Matching of WKB solutions to other solutions

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We comment on a perturbation procedure for the Schrödinger equation which permits the derivation of several similarly constructed pairs of solutions. In particular we establish the matching of these solutions to the WKB solutions, and we point out their usefulness, e.g., in deriving the eigenvalue gaps characteristic of symmetric potentials.

I. INTRODUCTION

Recently we have formulated[1] and tested[2] a perturbation procedure for solving wave equations which has certain advantages over such customary methods of approximation as the WKB method. In particular we have shown that two *similarly constructed* pairs of solutions can be derived (belonging to one and the same eigenvalue in the discrete sector of the spectrum), and that these solutions can be matched in regions of common validity.

A point that we did not elaborate on previously which, however, is vital for the specification of the solutions over the entire domain of the variable is the relation of our type of solutions[1,2] to the well-known WKB solutions[3,4] as well as their matching across Stokes discontinuities.[3] A further point which we did not discuss in Ref. 1 is the asymptotic degeneracy of eigenvalues resulting from the symmetry of a potential. It is these points we wish to comment on in this addendum to Refs. 1 and 2; in particular we wish to stress the importance and usefulness of our WKB-type solutions in linking the solutions in the neighborhood of an extremum to those in the neighborhood of a turning point.

This investigation was motivated by the recent upsurge of interest in the double-well potential and its significance in relation to instanton phenomena.[5-8] However, for ease of presentation we discuss our points here for the important and equally ubiquitous case of a periodic potential, i.e., the Mathieu equation, which in view of the existing literature[9,10] obviates the need for a detailed derivation of solutions. The method is, of course, much more general.

II. OSCILLATOR-LIKE, WKB-TYPE, AND WKB SOLUTIONS AND THEIR MATCHING

We consider the equation

$$\psi'' - f(x)\psi = 0, \quad f(x) \equiv V(x) - E\,, \qquad V(x) = 2h^2\cos 2x\,. \tag{1}$$

It follows from the symmetry of the equation that if $\psi(x;h)$ is a solution, the following functions are also solutions:

$$\psi(x \pm n\pi; \pm h), \quad \psi(-x \pm n\pi; \pm h), \tag{2a}$$

$$\psi\left(x + \frac{\pi}{2}; \pm ih\right), \quad \psi\left(x - \frac{\pi}{2}; \pm ih\right), \tag{2b}$$

where n is an integer. It suffices to consider the domain $-\pi/2 \leq x \leq \pi/2$; in other domains the solutions simply repeat themselves in view of the periodicity of the potential (there are solutions of periods π and 2π).

The eigenvalues E associated with solutions around a minimum of $V(x)$ are given by[9]

$$E = -2h^2 + 2hq + \tfrac{1}{8}\Delta\left(q, \frac{1}{h}\right), \tag{3}$$

where q is approximately (see below) an odd integer, and Δ is a known function of q and $1/h$. It is important to distinguish between the domains around $x = -\pi/2$ and $x = +\pi/2$. The solution around $+\pi/2$ is[9]

$$\psi_B(x, q, h) = e^{2h\sin x} \sum_{i=0}^{\infty} \frac{1}{(2^7 h)^i} \sum_{\substack{j=-i \\ j\neq 0}}^{i} P_i(q, q+4j) B_q(z(x)), \tag{4}$$

where

$$B_q(z(x)) = \frac{H_{(q-1)/2}(z)}{2^{(q-1)/4}[\frac{1}{4}(q-1)]!},$$

$$z(x) = 4h^{1/2}\cos(\tfrac{1}{2}x + \tfrac{1}{4}\pi),$$

and

$$|z(x)| \ll h^{1/2}, \quad \text{i.e., } x \simeq \pi/2\,.$$

Here H is a Hermite function and P are known coefficients which are independent of h. The solution is valid around $x = \pi/2$. The corresponding solution $\psi_C(x, q, h)$ valid for $|x(-x)| \ll h^{1/2}$, i.e., around $x = -\pi/2$, is obtained[9] by replacing B_q by C_q with

$$C_q(z(-x)) = 2^{(q+1)/4}[\tfrac{1}{4}(q-3)]!\,H^*_{-(q+1)/2}(z) \tag{5}$$

and $H_m^*(z) = (-i)^m H_m(iz)$.

In each of these two cases an associated solution $\bar{\psi}$ is obtained by changing throughout the sign of x. These associated solutions $\bar{\psi}_B$ and $\bar{\psi}_C$ are valid around $x = \mp\pi/2$, respectively (see Fig. 1). Thus, e.g., the general solution around $x = +\pi/2$ is (with constants α, β)

$$\psi(x,q,h) = \alpha\psi_B + \beta\bar{\psi}_C . \tag{6}$$

The solutions around a maximum of $V(x)$ are obtained by transforming the solutions (2a) to (2b) (then the factors $e^{\pm 2h\sin x}$ become $e^{\pm 2ih\cos x}$). There, of course, q is no longer (approximately) an odd integer; rather, it is a parameter determined by Eq. (3). Thus, a solution valid around $x = 0$ is $\psi_B(x - \pi/2, q, ih)$ and the associated solution is $\bar{\psi}_C(x - \pi/2, q, ih)$. We dub all these solutions which involve Hermite functions "oscillator-like."

In the region above the minimum of the potential but far below the turning point a solution $\psi(x,q,h)$ is[9]

$$\psi_A(x,q,h) = e^{2h\sin x} \sum_{i=0}^{\infty} \frac{1}{(2^7 h)^i} \sum_{\substack{j=-i \\ j\neq 0}}^{i} P_i(q, q+4j) A_q(x) , \tag{7}$$

where

$$A_q(x) = \frac{\cos^{(q-1)/2}(\frac{1}{2}x + \frac{1}{4}\pi)}{\sin^{(q+1)/2}(\frac{1}{2}x + \frac{1}{4}\pi)} = \frac{2^{1/2}}{(\cos x)^{1/2}} \exp\left(-\frac{q}{2}\int \frac{dx}{\cos x}\right)$$

and the coefficients P_i are the same as in (4). The associated solution $\bar{\psi}_A$ is obtained by changing throughout the sign of x. Both solutions are valid where

$$|\cos(\tfrac{1}{4}\pi \pm \tfrac{1}{2}x)| \gg \frac{1}{h^{1/2}} .$$

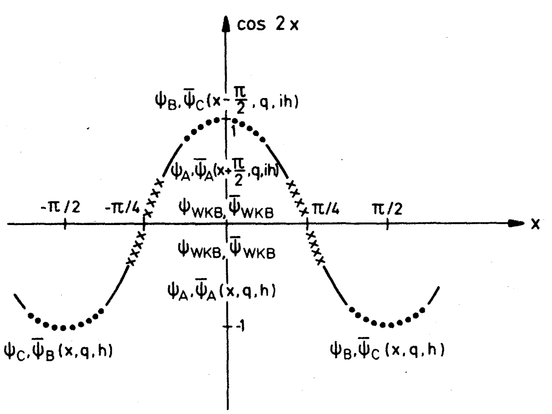

FIG. 1. The periodic potential cos $2x$. The domains of the various solutions are indicated by dots, continuous lines, and crosses.

The corresponding solutions below a maximum of $V(x)$ but above a turning point are again obtained by transforming the solutions (2a) to 2(b), etc., as explained above. We dub the solutions of type (7) "WKB-type." Finally, we note that the solutions ψ_A^* and $\bar{\psi}_A$ can easily be matched to the solutions ψ_B and $\bar{\psi}_C$ in their common region of validity by using the asymptotic expansion of $H_{(q-1)/2}(z)$. Thus, in these regions[9]

$$\psi_B(x,q,h) = \alpha(q,h)\psi_A(x,q,h) ,$$

$$\alpha(q,h) = \frac{(8h)^{(q-1)/4}}{[\frac{1}{4}(q-1)]!}\left[1 + O\left(\frac{1}{h}\right)\right] ,$$

and (8)

$$\bar{\psi}_C(x,q,h) = \bar{\alpha}(q,h)\bar{\psi}_A(x,q,h) ,$$

$$\bar{\alpha}(q,h) = \frac{[\frac{1}{4}(q-3)]!}{(8h)^{(q+1)/4}}\left[1 + O\left(\frac{1}{h}\right)\right] .$$

In the region above the minimum of the potential but just below the turning point a solution $\psi(x,q,h)$ is

$$\psi_{\text{WKB}}(x,q,h) = \frac{1}{f^{1/4}} \exp\left(\int^x f^{1/2}dx\right) Y(x,q,h) , \tag{9}$$

where Y satisfies an equation which has been given and solved by Dingle.[11] Since

$$f = V - E = 4h^2\cos^2 x - 2hq - \cdots ,$$

we have (for x close to $\pm\pi/4$)

$$f^{1/4} \simeq (2h\cos x)^{1/2}$$

and (10)

$$\int f^{1/2}dx \simeq 2h\sin x - \frac{q}{2}\int \frac{dx}{\cos x} .$$

Thus, on expanding $f^{1/2}$ in the domain just below $x = \pm\pi/4$ (i.e., where $\cos x \neq 0$), we recover the solution (7). This shows that the solution ψ_{WKB} joins smoothly on to the solution (7), i.e., in their common domain

$$\psi_A(x,q,h) = 2h^{1/2}\left[1 + O\left(\frac{1}{h}\right)\right]\psi_{\text{WKB}}(x,q,h) . \tag{11}$$

Again an associated solution $\bar{\psi}_{\text{WKB}}$ is obtained by changing throughout the sign of x. The corresponding solutions on the other side of the turning point, i.e., far below a maximum of $V(x)$, are again obtained as before. It should be observed that the solution (7) is singular at the nearest extremum point. In effect the expansion (7) shifts the turning point to the extremum thereby hiding it in the solution (7).

The matching of the WKB-type solutions (7) in the domain below a turning point to the appropriate

WKB-type solutions above the turning point is now seen to be achieved by matching the WKB solutions in the usual way and then matching these to our WKB-type solutions. The WKB matching relation for the leading terms is[12]

$$\frac{1}{f^{1/4}}\exp\left(\pm\int^{x} f^{1/2}dx\right)\longrightarrow\begin{pmatrix}1\\2\end{pmatrix}\frac{1}{(-f)^{1/4}}\times\begin{pmatrix}\cos\\\sin\end{pmatrix}\left[\int^{x}(-f)^{1/2}dx+\tfrac{1}{4}\pi\right],$$

i.e.,

$$\psi_{\rm WKB}(x,q,h)\longrightarrow\tfrac{1}{2}[\psi_{\rm WKB}(x,q,h)+i\bar{\psi}_{\rm WKB}(x,q,h)]\,. \quad (12)$$

In the domain above the turning point (i.e., on the oscillatory side) each of the solutions $\psi_{\rm WKB}$ on the right-hand side of this relation is to be continued to solutions ψ_A and $\bar{\psi}_A$ as discussed previously. These solutions would now, however, be expanded with respect to the nearest maximum of the potential. Equation (3) then becomes an equation from which the (nonintegral) parameter q is to be determined. This then completes the continuation of the solutions into any domain. The domains of the various solutions are indicated in Fig. 1.

III. THE PARAMETER q AND THE ASYMPTOTIC DEGENERACY OF EIGENVALUES

In the range under consideration our potential has two symmetric wells. This has the consequence that the actual eigenstates must be even or odd about the axis passing through the central maximum; moreover, the degeneracy is split by the perturbation so that the symmetric state lies slightly below the antisymmetric one. This splitting has been calculated previously[9] and has been treated rigorously by Harrell[6,7] recently. We have nothing new to add here except that the above reasoning would be incomplete without a specification of the parameter q. The even and odd Mathieu functions $\psi_\pm$ are most conveniently defined in terms of ψ_A and $\bar{\psi}_A$; thus (apart from an overall constant)

$$\psi_\pm=\psi_A(x,q,h)\pm\bar{\psi}_A(x,q,h) \quad (13)$$

for

$$|\cos(\tfrac{1}{4}\pi\pm\tfrac{1}{2}x)|\gg\frac{1}{h^{1/2}}\,.$$

There are two types of functions—those of period 2π and those of period π—and the functions of integral order are defined by equating to zero the following particular values[9,10]:

$$\psi_+(x=\tfrac{1}{2}\pi)=0,\quad \frac{\partial\psi_-}{\partial x}(x=\tfrac{1}{2}\pi)=0\,,$$

$$\psi_-(x=\tfrac{1}{2}\pi)=0,\quad \frac{\partial\psi_+}{\partial x}(x=\tfrac{1}{2}\pi)=0\,.$$

Inserting in $\psi_\pm$ the continuations of ψ_A and $\bar{\psi}_A$ into the domain of $x=\frac{1}{2}\pi$ [i.e., $\psi_A=(1/\alpha)\psi_B$, etc.] and solving the resulting equations for q near an odd integer q_0, one obtains[9] (for $\psi_\pm$, respectively)

$$q=q_0\mp O(h^{q_0/2}e^{-4h})\,.$$

Then

$$E\equiv E(q)\simeq E(q_0)+\left(\frac{\partial E}{\partial q}\right)_{q_0}(q-q_0)$$

shows that the state corresponding to the symmetric solution has a lower energy than the state corresponding to the antisymmetric solution. This, therefore, determines q and the splitting of the eigenvalue degeneracy.

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