PHYSICAL REVIEW A VOLUME 22, NUMBER 5 NOVEMBER 1980

Construction of a symmetric potential barrier from tunneling transmission coefficients

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(Received 12 May 1980)

For a symmetric potential barrier with two turning points there exists an inversion procedure which is closely related to the inversion of scattering phase shifts. The inversion formulas correct to first order in $\hbar^2$ are derived in the WKB approximation. To illustrate the applicability and limitation of the proposed procedure, we construct the quartic potential barrier $U(X) = -X^4$, from its transmission coefficients.

I. INTRODUCTION

The WKB method is widely used in the inversion of molecular scattering data.[1] In this class of problems, one determines the spherically symmetric potential from the phase shifts $\eta(E,l)$. At a fixed energy, the potential can be determined from the angular momentum dependence of the phase shifts. On the other hand, at a fixed angular momentum, one can construct the potential from the energy dependence. Inversion formulas in the generalized WKB approximation have been developed correct to $\hbar^2$ for both cases.[2] The formulation for the latter case is closely related to the inversion procedure discussed in this paper.

Determination of the single-hump potential barrier was discussed by Cole and Good.[3] Their inversion formulas are correct to the zeroth order in $\hbar^2$. The objective of this paper is to derive an inversion formula which is correct to the first order in $\hbar^2$. To illustrate the contribution of the higher-order term, we choose to construct a quartic barrier $U(X)=-X^4$. Application of the higher-order correction improves the accuracy of the method by at least two orders of magnitude. However, the WKB method fails near the top of the barrier. This limitation was discussed in detail by Ford *et al.*[4]

II. INVERSION FORMULA CORRECT TO $\hbar^2$

In the WKB approximation, the transmission coefficient $T(E)$ is given by

$$T(E)=\{1+\exp[(8m)^{1/2}f(E)/\hbar]\}^{-1}, \tag{2.1}$$

where

$$f(E)=\int_{X_1}^{X_2}[U(X)-E]^{1/2}dX - \frac{1}{96}\left(\frac{\hbar^2}{2m}\right)\oint \frac{d^2U}{dX^2}dX\Big/[U(X)-E]^{3/2}. \tag{2.2}$$

X_1 and X_2 are the classical turning points. Equation (2.2) was used to calculate the transmission coefficients above and below the Eckart potential barrier.[5,6] Results showed that it is a fairly good approximation even for energies close to the height of the barrier.

To separate the zeroth- and first-order contributions, we define

$$f_0(E)=\int_{X_1}^{X_2}[U(X)-E]^{1/2}dX, \tag{2.3}$$

$$f_2(E)=-\frac{1}{96}\left(\frac{\hbar^2}{2m}\right)\oint\frac{d^2U}{dX^2}dX\Big/[U(X)-E]^{3/2} \tag{2.4a}$$

$$=-\frac{1}{48}\left(\frac{\hbar^2}{2m}\right)\frac{d}{dE}\oint U''dX/[U(X)-E]^{1/2}. \tag{2.4b}$$

The zeroth-order expression was derived by Cole and Good.[3] We shall not duplicate their efforts but quote their result [Eq. (2.2b) in Ref. 3] as follows:

$$X_2(E)-X_1(E)=-\frac{2}{\pi}\int_E^{U_{\max}}\frac{df}{dE'}\frac{dE'}{(E'-E)^{1/2}}. \tag{2.5}$$

For a symmetric potential, we can rewrite (2.5) as

$$\bar{X}_0(E)=-\frac{1}{\pi}\int_E^{U_{\max}}\frac{df}{dE'}\frac{dE'}{(E'-E)^{1/2}}, \tag{2.6}$$

where the subscript 0 shows explicitly that this formula is correct to zeroth order in $\hbar^2$.

Since $\bar{X}_0(E)=\bar{X}(E)+\hbar^2\bar{X}_2(E)$, we have the following higher-order expression:

$$\bar{X}_2(E)=-\frac{1}{\pi}\int_E^{U_{\max}}\frac{df_2(E')}{dE'}\frac{dE'}{(E'-E)^{1/2}}. \tag{2.7}$$

Integrating by parts, we can write Eq. (2.7) in the following form:

$$\bar{X}_2(E)=-\frac{1}{\pi}\frac{d}{dE}\int_E^{U_{\max}}\frac{f_2(E')dE'}{(E'-E)^{1/2}}. \tag{2.8}$$

Substitute (2.4b) into (2.8)

$$\bar{X}_2(E) = -\frac{1}{24\pi}\left(\frac{1}{2m}\right)\frac{d}{dE}\left\{\int_E^{U_{max}} \frac{d}{dE}(E'-E)^{1/2} \times\left(\frac{d}{dE'}\oint\frac{U''d\bar{X}}{(U-E')^{1/2}}\right)dE'\right\}$$
$$= -\frac{1}{24\pi}\left(\frac{1}{2m}\right)\frac{d^2}{dE^2}\left\{\int_E^{U_{max}}(E'-E)^{1/2} \times\left(\frac{d}{dE'}\oint\frac{U''d\bar{X}}{(U-E')^{1/2}}\right)dE'\right\}. \quad (2.9)$$

Integrating by parts, we obtain

$$\bar{X}_2(E) = -\frac{1}{12\pi}\left(\frac{1}{2m}\right)\frac{d^2}{dE^2}\int_E^{U_{max}}\frac{dE'}{(E'-E)^{1/2}} \times\int_{E'}^{U_{max}}\frac{U''}{(U-E')^{1/2}}\frac{d\bar{X}}{dU}dU. \quad (2.10)$$

Interchanging the integrations,

$$\bar{X}_2(E) = -\frac{1}{12\pi}\left(\frac{1}{2m}\right)\frac{d^2}{dE^2} \times\int_E^{U_{max}}U''\frac{d\bar{X}}{dU}dU\int_E^U\frac{dE'}{[(E'-E)(U-E')]^{1/2}}$$
$$=\frac{1}{12}\left(\frac{1}{2m}\right)\frac{d^2}{dE^2}\int_{U_{max}}^E U''\frac{d\bar{X}}{dU}dU. \quad (2.11)$$

Hence the correction is

$$\hbar^2\bar{X}_2(E) = -\frac{\hbar^2}{24m}\left(\frac{\bar{X}_0'''\bar{X}_0' - 2\bar{X}_0''^2}{\bar{X}_0'^3}\right), \quad (2.12)$$

where the prime is interpreted as d/dE. Equation (2.12) is similar to an expression derived by Vasilevsky and Zhirnov[2] for the inversion of phase shifts at a fixed angular momentum.

III. CONSTRUCTION OF THE QUARTIC POTENTIAL BARRIER $U(\bar{X}) = -\bar{X}^4$

In the following calculation, we choose $\hbar = 2m = 1$. The input to our inversion procedure is $f(E')$ which is approximated by Eq. (2.2). In terms of complete elliptic integrals of the first and second kind,[7,8]

$$f(E') = \frac{2\sqrt{2}}{3}F\left(\frac{\pi}{2},\frac{1}{\sqrt{2}}\right)|E'|^{3/4} - \frac{\sqrt{2}}{4}\frac{1}{|E'|^{3/4}}\left[E\left(\frac{\pi}{2},\frac{1}{\sqrt{2}}\right)-\tfrac{1}{2}F\left(\frac{\pi}{2},\frac{1}{\sqrt{2}}\right)\right], \quad (3.1)$$

where

TABLE I. $\bar{X}(E)$ for different energies E. (a) Exact value given by $|E|^{1/4}$. (b) WKB result correct to zeroth order in $\hbar^2$. (c) WKB result correct to first order in $\hbar^2$.

$\|E\|$	(a)	(b)	(c)
10	1.778 3	1.781	1.778 5
20	2.114 74	2.116	2.114 78
30	2.340 35	2.341	2.340 36
40	2.514 867	2.5154	2.514 872
50	2.659 148	2.6596	2.659 151
60	2.783 158	2.7835	2.783 159
70	2.892 508	2.8928	2.892 509
80	2.990 697 6	2.9910	2.990 698 3

$$F\left(\frac{\pi}{2},\frac{1}{\sqrt{2}}\right) = 1.854\,074\,677\,301\,372,$$
$$E\left(\frac{\pi}{2},\frac{1}{\sqrt{2}}\right) = 1.350\,643\,881\,047\,676.$$

The zeroth-order result is

$$\bar{X}_0(E) = -\frac{1}{\pi}\int_E^0\frac{df_0}{dE'}\frac{dE'}{(E'-E)^{1/2}} - \frac{1}{\pi}\frac{d}{dE}\int_E^0\frac{f_2(E')dE'}{(E'-E)^{1/2}}$$
$$=\frac{4}{\pi}F\left(\frac{\pi}{2},\frac{1}{\sqrt{2}}\right)|E|^{1/4}\left(1+\frac{1}{16|E|^{3/2}}\right) \times\left[E\left(\frac{\pi}{2},\frac{1}{\sqrt{2}}\right)-\tfrac{1}{2}F\left(\frac{\pi}{2}\,\frac{1}{\sqrt{2}}\right)\right]. \quad (3.2)$$

The higher-order correction $\bar{X}_2(E)$ is obtained by differentiating (3.2) as specified by Eq. (2.12). $(\bar{X}_0 - \bar{X}_2)$ gives us the final result which should be close to $E^{1/4}$, the exact value. The numerical results are shown in Table I. Our approximation works fine when E is large since the WKB method is essentially semiclassical. It fails, however, when E is close to the top of the barrier. We should expect that our correction is not good for small E because Eq. (3.1) is essentially an asymptotic expansion.

In more realistic applications, the correction term is necessary only if the experimental data are relatively noise-free so that numerical differentiation is feasible.

ACKNOWLEDGMENT

One of us (P.L.) wants to acknowledge the financial assistance received from the Provost's Research Fund of Arizona State University. He also wishes here to express his appreciation to Professor A. P. Wang and Professor C. Y. Wang for their kind comments.

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