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Multidimensional WKB Approximation for Tunneling Along Curved Escape Paths

J. Zamastil[1,2,3] and L. Skála[1,2]

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Asymptotics of the perturbation series for the ground state energy of the coupled anharmonic oscillators for the positive coupling constant is related to the lifetime of the quasistationary states for the negative coupling constant. The latter is determined by means of the multidimensional WKB approximation for tunneling along curved escape paths. General method for obtaining such approximation is described. The cartesian coordinates (x, y) are choosen in such a way that the x-axis has the direction of the probability flux at large distances from the well. The WKB wave function is then obtained by the simultaneous expansion of the wave function in the coordinate y and the parameter γ determining the curvature of the escape path. It is argued, both physically and mathematically, that these two expansions are mutually consistent. Several simplifications in the integrations of equations are pointed out. It is shown that to calculate outgoing probability flux it is not necessary to deal with inadequacy of the WKB approximation at the classical turning point. The WKB formulas for the large-order behavior of the perturbation series are compared with numerical results and an excellent agreement between the two is found.

KEY WORDS: multidimensional wkb approximation; large-order behavior of the perturbation series.

1. INTRODUCTION

The study of the multidimensional WKB approximation for tunneling along curved escape paths was initiated by Banks and Bender in Banks and Bender (1973) in the context of quantum field theory. Later on, the theory found many other applications ranging from quantum cosmology (see e.g. Hackworth and Weinberg, 2005) to the high temperature superconductivity (see e.g. Blatter *et al.*, 1994).

[1]Department of Chemical Physics and Optics, Charles University, Faculty of Mathematics and Physics, Ke Karlovu 3, 121 16 Prague 2, Czech Republic.
[2] Department of Applied Mathematics, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada
[3] To whom correspondence should be addressed at; e-mail: zamastil@karlov.mff.cuni.cz

Banks and Bender studied the large-order behavior of the perturbation coefficients E_n for the ground state energy E of the system of two coupled oscillators

$$\left[-\frac{\partial^2}{\partial u^2} - \frac{\partial^2}{\partial z^2} + u^2 + z^2 + \gamma uz + \lambda(u^4 + \delta u^2 z^2 + z^4)\right]\psi = E(\lambda)\psi, \tag{1}$$

$$E(\lambda) = \sum_{n=0}^{\infty} E_n \lambda^n. \tag{2}$$

The perturbation coefficients E_n for $\lambda > 0$ are related to the imaginary part of the energy $\Im[E(\lambda)]$ for $\lambda < 0$ via the dispersion relation (Banks and Bender, 1973; Bender and Wu, 1973; Banks and Bender, 1972; Bender and Wu, 1971; Simon, 1970)

$$E_n = \frac{1}{\pi}\int_{-\infty}^{0} d\lambda \frac{\Im[E(\lambda)]}{\lambda^{n+1}}. \tag{3}$$

For $\lambda < 0$, the potential in Eq. (1) has no bound states. Due to tunneling the particle disappears to infinity. Therefore, the energy has the nonzero imaginary part. For $|\lambda| \ll 1$, the lifetime of the bound states are very long and the tunneling through the barrier can be calculated by means of the WKB method (Banks and Bender, 1973; Bender and Wu, 1973; Banks and Bender, 1972; Bender and Wu, 1971). For n very large the dominant contribution to the integral in Eq. (3) comes from the region of very small λ. Thus, the asymptotic behavior of the perturbation coefficients in Eq. (2) is determined by the behavior of the imaginary part of the energy in Eq. (1) for $\lambda = -\lambda'$ and $0 < \lambda' \ll 1$. Henceforth, we will drop the prime on λ. Therefore, λ is always positive henceforth.

In this paper we restrict ourselves to the case $\delta = 0$. Equation (1) then has all essential features of the more complicated problem $\delta \neq 0$, while is much more technically simpler to deal with. Setting $\delta = 0$ in Eq. (1) we see that the outgoing probability flux comes from the neighborhood of the u and z axes. Since Eq. (1) is symmetric with respect to the coordinates u and z, the outgoing probability flux equals twice the one coming from the neighborhood of u axis. We multiply Eq. (1) by ψ^*, then take complex conjugate of Eq. (1) and multiply it by ψ. Subtracting the resulting two equations and integrating by parts we obtain (Banks and Bender, 1973; Zamastil *et al.*, 2001)

$$\Im[E] = \frac{2J}{<\psi|\psi>}, \tag{4}$$

where the outgoing probability flux along u axis equals

$$J = \frac{1}{2i}\int_{-\infty}^{\infty} dz \lim_{u\to\infty}\left[\psi^*\frac{\partial}{\partial u}\psi - \psi\frac{\partial}{\partial u}\psi^*\right] \tag{5}$$

and the norm of the wave function equals

$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} du |\psi|^2. \tag{6}$$

Now, we calculate the imaginary part of the energy from the formula (4) in the limit of very small λ. The imaginary part of the energy has in this limit generic form (Banks and Bender, 1973; Bender and Wu, 1973; Banks and Bender, 1972; Bender and Wu, 1971; Zamastil *et al.*, 2001)

$$\Im[E] = M\lambda^{\beta} e^{-P/\lambda}(1 + R_1\lambda + \cdots) \tag{7}$$

where M, β, P and R_1 are parameters determined later. Replacing $\lambda \to -\lambda$ and inserting this equation into Eq. (3) we see that the coefficients E_n behave at large order as

$$E_n \sim P^{-n}\Gamma(n - 1 - \beta) \tag{8}$$

Taking the ratio of two succesive coefficients we get in the limit of very large n

$$P = \lim_{n\to\infty} \frac{nE_{n-1}}{E_n}. \tag{9}$$

In this paper we will be content with the determination of P.

Since the dominant contribution to the norm of the wave function comes from the interior of the potential well, we can replace in Eq. (6) the exact wave function by the wave function of two non-interacting harmonic oscillators corresponding to $\lambda = 0$. However, the norm of the wave function contributes only to the constant M (Banks and Bender, 1973; Bender and Wu, 1973; Banks and Bender, 1972; Bender and Wu, 1971; Zamastil *et al.*, 2001).

The dominant contribution to the outgoing probability flux comes from classically forbiden region $u^2 \approx \lambda u^4$ and $z^2 \approx \lambda z^4$. To make the terms u^2 and λu^4 of the same order of magnitude we rescale the coordinate u as

$$u = \lambda^{-1/2}x. \tag{10}$$

Likewise, to make the terms z^2 and λz^4 of the same order of magnitude we rescale the coordinate z as

$$z = \lambda^{-1/2}y. \tag{11}$$

Inserting these substitutions into Eq. (1) and searching for the wave function in the WKB form

$$\psi(x, y) = \exp\left\{\frac{1}{\lambda}S_0(x, y) + S_1(x, y) + \cdots\right\} \tag{12}$$

we get from Eq. (1) at the order λ^{-1}

$$\left(\frac{\partial S_0}{\partial x}\right)^2 + \left(\frac{\partial S_0}{\partial y}\right)^2 = V(x, y), \tag{13}$$

where the potential $V(x, y)$ equals

$$V(x, y) = x^2 + y^2 + \gamma xy - x^4 - y^4. \tag{14}$$

At the order λ^0 we get from Eq. (1)

$$2\frac{\partial S_0}{\partial x}\frac{\partial S_1}{\partial x} + 2\frac{\partial S_0}{\partial y}\frac{\partial S_1}{\partial y} + \frac{\partial^2 S_0}{\partial x^2} + \frac{\partial^2 S_0}{\partial y^2} = -E_0, \tag{15}$$

where we used expansion (2) for the energy.

Advantage of the scaling (10) and (11) is now apparent. It enables us to obtain an approximation to the wave function in the tunneling region as the WKB expansion in the coupling constant λ.

The difficulty of finding a solution of Eq. (13) was the main obstacle in development of the multidimensional WKB method. The difficulty lies in the non-linearity of the equation. Equation (15) for the function $S_1(x, y)$ as well as for the higher order terms $S_2(x, y)$, $S_3(x, y)$ in Eq. (12) are linear.

It was argued by Banks and Bender (Banks and Bender, 1973) that the solution of Eq. (13) is obtained by integrating the right-hand side of Eq. (13) along the trajectory that minimizes the right-hand side of Eq. (13). This trajectory is called the escape path and it is a curved line for the potential (14). Further, Banks and Bender argued that the trajectory can be obtained by solving the classical equations of motion. The function $S_0(x, y)$ is then given as Banks and Bender (1973)

$$S_0(x, y) = \int_{s_0}^{s_1} [V(x, y)]^{1/2} ds \tag{16}$$

where s parametrizes the classical trajectory, $x = x(s)$, $y = y(s)$, and s_0 and s_1 are the classical turning points.

This approach, though generally adopted (see e.g. Takatsuka *et al.*, 1999), does not seem to be suitable for actual calculations. Solution of the classical equations of motion involves solution of the coupled nonlinear ordinary differential equations. Consequently, parametrization of the classical trajectory is generally rather complex and the contour integration in Eq. (16) is difficult to perform. To carry out the calculation to the end Banks and Bender considered perturbation theory for slightly curved escape paths starting from the approximation of the straight line escape path. The case of straight line escape path corresponding to $\gamma = 0$ in Eq. (14) is much simpler to deal with. In contrast to the problem of the curved escape paths that is intrinsically two-dimensional, the problem of straight lines is quasi-one-dimensional (Banks and Bender, 1973; Zamastil *et al.*, 2001).

In this paper we show how to develop this perturbation theory directly without invoking any correspondence with classical mechanics. Particulary we show that *it is not advantageous and in fact not at all necessary to solve classical equations of motion*. Further, it is not necessary to find parametrization of the escape path and to calculate the curve line integral (16).

The paper is organized as follows. First, in the Section 2. the precise relation between the solution of Eq. (13) and the parameter P determining the large-order behavior of the perturbation series (2) is established. This connection provides precise numerical test of the soudness of the suggested WKB method. In Section 3. a method for solution of Eq. (13) is suggested. The method consists of double expansion of the wave function in the coordinate y and the parameter γ determining the curvature of the escape path. It is shown that the suggested approximation of the wave function provides systematic approximation to the parameter P; the parameter P is obtained as the series in the parameter γ. In Section 4. the first three orders of this series are explicitly calculated. Several simplifications in the integration of equations are pointed out. Particulary, it is stressed that it is not necessary to replace the WKB approximation by some better approximation in the vicinity of the classical turning points. To show that the methods developed in Sections 3. and 4. are not limited to the special case of the coupled oscillators, the calculations are done first for a general potential $V(x, y)$ in Eq. (13) and only then for the special case of the coupled oscillators. In Section 5. a numerical verification of the WKB results is performed. Finally, in Section 6. summary of the achieved results and perspectives of further development are outlined. We note that brief account of the work presented here was given in Zamastil (2005).

2. RELATION BETWEEN SOLUTION OF EQ. (13) AND THE PARAMETER *P*

We are interested in the outgoing probability flux for very large u, Eq. (5). Considering limit $x \to \infty$ in Eqs. (13) and (15) for finite y we get

$$\left(\frac{\partial S_0}{\partial x}\right)^2 \to (-x^4) \tag{17}$$

and

$$2\frac{\partial S_0}{\partial x}\frac{\partial S_1}{\partial x} + \frac{\partial^2 S_0}{\partial x^2} \to 0. \tag{18}$$

Solving the last equation for S_1 we get

$$S_1(x \to \infty) \to -\frac{1}{4}\ln(-x^4) = -\frac{1}{4}\ln(-\lambda^2 u^4). \tag{19}$$

Inserting this result into Eq. (12) we see that the behavior of the wave function for large u reads

$$\psi(u, z) \to \frac{e^{S_0(u,z)/\lambda}}{e^{i\pi/4}\lambda^{1/2}u}. \tag{20}$$

At the leading order of u, the derivative of this function with respect to u equals

$$\frac{\partial \psi}{\partial u} \to u\, e^{i\pi/4} e^{S_0(u,z)/\lambda}, \tag{21}$$

where we used Eq. (17). As it will be clear from the resulting equations for $S_0(u, z)$ the differentiation of the other terms in $S_0(u, z)$ yields contribution to the outgoing probability flux that vanishes for u going to infinity. Inserting Eqs. (20) and (21) into Eq. (5) we obtain that the outgoing probability flux for very large u is proportional to

$$J \sim \int_{-\infty}^{\infty} dz \lim_{u\to\infty} \exp\{2\Re[S_0(u, z)]/\lambda\}, \tag{22}$$

where $\Re$ denotes the real part. Here, we neglected the factor $\lambda^{-1/2}$ coming from Eq. (20) and the term S_1 in Eq. (12). These terms influence the form of M and β in Eq. (7), but not that of P (Banks and Bender, 1973; Bender and Wu, 1973; Banks and Bender, 1972; Bender and Wu, 1971; Zamastil *et al.*, 2001). The integration over variable z can be performed as follows. First, we find an extreme of $S_0(u, z)$ in the direction of the z axis

$$\Re\left[\left.\frac{\partial S_0(x, y)}{\partial y}\right|_{y=\Delta}\right] = 0. \tag{23}$$

We note that this extreme corresponds to the escape path. Around this extreme we expand the function $S_0(x, y)$ as

$$S_0(x, y) \approx S_0(x, \Delta) + \frac{(y-\Delta)^2}{2!}\left.\frac{\partial^2 S_0(x, y)}{\partial y^2}\right|_{y=\Delta} + \cdots. \tag{24}$$

Inserting this expansion into Eq. (22) we see that the first term is independent of z and can be pushed out of the integral. The integration of the second term contributes to M and β in Eq. (7), but not to P. Therefore, to the required accuracy we get

$$J \sim \exp\{2\Re[S_0(x \to \infty, \Delta)]/\lambda\}. \tag{25}$$

Inserting Eq. (25) into Eq. (4) and comparing it with Eq. (7) we see that P equals to

$$P = 2\Re\,[S_0(x \to \infty, \Delta)]. \tag{26}$$

In other words, P equals twice the real part of the value of $S_0(x, y)$ for y lying on the escape path and x approaching infinity. This is the equation we searched for.

It provides connection between the parameter P determing the asymptotics of the perturbation series and the solution of Eq. (13).

3. WKB METHOD

We now turn to the solution of Eq. (13). We shall proceed with greater generality than it is actually needed; we discuss the solution of Eq. (13) for a general potential $V(x, y)$ to show that the suggested method is not limited to the special case of the coupled oscillators.

3.1. Approximate Solution of Eq. (13)

In the neighbourhood of the x axis, the potential can be expanded as

$$V(x, y) = V_0(x) + \gamma V_1(x)\, y + V_2(x)\, y^2 + \gamma V_3(x)\, y^3 + V_4(x)\, y^4 + \ldots, \quad (27)$$

where the meaning of the parameter γ will be made clear later. By comparing Eqs. (14) and (27) we see that for the special case of the coupled oscillators we have

$$V_0(x) = x^2 - x^4, \quad (28)$$

$$V_1(x) = x, \quad (29)$$

$$V_2(x) = 1, \quad (30)$$

$$V_3(x) = 0 \quad (31)$$

and

$$V_4(x) = -1. \quad (32)$$

Let us first consider the case $\gamma = 0$. Then the particle moves inside the potential that is in the first approximation parabolic in the coordinate y (Zamastil *et al.*, 2001; Banks and Bender, 1973). Henceforth, under the first approximation we understand neglection of the terms having higher than the second power of y. Then, the wave function in this approximation is that of the harmonic oscillator, namely

$$S_0(x, y, \gamma = 0) = f_0(x) + f_2(x) y^2/2! + \cdots. \quad (33)$$

This is the case that is usually refered to as the straight line escape path (Zamastil *et al.*, 2001; Banks and Bender, 1973). Now, the first key idea toward the solution of Eq. (13) is that for $\gamma \neq 0$, the wave function of the particle is in the first approximation that of the *shifted* harmonic oscillator, namely

$$S_0(x, y) = f_0(x) + f_1(x)\, y + f_2(x)\, y^2/2! + f_3(x)\, y^3/3! + f_4(x)\, y^4/4! + \ldots. \quad (34)$$

By inserting this expansion into Eq. (13) and comparing the terms proportional to the zeroth power of y we obtain

$$[f_0'(x)]^2 + [f_1(x)]^2 = V_0(x), \tag{35}$$

in the first power of y

$$2f_0'(x)f_1'(x) + 2f_2(x)f_1(x) = \gamma V_1(x) \tag{36}$$

in the second power of y

$$f_0'(x)f_2'(x) + [f_1'(x)]^2 + f_1(x)f_3(x) + [f_2(x)]^2 = V_2(x) \tag{37}$$

and so on. Here, the prime denotes the differentiation with respect to x. The second key idea is that comparing Eqs. (33) and (34) we see that in case $\gamma = 0$ the terms proportional to the odd powers of y vanish and the terms proportional to the even powers of y remain. This suggests the following expansion of the functions in Eq. (34):

$$f_{2i}(x) = f_{2i,0}(x) + \gamma^2 f_{2i,2}(x) + \gamma^4 f_{2i,4}(x) + \cdots \tag{38}$$

and

$$f_{2i+1}(x) = \gamma f_{2i+1,1}(x) + \gamma^3 f_{2i+1,3}(x) + \gamma^5 f_{2i+1,5}(x) + \cdots, \tag{39}$$

where $i = 0, 1, 2, \ldots$.

3.2. Approximate Determination of the Parameter *P*

Before writing down the explicit form of the equations for the functions $f_{i,j}(x)$ let us show that the expansions (34), (38) and (39) provide systematic approximation to the parameter P. First we show that these expansions provide systematic approximation to the escape path. By inserting Eq. (34) into Eq. (23) we obtain

$$\Re[f_1(x)] + \Delta(x)\Re[f_2(x)] + \frac{\Delta^2(x)}{2!}\Re[f_3(x)] + \frac{\Delta^3(x)}{3!}\Re[f_4(x)] + \cdots = 0. \tag{40}$$

Here, we wrote explicitly the extreme Δ in the direction of the y-axis as a function of the coordinate x. This is the expression of the fact that the escape path is curved.

Searching for the solution of Eq. (40) in the form

$$\Delta(x) = \Delta_1(x)\gamma + \Delta_3(x)\gamma^3 + \cdots, \tag{41}$$

inserting the expansions (38) and (39) into Eq. (40) and comparing the terms of the same order of γ we obtain equations for the functions $\Delta_i(x)$. For example, for $i = 1$ we obtain

$$\Delta_1(x) = -\frac{\Re[f_{1,1}(x)]}{\Re[f_{2,0}(x)]}. \tag{42}$$

By inserting the expansion (34) into Eq. (26) we obtain

$$P = \lim_{x\to\infty} 2\bigg(\Re[f_0(x)] + \Delta(x)\Re[f_1(x)] + \frac{[\Delta(x)]^2}{2!}\Re[f_2(x)] + \frac{[\Delta(x)]^3}{3!}\Re[f_3(x)] + \frac{[\Delta(x)]^4}{4!}\Re[f_4(x)] + \cdots\bigg). \tag{43}$$

By inserting the expansions of the functions $f_i(x)$, Eqs. (38) and (39), the expansion of the escape path, Eq. (41), and the expression for $\Delta_1(x)$ and $\Delta_3(x)$ we obtain the following expansion of the parameter P in the powers of γ

$$P = P(\gamma) = P_0 + \gamma^2 P_2 + \gamma^4 P_4 + \cdots \tag{44}$$

where

$$P_0 = \lim_{x\to\infty} 2\Re[f_{0,0}(x)] \tag{45}$$

$$P_2 = \lim_{x\to\infty} \left\{2\Re[f_{0,2}(x)] - \frac{(\Re[f_{1,1}(x)])^2}{\Re[f_{2,0}(x)]}\right\} \tag{46}$$

and

$$P_4 = \lim_{x\to\infty} \left\{2\Re[f_{0,4}(x)] - 2\frac{\Re[f_{1,3}(x)]\Re[f_{1,1}(x)]}{\Re[f_{2,0}(x)]} + \frac{\Re[f_{2,2}(x)](\Re[f_{1,1}(x)])^2}{(\Re[f_{2,0}(x)])^2} - \frac{\Re[f_{3,1}(x)](\Re[f_{1,1}(x)])^3}{3(\Re[f_{2,0}(x)])^3} + \frac{\Re[f_{4,0}(x)](\Re[f_{1,1}(x)])^4}{12(\Re[f_{2,0}(x)])^4}\right\} \tag{47}$$

and so on. We would like to conclude this section with few remarks.

First, it is obvious that the suggested approximation of the wave function provides systematic approximation of the parameter P determining the large-order behavior of the perturbation series.

Second, it is evident that the simultaneous expansion of the wave function in y and γ is mutually consistent from the mathematical point of view. It is understandable also from the physical point of view. Since γ determines how much the escape path of the particle deviates from the straight line, going to higher powers of γ one has to take into account the behavior of the wave function at larger distances from the x-axis. To describe this behavior one has to go to higher powers of y.

Finally, it is seen from the last three equations, that to calculate the parameter P in p-th order of γ, we need to calculate the functions $f_{i,j}(x)$, where the sum of the indices $i + j$ equals p.

4. INTEGRATION OF EQUATIONS

In this Section, the first three orders of the series in Eq. (44) are explicitly calculated.

4.1. Zeroth Order Calculation

Comparison of the terms proportional to zeroth power of γ in Eq. (35) yields equation for the function $f_{0,0}(x)$

$$[f'_{0,0}(x)]^2 = V_0(x). \tag{48}$$

For the case of the coupled oscillators, Eq. (28) yields

$$f'_{0,0}(x) = -\sqrt{x^2 - x^4}. \tag{49}$$

Here, we choose the solution with the minus sign since for x approaching zero we have to get from Eqs. (12), (34), (38) and (39) the wave function of two non-interacting harmonic oscillators

$$\begin{aligned}\psi_0(u,z) &= \exp\left\{-\frac{u^2+z^2}{4}\left(\sqrt{1+\frac{\gamma}{2}}+\sqrt{1-\frac{\gamma}{2}}\right)-\frac{uz}{2}\left(\sqrt{1+\frac{\gamma}{2}}-\sqrt{1-\frac{\gamma}{2}}\right)\right\}\\ &= \exp\left\{-\frac{u^2+z^2}{2}\left(1-\frac{\gamma^2}{32}-\frac{5\gamma^4}{2048}+\cdots\right)-\frac{uz}{4}\left(\gamma+\frac{\gamma^3}{32}+\cdots\right)\right\}. \end{aligned} \tag{50}$$

For further calculation, it is advantageous to make the substitution

$$w = \frac{1-(1-x^2)^{1/2}}{2}. \tag{51}$$

Then, we get from Eq. (49)

$$\frac{df_{0,0}(w)}{dw} = -2(1-2w)^2. \tag{52}$$

Obviously, for x larger than 1, the integrand in Eq. (52) is purely imaginary. Therefore, we can stop the integration at the point $x = 1$. Further, to match the WKB function to the bound state function (50) we take the lower bound of the integration $x = 0$. Thus, integrating Eq. (52) from $w = 0$ to $w = 1/2$ and multiplying it by 2 we get

$$P_0 = -\frac{2}{3}. \tag{53}$$

It is not surprising that it is the same result as for the case $\gamma = 0$ found in Zamastil *et al.* (2001), Banks and Bender (1973).

4.2. Second Order Calculation

4.2.1. General Case

Comparing the terms of the order γ^0 in Eq. (37) we obtain the equation for the function $f_{2,0}(x)$

$$f'_{0,0}(x)f'_{2,0}(x) + [f_{2,0}(x)]^2 = V_2(x). \tag{54}$$

Comparing the terms of the order γ in Eq. (36) we get equation for the function $f_{1,1}(x)$

$$2f'_{0,0}(x)f'_{1,1}(x) + 2f_{2,0}(x)f_{1,1}(x) = V_1(x) \tag{55}$$

and finally comparing the terms of the order γ^2 in Eq. (35) we get equation for the function $f_{0,2}(x)$

$$2f'_{0,0}(x)f'_{0,2}(x) + [f_{1,1}(x)]^2 = 0. \tag{56}$$

Equation (54) is a non-linear first order differential equation. By means of the substution

$$f_{2,0}(x) = f'_{0,0}(x)(\ln\varphi(x))', \tag{57}$$

it can be converted to the linear second order differential equation

$$f'_{0,0}(x)[f'_{0,0}(x)\varphi'(x)]' = V_2(x)\varphi(x). \tag{58}$$

We note that sometimes it is more advantageous to solve the original equation (54).

Equation (55) is a linear inhomogenous first-order differential equation. By the substitution

$$f_{1,1}(x) = \varphi^{-1}(x)F_{1,1}(x) \tag{59}$$

it can be simplified to

$$F'_{1,1}(x) = \frac{V_1(x)\varphi(x)}{2f'_{0,0}(x)}. \tag{60}$$

As it becomes apparent later it is advantageous to introduce another function $\phi(x)$ via the relation

$$\phi'(x) = -\frac{F_{1,1}(x)}{f'_{0,0}(x)[\varphi(x)]^2}. \tag{61}$$

Equation (56) then takes the form

$$f'_{0,2}(x) = \frac{1}{2}\phi'(x)F_{1,1}(x) \tag{62}$$

where we inserted Eq. (59). Integrating the last equation by parts and using Eq. (60) the solution of the last equation can be written as

$$f_{0,2}(x) = \xi_{0,2}(x) + \frac{\phi(x)F_{1,1}(x)}{2}, \tag{63}$$

where the derivative of the function $\xi_{0,2}(x)$ equals

$$\xi'_{0,2}(x) = -\frac{V_1(x)\varphi(x)\phi(x)}{4f'_{0,0}(x)}. \tag{64}$$

4.2.2. Coupled Oscillators

The solution of Eq. (54) with $f'_{0,0}(x)$ given by Eq. (49) and with the potential $V_2(x)$ given by Eq. (30) reads

$$f_{2,0}(x) = -1. \tag{65}$$

The other possible solution is discarded here. Only the solution (65) yields for x approaching zero the bound state function (50), compare Eqs. (12) and (34) with Eq. (50). Integrating Eqs. (57), (60) and (61) we get succesively

$$\varphi(w) = \sqrt{\frac{w}{1-w}}, \tag{66}$$

$$F_{1,1}(w) = \frac{\ln(1-w)}{2} \tag{67}$$

and

$$\phi(w) = \frac{1}{4}\left[-\frac{\ln(1-w)}{w} + \ln\left(\frac{1-w}{w}\right)\right], \tag{68}$$

where Eqs. (51) and (52) were used.

4.2.3. Calculation of P_2

It is seen from Eq. (51) that for x approaching to infinity, w approaches to i times infinity and the functions $\varphi(x)$, $\phi(x)$ and $F_{1,1}(x)$ tend to

$$\varphi(x \to \infty) \to (-1)^{1/2} = i, \tag{69}$$

$$\phi(x \to \infty) \to \frac{\ln(-1)}{4} = \frac{i\pi}{4} \tag{70}$$

and

$$\Im[F_{1,1}(x \to \infty)] \to \Im\left[\frac{\ln(-1)}{4}\right] = \frac{\pi}{4}. \tag{71}$$

Thus, in the case of the coupled oscillators, for x approaching infinity both the functions $\varphi(x)$ and $\phi(x)$ are purely imaginary. Assuming that this holds generally, we put $\phi(x) = i\tilde{\phi}(x)$ and $\varphi(x) = i\tilde{\varphi}(x)$. By inserting Eqs. (59) and (63) into Eq. (46) we obtain

$$P_2(x) = \lim_{x\to\infty} \left\{2\Re[\xi_{0,2}(x)] - \Im[F_{1,1}(x)]\tilde{\beta}(x)\right\}, \tag{72}$$

where the function $\tilde{\beta}(x)$ equals

$$\tilde{\beta}(x) = \tilde{\phi}(x) + \frac{\Im[F_{1,1}(x)]}{\Re[f_{2,0}(x)][\tilde{\varphi}(x)]^2}. \tag{73}$$

Since we have the freedom in determining the integration constant for the function $\phi(x)$ we can adjust this constant to put the function $\tilde{\beta}(x)$ in Eq. (72) equal to zero for x approaching infinity. Then all we have to do to calculate P_2 is to integrate Eq. (64). The simplification achieved by vanishing the function $\tilde{\beta}(x)$ at infinity becomes even more apparent when calculating P_4.

It is clear from Eqs. (65), (69), (70) and (71) that with the choice of the integration constant made in Eq. (68) in the case of the coupled oscillators the function $\tilde{\beta}(x)$ vanishes for x approaching infinity. Making the substitution (51) and inserting Eqs. (52), (66), (67) and (68) into Eq. (64) we obtain

$$\xi_{0,2}(w) = -\frac{1}{16}\int_0^w dw' \left[\frac{\ln(1-w')}{w'} + \frac{\ln(w')}{1-w'}\right]. \tag{74}$$

Although it is not immediately seen, little algebra shows that the right hand side of Eq. (64) is purely imaginary for $x > 1$. Therefore, to calculate P_2 from Eq. (72) it is sufficient to stop the integration in Eq. (74) at the point $w = 1/2$ corresponding to the point $x = 1$.

Therefore, the coefficient P_2 given by Eq. (72) reads

$$P_2 = 2\xi_{0,2}(w = 1/2) = \frac{\pi^2}{48} = 0.20561675835. \tag{75}$$

4.3. Fourth Order Calculation

4.3.1. General Case

To get the equation for the function $f_{4,0}(x)$ we have to compare the terms in Eq. (13) proportional to y^4 and γ^0. The function $f_{3,1}(x)$ is obtained by comparing the terms in Eq. (13) proportional to y^3 and γ^1. Proceeding in this way we obtain generally

$$f'_{i,4-i}(x)f'_{0,0}(x) + if_{i,4-i}f_{2,0}(x) + f_{i+1,3-i}(x)f_{1,1}(x) = \eta_i(x)\frac{f'_{0,0}(x)}{[\varphi(x)]^i}, \tag{76}$$

with i descending from 4 to 0. The functions $\eta_i(x)$ has not to be precisely specified at this point. They can be obtained from Eqs. (13), (34), (38) and (39).

Equations (76) are linear first-order inhomogenous differential equations for the functions $f_{i,4-i}(x)$. Solution of homogenous equations is very simple. By means of Eq. (57) we find that $f_{i,4-i}(x) = F/[\varphi(x)]^i$, where F is constant. Using well-known method of variation of constants the solution of inhomogenous equations is searched for in the form

$$f_{i,4-i}(x) = \frac{F_{i,4-i}(x)}{[\varphi(x)]^i}. \tag{77}$$

By inserting Eq. (77) into Eq. (76) we obtain the equations

$$F'_{i,4-i}(x) = \eta_i(x) + \phi'(x)F_{i+1,p}(x) \tag{78}$$

where the function $\phi(x)$ is given by Eq. (61). As is clear from Eq. (47), to calculate P_4 we need to calculate the functions $f_{i,j}(x)$ where the sum of the indices $i + j$ equals to 4. Therefore, we need to solve system of Eqs. (78). We start with Eq. (78) for $i = 4$

$$F'_{4,0}(x) = \eta_4(x), \tag{79}$$

then decrease the index i by 1 till the index i has the value 0. The integration of these equations is difficult because the equations are mutually coupled. It means that before integrating Eq. (78) for $i = q$ to obtain function $F_{q,4-q}(x)$ we have to integrate $q - 1$ equations (78) for $q - 1$ functions $F_{i,4-i}(x)$ with $q < i \leq 4$. However, as we show further by means of the function $\phi(x)$ and integration by parts the equations for the functions $F_{i,4-i}(x)$ can be *decoupled*. Integrating by parts we rewrite Eq. (78) for $i = 3$ into the form

$$F'_{3,1}(x) = \eta_3(x) + \left[\phi(x)F_{4,0}(x)\right]' - \phi(x)\eta_4(x), \tag{80}$$

where we used Eq. (79). The solution of this equation can be written as

$$F_{3,1}(x) = \xi_{3,1}(x) + \phi(x)\xi_{4,0}(x), \tag{81}$$

where we put $\xi_{4,0}(x) = F_{4,0}(x)$. The derivative of the function $\xi_{3,1}(x)$ with respect to x equals

$$\xi'_{3,1}(x) = \eta_3(x) - \phi(x)\eta_4. \tag{82}$$

Inserting solution (81) into Eq. (78) for $i = 2$, using Eq. (82) and integrating by parts we can write the solution of Eq. (78) for $i = 2$ as

$$F_{2,2}(x) = \xi_{2,2}(x) + \phi(x)\xi_{3,1}(x) + \frac{[\phi(x)]^2}{2}\xi_{4,0}(x). \tag{83}$$

By inserting the last equation into Eq. (78) for $i = 2$ we get the derivative of the function $\xi_{2,2}(x)$

$$\xi'_{2,2}(x) = \eta_2(x) - \eta_3(x)\phi(x) + \eta_4(x)\frac{[\phi(x)]^2}{2}. \tag{84}$$

Proceeding further in this way we obtain generally

$$F_{4-k,k}(x) = \sum_{l=0}^{k} \xi_{4-k+l,k-l}(x)\frac{\phi(x)^l}{l!}, \tag{85}$$

where the derivative of the functions $\xi_{4-k,k}(x)$ equals

$$\xi'_{4-k,k}(x) = \sum_{l=0}^{k} \eta_{4-k+l}(x)(-1)^l\frac{\phi(x)^l}{l!}. \tag{86}$$

4.3.2. Calculation of P_4

By inserting Eqs. (77) and (85) into Eq. (47) and using again the fact that the functions $\varphi(x)$ and $\phi(x)$ are purely imaginary for x approaching infinity we get

$$P_4 = \lim_{x\to\infty}\left\{2\Re[\xi_{0,4}(x)] - 2\Im[\xi_{1,3}(x)]\tilde{\beta}(x) - \Re[\xi_{2,2}(x)]\tilde{\beta}^2(x) + \frac{\Im[\xi_{3,1}(x)]\tilde{\beta}^3(x)}{3} + \frac{\Re[\xi_{4,0}(x)]\tilde{\beta}^4(x)}{12}\right\}. \tag{87}$$

The function $\tilde{\beta}(x)$ can be made vanish for x approaching the infinitly. Thus, we see that if we properly adjust the integration constant for $\phi(x)$, to calculate P_4 we have to integrate only Eq. (86) for $k = 4$.

It turns out that the right hand side of Eq. (86) for $k = 4$ can be expressed solely by means of the functions $f'_{0,0}(x)$, $f_{2,0}(x)$, $F_{1,1}(x)$, $\varphi(x)$ and $\phi(x)$. Taking into account the explicit form of the functions $\eta_i(x)$, Eq. (86) can be for $k = 4$ brought into the form

$$\xi'_{0,4}(x) = -\frac{[\varphi(x)]^2}{8[f'_{0,0}(x)]^3}\left\{\varphi(x)[f_{2,0}(x)\beta(x)]^2 + [V_1(x) - \varphi(x)\phi(x)V_2(x)]\phi(x)\right\}^2 - \frac{[\varphi(x)\phi(x)]^3[V_3(x) - \varphi(x)\phi(x)V_4(x)]}{2f'_{0,0}(x)}, \tag{88}$$

where the function $\beta(x)$ is given as

$$\beta(x) = \phi(x) - \frac{F_{1,1}(x)}{f_{2,0}(x)[\varphi(x)]^2}. \tag{89}$$

This form is very usefull both for theoretical considerations and practical calculations.

4.3.3. General Discussion of the Divergence of the WKB Function at the Classical Turning Point

We have seen on our example of the coupled oscillators that the outgoing probability flux at infinity equals the outgoing probability flux at the point $x = 1$. In other words, there is no additional contribution to the outgoing probability flux once particle passes through the point $x = 1$.

It is not surprising at all, if we realize that the point $x = 1$ corresponds to the classical turning point x_T. Indeed, the very notion of "tunneling through the potential barrier" implies that this tunneling is "done" once particle is outside the potential barrier in the classically allowed region $x > x_T$.

Therefore, it is very likely that the equality of the outgoing probability flux at infinity and at the classical turning point holds also in the higher order calculations and for a wide class of Hamiltonians. If this is true, as we will assume henceforth, then we can stop the integration in Eq. (88) at the point $x = 1$, or more generally at the point $x = x_T$. However, the situation is not so simple, since as will be shown below, the function $\xi_{0,4}(x)$ given by Eq. (88) diverges at the point x_T.

There is a large number of papers dealing with inadequacy of the WKB approximation around the classical turning point and its replacement by proper approximation at this region see e.g. Langer (1937), Silverstone (1985), Silverstone *et al.* (1985), Damburg and Kolosov (1978). The usual procedure is the approximation of the potential at the vicinity of the classical turning point by the straight line and matching the solution for the straight line, the Airy functions, to the WKB wave function. Disadvantage of this procedure is that it complicates the calculation in a substantial way.

It was shown in Zamastil *et al.* (2000) for the one-dimensional problems, that as far as the tunneling through the potential barrier is concerned, one does not need to replace the WKB approximation at the classical turning point by some better approximation at all. The main idea can be described as follows. Since we are interested in the outgoing probability flux at large distances from the origin, what we actually need is behavior of the wave function in the asymptotic region. At this region, the WKB approximation is an excellent approximation. Therefore, we split the expression for the WKB wave function in Eq. (88) into the part that is finite at the classical turning point and to the part that diverges at the classical turning point. The part that diverges at the classical turning point is determined analytically by means of the integration by parts. For example, the part in Eq. (88) that diverges at the classical turning point behaves around the classical turning point as $(x_T - x)^{-1/2}$, see below. Now, as was emphasized above, we are interested in the outgoing probability flux for x approaching infinity. Obviously, the term diverging at the turning point goes to zero for x approaching the infinity. Thus, the outgoing probability flux at infinity equals the *finite* part of the outgoing probability flux at the classical turning point.

From the practical point of view, the only difficulty in the method used in Zamastil *et al.* (2000) and described above is the integration by parts. For general potential, the integrand in Eq. (88) could be very complex and the isolation of the divergent part by means of this technique could be rather cumbersome. Therefore, we suggest below more practical method of identifying the divergent part of the function $\xi_{0,4}(x)$ at the turning point.

The method is based on the precise determination of the divergent part of the function $\xi_{0,4}(x)$ at the point x_T. For this aim we need to determine the behavior of the functions appearing on the right hand side of Eq. (88) in the vicinity of the classical turning point.

We shall assume that the potentials $V_0(x)$, $V_1(x)$, $V_2(x)$ and so on are smooth analytic functions at the classical turning point and can be expanded in the Taylor series as

$$V_i(x) = V_{i0} + V_{i1}(x_T - x) + \cdots, \quad i = 1, 2, \ldots, \tag{90}$$

where $V_{00} = 0$. It follows from Eq. (48) that the derivative of the function $f_{0,0}(x)$ behaves around the point x_T as

$$\begin{aligned} f'_{0,0}(x) &= [V_{01}]^{1/2}(x_T - x)^{1/2}\left[1 + \frac{V_{02}}{V_{01}}(x_T - x) + \cdots\right]^{1/2} \\ &= [V_{01}]^{1/2}(x_T - x)^{1/2} + \frac{V_{02}}{2[V_{01}]^{1/2}}(x_T - x)^{3/2} + \cdots. \end{aligned} \tag{91}$$

Inserting Eqs. (90) and (91) into Eq. (54) we obtain

$$f_{2,0}(x) = f^0_{2,0} + f^1_{2,0}(x_T - x)^{1/2} + \cdots. \tag{92}$$

Inserting the last equation and Eq. (91) into Eq. (57) we find

$$\varphi(x) = \varphi_0 + \varphi_1(x_T - x)^{1/2} + \cdots. \tag{93}$$

Further, by comparing the terms of the order $(x_T - x)^{-1/2}$ on both sides of Eq. (57) we get the relation

$$\varphi_1 = \frac{2 f^0_{2,0}\varphi_0}{[V_{01}]^{1/2}}. \tag{94}$$

By inserting Eqs. (90), (91) and (93) into Eq. (60) we obtain

$$F_{1,1}(x) = F^0_{1,1} + F^1_{1,1}(x_T - x)^{1/2} + \cdots. \tag{95}$$

Likewise, by inserting the last equation and Eqs. (91), and (93) into Eq. (61) we get

$$\phi(x) = \phi_0 + \phi_1(x_T - x)^{1/2} + \cdots. \tag{96}$$

Comparison of the terms of the power $(x_T - x)^{-1/2}$ on both sides of Eq. (61) provides the relation

$$\phi_1 = -\frac{2F_{1,1}^1}{[V_{01}]^{1/2}[\varphi_0]^2}. \tag{97}$$

By comparing Eq. (88) with the expansions (90)–(96) we see that the second term on the right hand side of Eq. (88) does not cause problems since it goes near the turning point like $(x_T - x)^{-1/2}$, so the integral from it is convergent at the point x_T. The problem is caused by the first term in Eq. (88). This term behaves near the turning point as $(x_T - x)^{-3/2}$. Therefore, to achieve our goal of precise determination of the divergent part of $\xi_{0,4}(x)$, we need to determine precisely the behavior of the first term on the right hand side of Eq. (88), i.e.

$$-\frac{[\varphi(x)]^2 \left\{\varphi(x)[f_{2,0}(x)\beta(x)]^2 + [V_1(x) - \varphi(x)\phi(x)V_2(x)]\phi(x)\right\}^2}{8[V_{01}(x_T - x)]^{3/2}}, \tag{98}$$

where Eq. (91) was inserted.

By inserting Eqs. (65), (66), (67) and (68) into Eq. (89) one can see that for the case of the coupled oscillators the function $\beta(x)$ vanishes at the turning point. Henceforth, we limit our discussion to the cases when this condition holds true. We shall also assume that the values of the functions $\varphi(x)$ and $\phi(x)$ at the turning point, φ_0 and ϕ_0, are real numbers.

Using the expansions (93)–(96) in Eq. (89) vanishing of the function $\beta(x)$ yields

$$F_{1,1}^0 = \phi_0 f_{2,0}^0[\varphi_0]^2. \tag{99}$$

Since the function $\beta(x)$ in Eq. (88) is squared it behaves in the vicinity of the turning point as $(x - x_T)$ and yields therefore convergent contribution. The "dangerous" term in the numerator equals

$$\{[V_1(x) - \phi(x)\varphi(x)V_2(x)]\phi(x)\varphi(x)\}^2. \tag{100}$$

Inserting the expansions (90), (93) and (96) into this term we get

$$\left\{(V_{10} - \phi_0\varphi_0 V_{20})\phi_0\varphi_0 + (\phi_0\varphi_1 + \phi_1\varphi_0)(V_{10} - \phi_0\varphi_0 V_{20})(x_T - x)^{1/2} + \cdots\right\}^2. \tag{101}$$

Now, inserting Eq. (99) into Eq. (97) and taking the ratio of Eqs. (97) and (94) we get

$$\frac{\varphi_1}{\phi_1} = -\frac{\varphi_0}{\phi_0}. \tag{102}$$

Thus, the term proportional to $(x_T - x)^{1/2}$ in Eq. (101) vanishes.

We are arriving to the conclusion that the divergent part of the integrand in Eq. (88) equals

$$-\frac{\{(V_{10}-\phi_0\varphi_0 V_{20})\phi_0\varphi_0\}^2}{[2V_{01}(x_T-x)]^{3/2}}. \tag{103}$$

The rest of the integrand yields convergent contribution. Thus, we rewrite the expression for $\xi'_{0,4}(x)$ into the form

$$\xi'_{0,4}(x)=\left[\xi'_{0,4}(x)+\frac{\{(V_{10}-\phi_0\varphi_0 V_{20})\phi_0\varphi_0\}^2}{[2V_{01}(x_T-x)]^{3/2}}\right]-\left[\frac{\{(V_{10}-\phi_0\varphi_0 V_{20})\phi_0\varphi_0\}^2}{[2V_{01}(x_T-x)]^{3/2}}\right]. \tag{104}$$

The first bracket yields convergent contribution at the turning point x_T. For x greater than x_T it is purely imaginary. Therefore, to calculate P_4 from Eq. (87), the first bracket is integrated *numerically* from the point x_0, determined by the matching of the WKB wave function (12) to the bound state function, to the classical turning point x_T. The second bracket is integrated *analytically* from the point x_0 till infinity where it vanishes.

In the next paragraph this procedure is illustrated on the example of two coupled anharmonic oscillators.

4.3.4. Coupled Oscillators

Making substitution (51) into Eq. (88) we get

$$\begin{aligned}\frac{d\xi_{0,4}(w)}{dw}=&-\frac{[\varphi(w)]^2}{\left[2\frac{df_{0,0}(w)}{dw}\right]^3\left[\frac{dw}{dx}\right]^4}\big\{\varphi(w)[f_{2,0}(w)\beta(w)]^2\\&+[V_1(w)-\varphi(w)\phi(w)V_2(w)]\phi(w)\big\}^2\\&-\frac{[\varphi(w)\phi(w)]^3[V_3(w)-\varphi(w)\phi(w)V_4(w)]}{2\frac{df_{0,0}(w)}{dw}\left[\frac{dw}{dx}\right]^2}.\end{aligned} \tag{105}$$

With the additional term coming from the substitution (51) into the differential dx, the divergent part (103) reads in this case

$$-\frac{\{[V_1(w)-\varphi(w)\phi(w)V_2(w)]\varphi(w)\phi(w)\}^2}{(-4)^3\,[w(1-w)]^2}\bigg|_{w=1/2}\frac{1}{(1-2w)^2}=\left[\frac{\ln 2(\ln 2-2)}{8(1-2w)}\right]^2. \tag{106}$$

With some effort, one can again show that the right hand side of Eq. (88) is purely imaginary for x greater than 1. Therefore, there is no contribution to the outgoing probability flux, once particle passes through the classical turning point.

The outgoing probability flux at infinity equals the finite part of the outgoing probability flux at the turning point. We obtain for P_4 from Eq. (87)

$$P_4 = 2\int_0^{1/2} dw \left\{ \frac{d\xi_{0,4}(w)}{dw} - \left[\frac{\ln 2(\ln 2 - 2)}{8(1-2w)}\right]^2 \right\} - \left. \frac{[\ln 2(\ln 2 - 2)]^2}{64(1-2w)} \right|_{w=0}^{w=i\infty} = 0.01132591784. \tag{107}$$

5. NUMERICAL VERIFICATION

We calculated 100 perturbation energies E_n for the eigenvalue problem (1) numerically in 200 digits arithmetics using the language MAPLE. The perturbation energies were calculated by means of the difference-equation method described in Banks and Bender (1973). We note that for calculation of the perturbation energies it is advantageous to make the rotation of the coordinates u and z in Eq. (1) about $\pi/2$, i.e. to perform the substitution $u \to (u+z)/2^{1/2}$, $z \to (u-z)/2^{1/2}$.

Further, we extrapolated Eq. (9) from the interval $n = 90$ to $n = 100$ by means of the Thiele-Padé extrapolation for different values of γ and obtained $P(\gamma = 1/10) = -0.664609364466$, $P(\gamma = 1/20) = -0.6661525539521$ and $P(\gamma = 1/30) = -0.6664381896164$. We checked these numbers by extrapolating Eq. (9) from the interval $n = 80$ to $n = 90$. Only the numbers that agree in both cases are given here. By inserting the values of γ into Eq. (44) with P_0, P_2 and P_4 given by Eqs. (53), (75) and (107) we obtained $P(\gamma = 1/10) = -0.664609366491$, $P(\gamma = 1/20) = -0.666152553983$ and $P(\gamma = 1/30) = -0.6664381896192$, an excellent agreement indeed. We tried to use the first three term of the series (44) also in the case when the parameter γ is not small. From numerical analysis we obtained $P(\gamma = 1) = -0.447$, while from the series (44) we get $P(\gamma = 1) = -0.449$. It is seen that the first three terms yield semi-quantitative information even in the case of moderetaly curved escape paths.

6. CONCLUSIONS

In this paper, the multidimensional WKB approximation for particle tunneling along the curved escape paths was suggested. The method is based on the simultaneous expansion of the function $S_0(x, y)$ in the coordinate y and the parameter γ determining the curvature of the escape path. It was shown that these expansions provide systematic approximation to the parameter P determining the large-order behavior of the perturbation series for the ground state of the coupled oscillators. We explicitly calculated first three orders of the series for the parameter

P. It was shown that the calculation of the first three orders is generally feasible. It was pointed out that to calculate the outgoing probability flux at infinity it is not necessary to deal with inadequacy of the WKB approximation in the vicinity of the classical turning point. From the technical point of view it involves only solution of one linear second-order differential equation and quadratures. Further, it was shown that for the case of the coupled oscillators the first three terms of the series can be used also for moderately curved escape paths. However, the complexity of the calculation quickly grows when going to the higher orders of the method.

It is likely that the expansion (44) has a finite radius of convergence and that this radius is smaller than the interval of physically relevant values of the parameter γ. In other words, starting from some critical value of the parameter γ there could be qualitative change of the dependence of the outgoing probability flux on the parameter γ.

Therefore, future extension of the method should be aimed at larger number of the coefficients in Eq. (44). From large number of the perturbation coefficients one can get information about the analytic structure of the expanded function (Zamastil and Vinette, 2005).

The extension of the method to more than two dimensions is straightforward in principle, though the complexity of the problem grows with increasing number of dimensions.

From the discussion in Sections 3 and 4. it is clear that the method suggested in this paper is not restricted to the case of the coupled oscillators and to quantum mechanics in general. Indeed, we believe that the basic ideas, as expressed by Eqs. (34), (38) and (39) can find applications e.g. in the geometric optics.

Finally, from the mathematical point of view, considerations presented in this paper are rather heuristic. It would be highly desirable to put them into the rigorous form in the spirit of Harrell and Simon (1980), Hellfer (1998), Maslov and Fedoriuk (1981).

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