Once again: Instanton method vs. WKB

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Abstract

A recent analytic test of the instanton method performed by comparing the exact spectrum of the Lamé potential (derived from representations of a finite dimensional matrix expressed in terms of $su(2)$ generators) with the results of the tight–binding and instanton approximations as well as the standard WKB approximation is commented upon. It is pointed out that in the case of the Lamé potential as well as others the WKB–related method of matched asymptotic expansions yields the exact instanton result as a result of boundary conditions imposed on wave functions which are matched in domains of overlap.

1 Introduction

We comment on ref.[1]. Ever since the instanton method of evaluating path integrals became popular, the question was raised as to whether this method and that of the Schrödinger equation lead to identical results in the dominant approximation. In view of the significance of both methods this is an important question. Generally one would argue that in the 1–loop approximation of the path integral the results of both methods should agree – and, in fact, this is the widely accepted opinion. However, there are few models which allow explicit verification, and some detailed investigations of even these are not well known. Thus recently in a study of Lamé instantons [1],

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a parallel consideration of the standard WKB method (i.e. that with linear connection relations) was found to lead to a result which is off by an overall factor of $\sqrt{e/\pi}$ – very similar to an observation made long ago in ref.[2] in the case of the well known double well potential. In the following we point out that in both cases, the WKB method employed is too simple, and complete agreement between the result of the path integral method and that of the Schrödinger equation in all the examples referred to can be achieved with the method of matched asymptotic expansions *.

The best known examples for such considerations are the scalar theory with the double well potential and the sine–Gordon theory of the periodic potential. The case considered in ref.[1] with the Lam*é* potential is not so well known but has recently found widespread consideration in various contexts, such as supersymmetric quantum mechanics [5] and spin tunneling (cf. e.g. [6]), and includes in a particular limit the sine-Gordon case. In the following we sketch the main points of the method and recall the level splitting calculated long ago for the Lam*é* (and more generally ellipsoidal) wave equation [7] even for an arbitrary excited state, and consider limits and special cases to demonstrate the agreement with the result of the instanton method, or more generally the path integral method, in particular that of the ground state case of ref.[1]. For details of the calculations we refer to the literature, where many details are given.

2 The Lam*é* level splitting and consequences

The Lam*é* equation [8]

$$y'' + \Big\{\Lambda - \kappa^2 sn^2 u\Big\} y = 0, \quad \kappa^2 = n(n+1)k^2, \tag{1}$$

with elliptic modulus $|k| < 1$ and $n > -1/2, 0 < u < 2\mathcal{K}$, can be looked at as a Schrödinger equation with periodic potential $\kappa^2 sn^2 u$, where snu is

*The source of the discrepancy can be traced to a mismatch between the normalization of the WKB wave functions and the harmonic oscillator wave functions, as explained in ref. [3], and also commented on in ref. [4]. We thank the referee for pointing this out. Our solutions involving the function $B[z(u)]$ in terms of Hermite functions correspond to the harmonic oscillator wave functions of ref. [3]. Matching WKB- or WKB-like functions (like our functions involving $A(u)$) to these therefore avoids the mismatch one of the Jacobian elliptic functions with period $2\mathcal{K}$, and $\mathcal{K}$ is one of the complete elliptic integrals. (In the comparison with the Schrödinger equation, the usual factor $-\hbar^2/2m$ in front of the second derivative has to be kept in mind, where m is the mass).

We recapitulate briefly the main steps in the method of matched asymptotic expansions (of wave functions) as applied to the periodic Lamé equation (1) (for the simplest application of the method see ref. [9]). The first step is to write the eigenvalue Λ as

$$\Lambda(q,\kappa) := q\kappa + \frac{\triangle(q,\kappa)}{8}, \tag{2}$$

where $q \to q_0 = 2N+1, N = 0,1,2,\cdots$ in the case of $\kappa \to \infty$, i.e. very high potential barriers (i.e. harmonic oscillator approximation around a minimum of the potential). For barriers of finite height the parameter q is only approximately an odd integer q_0 in view of tunneling effects. The difference $q - q_0$ is obtained by imposing boundary conditions at extrema of the potential (see below). The second step is to insert (2) into the equation, i.e. (1), and to write

$$\begin{aligned} y &= A(u)exp\Big\{-\int \kappa snu du\Big\} \\ &= A(u)[f(u)]^{\kappa/2k} \end{aligned} \tag{3}$$

where

$$f(u) = \Big(\frac{dnu + kcnu}{dnu - kcnu}\Big).$$

For large κ the equation for $A(u)$ can be solved iteratively resulting in an asymptotic expansion for $A(u)$ and concurrently one for the remainder in eq. (2), i.e. $\triangle$. A second solution is written

$$y = \bar{A}(u)exp\Big\{+\int \kappa snu du\Big\}. \tag{4}$$

The very useful property of these solutions is that for the same value of $\triangle$ (which remains unchanged under the combined replacements $q \to -q, \kappa \to -\kappa$)

$$\begin{aligned} \bar{A}(u) &= A(u + 2\mathcal{K}), \\ \bar{A}(u,q,\kappa) &= A(u,-q,-\kappa). \end{aligned} \tag{5}$$

The domain of validity of these solutions is that away from an extremum of the potential, more precisely for

$$\left|\frac{dnu \mp cnu}{dnu \pm cnu}\right| >> \frac{1}{\kappa}.$$

Thus one can construct solutions $Ec(u), Es(u)$, which are respectively even in u (or snu) or odd, i.e.

$$\begin{matrix} Ec(u) \\ Es(u) \end{matrix} \propto A(u)[f(u)]^{\kappa/2k} \pm \bar{A}(u)[f(u)]^{-\kappa/2k} \tag{6}$$

Since these expansions are not valid at the extrema of the potential (where the boundary conditions are to be imposed), one has to derive new sets of solutions there and match these to the former (i.e. determine their proportionality factors) in domains of overlap (their extreme regions of validity).

Thus in the third step two more pairs of solutions $B, \bar{B}$ and $C, \bar{C}$ replacing $A, \bar{A}$ are derived, one pair in terms of Hermite functions of a real variable, the other in terms of those of an imaginary variable, by transforming the equations for $A, \bar{A}$ into equations in terms of

$$z(u) = \frac{\sqrt{8\kappa}}{k'}\left(\frac{dnu \mp cnu}{dnu \pm cnu}\right)^{1/2}, \quad k' = \sqrt{1-k^2}. \tag{7}$$

Solving the resulting equations iteratively as before, one obtains again the same expansion for Λ, but solutions B, C replacing A, which are valid for

$$\left|\frac{dnu \pm cnu}{dnu \mp cnu}\right| << 1.$$

In their regions of overlap one can determine the proportionality factors $\alpha, \bar{\alpha}$ of

$$B = \alpha A, \quad \bar{C} = \bar{\alpha}\bar{A} \tag{8}$$

(again in the form of asymptotic expansions). Then

$$\begin{matrix} Ec(u) \\ Es(u) \end{matrix} \propto \frac{B[z(u)]}{\alpha}[f(u)]^{\kappa/2k} \pm \frac{\bar{C}[z(u)]}{\bar{\alpha}}[f(u)]^{-\kappa/2k} \tag{9}$$

In the fourth and final step one now applies the appropriate boundary conditions (cf. ref.[8]) on these solutions (9), i.e. one sets

$$\begin{aligned}
Ec(u=2\mathcal{K}) &= Ec(u=0)=0, \\
Es(u=2\mathcal{K}) &= Es(u=0)=0, \\
\left(\frac{\partial Ec}{\partial u}\right)_{u=2\mathcal{K}} &= \left(\frac{\partial Ec}{\partial u}\right)_{u=0}=0, \\
\left(\frac{\partial Es}{\partial u}\right)_{u=2\mathcal{K}} &= \left(\frac{\partial Es}{\partial u}\right)_{u=0}=0.
\end{aligned} \tag{10}$$

These conditions define respectively functions of period $4\mathcal{K}, 2\mathcal{K}, 2\mathcal{K}$ and $4\mathcal{K}$. Evaluating these one obtains (from factors of factorials in q and $-q$) expressions $\cot\{\pi(q-1)/4\}=\cdots, \tan\{\pi(q-1)/4\}=\cdots$, from which the difference $q-q_0$ is obtained by expansion around zeros. Finally expanding

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

one obtains the eigenvalues from which the level splitting can be deduced.

In view of its periodicity the periodic potential avoids the necessity of matching across turning points in the above calculation. In the case of the double well potential this is different, as explained in detail in ref. [10], and one has to impose boundary conditions not only at the minimum but also at the central maximum, again, of course, on even and odd solutions constructed parallel to those above.

The perturbatively derived wave functions of ref.[7] (for large values of κ^2), when matched in domains of overlap and so extended over the entire domain of the variable u, and subjected to periodic boundary conditions as described above define two pairs of eigenfunctions, in each case with one even and one odd, of periods $2\mathcal{K}$ and $4\mathcal{K}$ respectively. These four conditions together imply for large values of κ^2 the following asymptotic expansion of the eigenvalues Λ as shown in ref. [7]:

$$\Lambda_{\pm}(q_0)=\Lambda(q_0)\pm\frac{2\kappa\left(\frac{2}{\pi}\right)^{\frac{1}{2}}}{[\frac{1}{2}(q_0-1)]!}\left(\frac{1+k}{1-k}\right)^{-\frac{\kappa}{k}}\left(\frac{8\kappa}{1-k^2}\right)^{\frac{1}{2}q_0}\left[1+O\left(\frac{1}{\kappa}\right)\right] \tag{11}$$

Here $q_0=2N+1, N=0,1,2,\cdots$ and $\Lambda(q_0)$ is the purely perturbative contribution which represents effectively the eigenvalues of degenerate oscillators of the periodic potential in the case of very high barriers. It is the boundary conditions imposed on the perturbatively derived solutions which yield the nonperturbative effects equivalent to those of the instanton. Thus the factor

$$\left(\frac{1+k}{1-k}\right)^{-\kappa/k}$$

is, in fact $exp(-S_0)$, where S_0 is the Euclidean action of the instanton.

We first verify the result (11) by reduction to the sine–Gordon case. With $\kappa = \pm 2h$ finite while $n \to \infty$ and $k \to 0$ the Jacobian elliptic function snu reduces to $\sin u$ and eq.(1) becomes by replacing u by $x \pm \pi/2$ the Mathieu equation

$$y'' + \left\{\lambda - 2h^2\cos^2 2x\right\}y = 0, \quad \lambda \equiv \Lambda - 2h^2. \tag{12}$$

Under the conditions stated the eigenvalues become

$$\lambda_{\pm}(q_0) = \lambda(q_0) \pm \frac{4h(\frac{2}{\pi})^{\frac{1}{2}}(16h)^{\frac{q_0}{2}}}{[\frac{1}{2}(q_0-1)]!}e^{-4h}\Big[1 + O\Big(\frac{1}{h}\Big)\Big] \tag{13}$$

in agreement with established results in this case [9, 10, 11].

Next we consider k approaching 1 in the case of the Lamé eigenvalues (11)(terms up to and including those of $O(1/\kappa^2)$ in the level splitting and up to and including those of $O(1/\kappa^4)$ in the perturbative part have been given in ref. [7] for any q_0). One readily obtains

$$\Lambda_{\pm}(q_0) = \Lambda(q_0) \pm \frac{(8\kappa)^{\frac{q_0}{2}+1}(1-k)^{\kappa-\frac{1}{2}q_0}}{[\frac{1}{2}(q_0-1)]!(2\pi)^{1/2}2^{\kappa+1+\frac{q_0}{2}}}\Big[1+(1-k)\{\kappa(\frac{1}{2}-\ln 2)+\frac{q_0}{4}\}+O\Big(\frac{1}{\kappa}\Big)\Big] \tag{14}$$

For the two lowest levels $q_0 = 1$ and one obtains

$$\Lambda_{\pm}(1) = \Lambda(1) \pm \frac{(4\kappa)^{3/2}(1-k)^{\kappa-\frac{1}{2}}}{(2\pi)^{1/2}2^{\kappa}}\Big[1+(1-k)\{\kappa(\frac{1}{2}-\ln 2)+\frac{1}{4}\}+O\Big(\frac{1}{\kappa}\Big)\Big] \tag{15}$$

Thus the separation of the two lowest levels is

$$\triangle\Lambda(1) \simeq \frac{2(4\kappa)^{3/2}(1-k)^{\kappa-\frac{1}{2}}}{(2\pi)^{1/2}2^{\kappa}}\Big[1 + (1-k)\{\kappa(\frac{1}{2} - \ln 2) + \frac{1}{4}\} + O\Big(\frac{1}{\kappa}\Big)\Big] \tag{16}$$

This result agrees with formula (13) of ref.[1] in the limit of (in our notation) large κ and $k \to 1$ (in particular this agrees also with our power $\kappa - 1/2$ of $(1-k)$ where in [1] the $-1/2$ has been ignored). The higher order contributions are, presumably, somewhat model or approximation dependent. We thus have agreement with the instanton result of ref.[1] (there ν is our k^2, so that for $k \to 1$ one has $(1-\nu) \to 2(1-k)$).

Hence in the case of the periodic cosine potential, as well as in the case of the Lamé potential, the method of matched asymptotic solutions of refs.[7, 9] – yields the same result as the instanton method in the 1–loop approximation, as one would expect. In ref.[1] reference is made to the well known case of the double well potential. For this case also it has been shown in ref. [10] that the method of matched perturbation expansions – which one might argue amounts to an improved form of the standard WKB method (since it gives the correct eigenvalues) – yields the same result as the instanton method, again for any arbitrary level, whether ground state or excited [10].

3 Conclusions

In the above we have demonstrated that the method of matched asymptotic expansions of refs. [7, 9, 10] which, incidentally, was also developed and used to determine the large order behaviour of the perturbation expansion (cf. ref.[13]), leads to the same result as the instanton calculation in the 1–loop approximation and thus is superior to a WKB calculation. The essential difference is that WKB solutions alone, or rather our WKB–like solutions involving the function A, (which are not valid at an extremum of the potential) do not suffice; one has to match these to solutions valid around the extrema. We may conclude that to obtain from the Schrödinger equation and perturbation theory results agreeing with those of the path integral method with expansion around the instanton, one has to use the full method of matched asymptotic expansions as developed in refs.[9] and [7, 10] (which has also been applied to other cases such as spheroidal wave equations[14]). In purely quantum mechanical cases, such as those considered above, the method of matched asymptotic expansions seems to be simpler and yields the splitting of excited oscillator states with the same ease as that of the ground state, whereas in the case of the path integral method, one has to use periodic instantons, as in e.g. refs. [12, 15]. This may be worth noting in connection with models of spin tunneling which attracted considerable interest recently, since these can – in certain cases and with certain approximations (and coherent states) – be related to periodic differential equations. Thus in ref.[5] the case of the Hamiltonian $\hat{H} = K_1\hat{S}_z^2 - K_2\hat{S}_x^2$ describing a ferromagnetic particle with large spin has been considered and related to Mathieu and Lamé equations. In particular the specific Lamé instanton of ref. [1] has been used in ref.[16]. Finally we add that the introduction of the parameter q in conjunction with the construction of solutions with the properties of eq. (5) has been shown to be extremely useful in other but related contexts as may be seen from the calculation of the scattering matrix in ref.[17].

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