Simple calculation of the level splitting for the double-well potential

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It is shown that for the double-well potential three similarly constructed pairs of solutions of the Schrödinger equation can be derived which are such that they can be linked in regions of common validity. Evaluating the boundary conditions satisfied by the even and odd wave functions at a minimum, several analogous transcendental equations are obtained from which the splitting of (asymptotically degenerate) eigenvalues can be deduced.

I. INTRODUCTION

The nonrelativistic treatment of the double-well potential has attracted considerable interest in recent years in view of its adaptability as a model for illustrating some deep and nontrivial physical phenomena which play a significant role in field-theoretic or other considerations. Some of these phenomena are symmetry breaking as a result of degenerate vacuums, semiclassical tunnelings between these vacuums, which are generally treated under the name of instantons,[1] and the existence of long-range order in statistical systems related to the critical behavior at a phase transition.[2] The nonrelativistic treatment of the double-well potential has recently also been the subject of rigorous mathematical investigations.[3,4]

One aspect of the double-well potential which is generally not particularly easy to deal with is the explicit calculation of the splitting of the asymptotically degenerate energy levels. The root of this difficulty is that this splitting is exponentially small, representing effectively a large-distance effect, and thus can be obtained by perturbation theory at best indirectly.

In the following we develop a straightforward method for estimating the splitting of asymptotically degenerate energy levels. The method is formulated along the pattern of a previous investigation[5] of the Mathieu equation. The present case, however, does not possess the exceptional simplicity of the corresponding considerations of the Mathieu equation. In particular we demonstrate that three pairs of eigensolutions of the Schrödinger equation can be derived which all belong to one and the same expansion of the eigenvalue. The solutions can be linked in regions where they overlap and the physically relevant even and odd solutions can be constructed. By continuing the latter to the domain of a minimum of the potential and applying the appropriate boundary conditions, certain transcendental equations are obtained from which the splitting can be deduced.

The level splitting for the double-well potential has also been considered by Damburg and Propin.[6] Compared with our approach their procedure is much less systematic, and, in particular, since they do not employ the nonintegral parameter q that we are using (which turns out to be a particularly convenient quantity to use here) their calculations are cumbersome.

II. THE FIRST PAIR OF SOLUTIONS

We consider the equation

$$\psi''+[\lambda-V(x)]\psi=0 \tag{1}$$

for

$$V(x)=-ax^2(b-x)(b+x)\ , \tag{2}$$

where $a,b>0$. The minima of $V(x)$ are located at $x\equiv x_0=\pm b/2^{1/2}$. The approximate behavior of the eigenvalues λ can be estimated by expanding $V(x)$ around x_0. The potential is then approximately harmonic and we obtain

$$\lambda\simeq V(x_0)+\tfrac{1}{2}qh^2\ ,$$

where $h=[2V^{(2)}(x_0)]^{1/4}$, and q is approximately an odd integer (i.e., not exactly because of the finite height of the central hump of the potential or the finiteness of x_0). We write

$$\lambda=V(x_0)+\tfrac{1}{2}qh^2+\Delta\ , \tag{3}$$

where Δ is a remainder to be determined by perturbation theory.

Inserting (3) into (1) and setting

$$z(x)=[V(x)-V(x_0)]^{1/2} \tag{4}$$

we obtain

$$\psi''+[\tfrac{1}{2}qh^2+\Delta-z^2(x)]\psi=0 \ . \tag{5}$$

Setting

$$\psi(x)=\phi(x)\exp\left[\pm\int^x z(x)dx\right] \tag{6}$$

we find that ϕ satisfies

$$\phi''\pm 2z(x)\phi'+[\tfrac{1}{2}qh^2+\Delta\pm z'(x)]\phi=0 \ . \tag{7}$$

We observe that one of the solutions (6) can be obtained from the other by changing the sign of x throughout. It is therefore sufficient to consider only the upper of equations (7). Since

$$z(x)=\tfrac{1}{2}h^2(x-x_0)+O((x-x_0)^2)$$

in approaching x_0, we have

$$\mathscr{D}_q^{(1)}(x)\phi(x)=O\left[\frac{1}{h}\right] , \tag{8}$$

where

$$\mathscr{D}_q^{(1)}=-\frac{4z(x)}{h^2}\frac{d}{dx}-q-\frac{2z'(x)}{h^2} \ . \tag{9}$$

The solution A_q of $\mathscr{D}_q^{(1)}A_q=0$ is (apart from an overall constant)

$$A_q(x)=\frac{1}{z(x)^{1/2}}\exp\left[-\tfrac{1}{4}qh^2\int^x\frac{dx}{z(x)}\right] \ . \tag{10}$$

The higher-order contributions to the solution and its appropriate eigenvalue (this is given in Ref. 7) can be obtained in our standard way[8] by using the relation $\mathscr{D}_q^{(1)}A_{q+j}=jA_{q+j}$. We do not go into further details here. We thus obtain the solutions

$$\begin{aligned}\psi_A(x)&=A(x)\exp\left[+\int^x z(x)dx\right] ,\\ \bar\psi_A(x)&=\bar A(x)\exp\left[-\int^x z(x)dx\right] ,\end{aligned} \tag{11}$$

where $A(x)=A_q(x)+O(1/h)$ and $\bar A(x)=A(-x)$. These solutions are valid in the domains

$$|x\mp x_0|>O(1/h) ,$$

which clearly exclude the neighborhoods of $\pm x_0$ and ensure that in (7) $|\phi''|<<|2z(x)\phi'|$ as in the well-known WKB procedure. Of course, $z(x)\simeq\frac{1}{2}h^2(x\mp x_0)+O((x\mp x_0)^2)$ only at the lower boundaries of these domains.

III. THE SECOND AND THIRD PAIRS OF SOLUTIONS

We now derive two further pairs of solutions; these involve Hermite functions, and are valid around the minima of the potential.

In the first of the two equations (7) we change the independent variable to $z(x)$. The equation then becomes

$$\frac{1}{4}\left[\frac{V'(x)}{z}\right]^2\frac{d^2\phi}{dz^2}+\left[V'(x)+\frac{V''(x)}{2z}-\frac{(V'(x))^2}{4z^3}\right]\frac{d\phi}{dz}+\left[\tfrac{1}{2}qh^2+\Delta+\frac{V'(x)}{2z}\right]\phi=0 \ . \tag{12}$$

Next we change the variable to

$$w(x)=\frac{2}{h}z(x) \ . \tag{13}$$

Then near x_0 where $w=h(x-x_0)+O((x-x_0)^2)$ Eq. (12) becomes

$$\mathscr{D}_q^{(2)}(w)\phi(w)=O\left[\frac{1}{h}\right] , \tag{14}$$

where

$$\mathscr{D}_q^{(2)}=-2\frac{d^2}{dw^2}-2w\frac{d}{dw}-(q+1) \ . \tag{15}$$

The solution B_q of $\mathscr{D}_q^{(2)}B_q=0$ is (apart from an overall constant)

$$\begin{aligned}B_q(w(x))=&\,2^{(q+1)/4}\Gamma(\tfrac{1}{4}(q+1))\\ &\times H^*_{-(q+1)/2}(w) ,\end{aligned} \tag{16}$$

where $H_m^*(w)=(-i)^mH_m(iw)$ is essentially a Hermite function of an imaginary variable, and the other factors have been inserted for convenience. Again the higher-order contributions to the solution ϕ and its appropriate eigenvalue can be obtained in our standard way by using the recurrence relation of Hermite functions and the relation $\mathscr{D}_q^{(2)}B_{q+j}=jB_{q+j}$. We thus obtain the solution

$$\psi_B(w(x))=B(w(x))\exp\left[+\int^x z(x)dx\right], \quad (17)$$

where

$$B(w(x))=B_q(w(x))+O\left[\frac{1}{h}\right]$$

is valid for $|x-x_0|<O(1/h)$. We also obtain an associated solution $\bar{\psi}_B$ by changing the sign of x throughout. Thus

$$\bar{\psi}_B(w(x))=\bar{B}(w(x))\exp\left[-\int^x z(x)dx\right], \quad (18)$$

where $\bar{B}(w(x))=B(w(-x))$ is valid for

$$|x+x_0|<O\left[\frac{1}{h}\right].$$

We can find another solution of (12) by changing the independent variable to

$$w(-x)=\frac{2}{h}z(-x). \quad (19)$$

Then $\mathscr{D}_q^{(2)}$ is replaced by

$$\mathscr{D}_q^{(3)}=-2\frac{d^2}{dw^2}+2w\frac{d}{dw}-(q-1) \quad (20)$$

and the solution of $\mathscr{D}_q^{(3)}C_q=0$ is

$$C_q(w(-x))=\frac{H_{(q-1)/2}(w)}{2^{(q-1)/4}\Gamma(\frac{1}{4}(q+3))}. \quad (21)$$

Proceeding as before we arrive at the solution

$$\psi_C(w(-x))=C(w(-x))\exp\left[+\int^x z(x)dx\right], \quad (22)$$

where

$$C(w(-x))=C_q(w(-x))+O\left[\frac{1}{h}\right]$$

valid for

$$|x+x_0|<O\left[\frac{1}{h}\right],$$

and the associated solution

$$\bar{\psi}_C(w(+x))=\bar{C}(w(+x))\times\exp\left[-\int^x z(x)dx\right], \quad (23)$$

where $\bar{C}(w(+x))=C(w(-x))$ valid for

$$|x-x_0|<O\left[\frac{1}{h}\right].$$

The two pairs of solutions defined above, one for the neighborhood of each minimum of the potential, have been constructed from the standard solution of Hermite's equation and its linearly independent partner. The coefficients inserted in (16) and (21) are such that B_q and C_q satisfy the same recurrence relation.

IV. LINKAGE OF THE SOLUTIONS

We now demonstrate the matching of our solutions in domains where they overlap.

Expanding $\psi_A(x)$ and $\bar{\psi}_A(x)$ close to x_0, we obtain

$$\psi_A(x)\simeq\left[\frac{2}{h^2}\right]^{1/2}\frac{\exp[\frac{1}{4}h^2(x-x_0)^2]}{(x-x_0)^{(q+1)/2}}e^{-h^2x_0^2/4}, \quad (24)$$

$$\bar{\psi}_A(x)\simeq\left[\frac{2}{h^2}\right]^{1/2}(x-x_0)^{(q-1)/2}\exp[-\tfrac{1}{4}h^2(x-x_0)^2]e^{+h^2x_0^2/4}. \quad (25)$$

Expanding $\psi_B(w(x))$ and $\bar{\psi}_C(w(-x))$ around x_0 and using the asymptotic relations

$$B_q(w)=\frac{2^{(q+1)/4}\Gamma(\frac{1}{4}(q+1))}{w^{(q+1)/2}}\left[1+O\left[\frac{1}{w^2}\right]\right],$$

$$\bar{C}_q(w)=\frac{w^{(q-1)/2}}{2^{(q-1)/4}\Gamma(\frac{1}{4}(q+3))}\left[1+O\left[\frac{1}{w^2}\right]\right], \quad (26)$$

we obtain

$$\psi_B(w(x))\simeq\frac{2^{(q+1)/4}\Gamma(\frac{1}{4}(q+1))}{(h(x-x_0))^{(q+1)/2}}e^{-h^2x_0^2/4}\exp[\tfrac{1}{4}h^2(x-x_0)^2]\,,$$
$$\bar\psi_C(w(x))\simeq\frac{(h(x-x_0))^{(q-1)/2}}{2^{(q-1)/4}\Gamma(\frac{1}{4}(q+3))}e^{h^2x_0^2/4}\exp[-\tfrac{1}{4}h^2(x-x_0)^2]\,. \tag{27}$$

Thus in their common domains of validity

$$\psi_A=\gamma\psi_B \text{ or } A=\gamma B \tag{28}$$

and

$$\bar\psi_A=\bar\gamma\bar\psi_C \text{ or } \bar A=\bar\gamma\bar C \tag{29}$$

with

$$\gamma\simeq\frac{h^{(q-1)/2}}{2^{(q-1)/4}\Gamma(\frac{1}{4}(q+1))}\left[1+O\left[\frac{1}{h}\right]\right] \tag{30}$$

and

$$\bar\gamma\simeq\frac{2^{(q+1)/4}\Gamma(\frac{1}{4}(q+3))}{h^{(q+1)/2}}\left[1+O\left[\frac{1}{h}\right]\right]. \tag{31}$$

V. THE SPLITTING OF EIGENVALUES

The even and odd solutions $\psi_\pm(x)$ are most easily defined in terms of solutions which are pure functions of x. Thus we write

$$\psi_\pm(x)=A(x)\exp\left[+\int^x z(x)dx\right]\pm\bar A(x)\exp\left[-\int^x z(x)dx\right]$$
$$=\gamma B(w(x))\exp\left[+\int^x z(x)dx\right]\pm\bar\gamma\bar C(w(x))\exp\left[-\int^x z(x)dx\right] \tag{32}$$

on using (28)—(31). The latter of expressions (32) represents the continuation of the defining expression into the region of $x=x_0$. We now require the solutions $\psi_\pm$ to satisfy the boundary conditions

$$\psi_-(x_0)=0,\quad \left[\frac{\partial\psi_+}{\partial x}\right]_{x_0}=0\,,\quad \left[\frac{\partial\psi_-(x)}{\partial x}\right]_{x_0}=-1,\quad \psi_+(x_0)=+1\,. \tag{33}$$

These conditions are such that the Wronskian of ψ_-,ψ_+ is $+1$.

To leading order in h the first two conditions imply

$$\frac{\gamma B_q(0)}{\bar\gamma\bar C_q(0)}\simeq e^{h^2x_0^2/2} \tag{34}$$

and

$$\left[\frac{\gamma\frac{d}{dw}B_q(w)}{\bar\gamma\frac{d}{dw}\bar C_q(w)}\right]_0\simeq -e^{h^2x_0^2/2}\,. \tag{35}$$

Inserting the expressions[5]

$$B_q(0)=-\frac{\pi^{1/2}\Gamma(\frac{1}{4}(q+1))\sin(\frac{1}{4}\pi(q-1))}{\Gamma(\frac{1}{4}(q+3))},\quad \bar C_q(0)=\frac{\pi^{1/2}}{\Gamma(\frac{1}{4}(q+3))\Gamma(-\frac{1}{4}(q-3))} \tag{36}$$

and

$$R\left[\frac{\partial B_q}{\partial w}\right]_0=(2\pi)^{1/2}\cos(\tfrac{1}{4}\pi(q-1)),\quad \left[\frac{\partial\bar C_q}{\partial w}\right]_0=-\frac{(2\pi)^{1/2}}{\Gamma(\frac{1}{4}(q+3))\Gamma(-\frac{1}{4}(q-1))} \tag{37}$$

(R meaning "real part of"), we arrive at the expressions

$$\left.\begin{matrix}\tan[(\pi/4)(q+1)]\\ \cot[(\pi/4)(q+1)]\end{matrix}\right\}\simeq\left[\frac{\pi}{2}\right]^{1/2}\frac{h^{q}e^{-h^2x_0^2/2}}{\Gamma(\frac{1}{2}(q+1))}\,, \tag{38}$$

where tan applies in the case of ψ_- and cot in the case of ψ_+. Expanding the tangent about $q_0=3, 7, 11, \ldots$ and the cotangent about $q_0=1, 5, 9, \ldots$ and retaining only the first nonvanishing term we obtain

$$q-q_0\simeq\pm 2\left[\frac{2}{\pi}\right]^{1/2}\frac{h^{q_0}e^{-h^2x_0^2/2}}{\Gamma(\frac{1}{2}(q_0+1))}\,, \tag{39}$$

the upper sign referring to ψ_- with $q_0=3, 7, 11, \ldots$ and the lower sign to ψ_+ with $q_0=1, 5, 9, \ldots$. Repeating these calculations for the last two of the boundary conditions (33), we again arrive at (39), this time, however, with $q_0=1, 5, 9, \ldots$ for ψ_- and $q_0=3, 7, 11, \ldots$ for ψ_+. Moreover, an additional term arising from ± 1 on the right-hand side of the last two conditions (33) and having a lower power of h is neglected. Thus, the result (39) holds for all values of q_0, the upper sign referring to ψ_-, and the lower to ψ_+.

In order to obtain the corresponding energy eigenvalues we expand $\lambda(q)$ of Eq. (3) in the neighborhood of q_0. Then

$$\lambda(q)\simeq\lambda(q_0)+(q-q_0)\left[\frac{\partial\lambda}{\partial q}\right]_{q_0}. \tag{40}$$

From the eigenvalue expansion (3) it can be seen that $(\partial\lambda/\partial q)_{q_0}$ is positive. Hence for any q_0 the level of the symmetric state lies below that of the antisymmetric state, the splitting being to leading order in h:

$$4\left[\frac{2}{\pi}\right]^{1/2}\frac{h^{q_0}e^{-h^2x_0^2/2}}{\Gamma(\frac{1}{2}(q_0+1))}\left[\frac{\partial\lambda}{\partial q}\right]_{q_0}.$$

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