,

$$\phi_n=H_n(S)\exp(-S^2/2),\quad(18)$$

where H_n is the nth Hermite polynomial. Also for this case one has

$$\int_{s1}^{s2}[P(\sigma)]^{-1}d\sigma=\pi,\quad(19)$$

$$A_n{}'^2=(2^n\pi^{\frac{1}{2}}n!)^{-1}.\quad(20)$$

Therefore the normalizing constant is given by

$$A_n{}^2=\pi^{\frac{1}{2}}\left\{2^n n!\int_{x1}^{x2}[p(\xi)]^{-1}d\xi\right\}^{-1}.\quad(21)$$

For a representative case such as the potential $V(x)$ used in reference 1, the approximate normalizing constant is correct to about three significant figures. This method of normalization should give as accurate results for high-energy levels as for low ones with no appreciable change in the labor of computation. A possible defect in this method is that there appears to be no way to estimate the error in the approximation. Also there does not seem to be any way to generalize the method to give matrix elements of general functions.