Multidimensional WKB approximation and the lifetime calculation

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A Wentzel-Kramers-Brillouin (WKB) approach for calculating the lifetime of the ground state of two coupled oscillators with the most probable escape path along one of the coordinate axes is suggested. The WKB approximation of the wave function in the neighborhood of this path is obtained by scaling the corresponding variable. An analytic formula for the lifetime is derived and numerically verified. The method is applied to the Henon-Heiles potentials. It is shown that the WKB method can be, in contrast to the numerical ones, easily extended to the problems of an arbitrary number of spatial dimensions.

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I. INTRODUCTION

The problem of harmonic oscillators coupled by a quartic interaction potential is of interest from the point of view of classical (see e.g., [1]) as well as quantum mechanics (see e.g., [2–5]) and even of general relativity [6].

Within quantum mechanics, the coupled oscillators serve as an important model system in the study of the unimolecular vibrational energy transfer (see e.g., [2–4]) or stationary states of the vibrational motion of the molecules (see e.g., [5]) and the energies of stationary states have been calculated in a number of papers [7–16].

In this paper, we investigate this problem from the point of view of the theory of resonances [17–19], i.e., we calculate the lifetime of the ground state of two coupled oscillators

$$\left[-\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}+V(x,y)\right]\psi=E\psi. \tag{1}$$

Here, the potential

$$V(x,y)=P(x,y)-\mu Q(x,y) \tag{2}$$

consists of the potential of two independent harmonic oscillators

$$P(x,y)=x^2+\omega^2y^2 \tag{3}$$

and the potential describing their coupling

$$Q(x,y)=x^4+\gamma x^2y^2+\delta y^4. \tag{4}$$

We assume that the coupling constant μ is small, $0<\mu\ll 1$ and ω, γ, and δ are real parameters.

Due to the form of the potential, the energy $E=\mathrm{Re}\,E+i\,\mathrm{Im}\,E$ has a small imaginary part $\mathrm{Im}\,E<0$, which can be calculated as a series in the coupling constant μ [17,18,20–22]. The lifetime is given by the equation $\tau=-1/(2\,\mathrm{Im}\,E)$.

To express $\mathrm{Im}\,E$ as a series in the coupling constant μ one usually proceeds as follows [17,20–22]. Starting from the time-independent version of the continuity equation for the probability density yielding ImE as a ratio of the probability current at infinity and the norm of the wave function, the wave function inside the potential barrier is approximated by the Rayleigh-Schrödinger perturbation theory (RSPT). Since the dominant contribution to the norm of the quasistationary wave function comes from the region around the origin, the RSPT approximation can be used to calculate the norm of the wave function. The wave function in the classically forbidden region and outside the potential barrier is approximated by the Wentzel-Kramers-Brillouin (WKB) wave function. Then, the WKB approximation is used to calculate the probability current at infinity. The same normalization of the RSPT and WKB approximations is guaranteed by the asymptotic matching of these functions in the overlap region of their mutual validity.

The most difficult step in this procedure is the calculation of the multidimensional WKB wave function. The standard formulation of the WKB method cannot be used for this aim. At the zeroth order of the method one has to solve the nonlinear equation

$$\left(\frac{\partial S_0(x,y)}{\partial x}\right)^2+\left(\frac{\partial S_0(x,y)}{\partial y}\right)^2=V(x,y)-\mathrm{Re}\,E, \tag{5}$$

the analytic solution of which is not known.

It was noted in [17] that to calculate $\mathrm{Im}\,E$ it is not necessary to know the approximate wave function for all x and y. The dominant contribution to the probability current at infinity comes from the neighborhood of the lines of the largest gradient of the potential, called the most probable escape paths (MPEP's). To calculate $\mathrm{Im}\,E$ it is sufficient to know these paths and the approximation of the wave function in their neighborhood.

In [17], the MPEP's were determined as a solution of the classical equations of motion and the WKB approximation in the neighborhood of these lines was obtained via semiclassical approximation. The analytic formula for $\mathrm{Im}\,E$ was derived for the case $\omega=1$. This result was rederived in [18] using the path-integral approach (see also [19]).

In this paper, we shall attack the problem from a different point of view. Due to the form of the coupling potential

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$Q(x,y)$, Eq. (4), the probability current at infinity comes from the neighborhood of four lines $y=0$ (x axis), $x=0$ (y axis), $y=x$ and $y=-x$ (see also [17]). In this paper we will restrict ourselves to the case when MPEP is directed along either x or y axes, i.e., to the first or second cases. In Sec. II, we calculate the imaginary part of the energy assuming that the MPEP is directed along the x axis. In the neighborhood of the MPEP we suggest a novel WKB approximation to the wave function. This approximation is obtained by scaling one of the variables. This is the main point of this paper. The rest of Sec. II is devoted to elaboration of this idea. First, we find the terms of the WKB expansion. Second, the asymptotic matching of the RSPT and WKB wave functions in the overlap region of mutual validity is performed in the same way as it was done for the one-dimensional problems [20]. Finally, we derive an analytic formula for $\mathrm{Im}\,E$ for the ground state of the problem, Eq. (1). In the Sec. III, this formula is generalized to the case of the MPEP along the y axis, to the problems of an arbitrary number of space dimensions and to the Hénon-Heiles Hamiltonians. The result for $\omega=1$ known from previous papers is obtained as a special case. New analytic results are verified numerically by means of the dispersion relation technique and complex scaling method in Sec. IV. It is shown that the multidimensional WKB method provides very accurate results for the states having a long lifetime. In the Appendix the properties of the special functions needed in the Sec. II are derived.

II. CALCULATION OF THE IMAGINARY PART OF THE ENERGY

In this section we perform the calculation of the imaginary part of the ground state energy at the zeroth order of the coupling constant μ. To be more concrete, we suppose that the MPEP is directed along the x axis. The case of the MPEP directed along the y axis is discussed later.

Performing the scaling $y\to y/\omega^{1/2}$ Eq. (1) becomes

$$\left[-\frac{\partial^2}{\partial x^2}+x^2+\omega\left(-\frac{\partial^2}{\partial y^2}+y^2\right)-\mu\left(x^4+\frac{\gamma}{\omega}x^2y^2+\frac{\delta}{\omega^2}y^4\right)\right]\psi=(\mathrm{Re}\,E+i\,\mathrm{Im}\,E)\psi. \tag{6}$$

Now we multiply Eq. (6) from the left by ψ^* and integrate in the plane xy. Further we take complex conjugate of Eq. (6), multiply it by ψ from the left and integrate. Subtracting the resulting two equations and integrating by parts we obtain

$$\int_{-\infty}^{\infty}\left[\psi(x,y)\frac{\partial\psi^*(x,y)}{\partial x}-\psi^*(x,y)\frac{\partial\psi(x,y)}{\partial x}\right]_{-\infty}^{\infty}dy+\omega\int_{-\infty}^{\infty}\left[\psi(x,y)\frac{\partial\psi^*(x,y)}{\partial y}-\psi^*(x,y)\frac{\partial\psi(x,y)}{\partial y}\right]_{-\infty}^{\infty}dx=2i\,\mathrm{Im}\,E\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|\psi(x,y)|^2dx\,dy. \tag{7}$$

Since we suppose that the dominant contribution to the probability current comes from the current along the x axis, we neglect the second term on the left-hand side of this equation. Because of the symmetry of the potential in Eq. (6) with respect to the inversion $x\to -x$, the probability current for $x\to\infty$ is the same as for $x\to-\infty$. Hence, the formula for $\mathrm{Im}\,E$ reads [17]

$$\mathrm{Im}\,E=\frac{1}{i}\frac{\int_{-\infty}^{\infty}\lim_{x\to\infty}[\psi(x,y)(\partial\psi^*(x,y)/\partial x)-\psi^*(x,y)(\partial\psi(x,y)/\partial x)]dy}{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|\psi(x,y)|^2dx\,dy}. \tag{8}$$

A. Norm of the wave function

The wave function $\psi(x,y)$ in the denominator of Eq. (8) can be at the zeroth order of μ replaced by the unperturbed wave function, i.e., by the zeroth-order RSPT approximation [17,20–22]

$$\psi_0(x,y)=e^{-(x^2+y^2)/2}. \tag{9}$$

The norm of this wave function equals

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|\psi_0(x,y)|^2dx\,dy=\pi. \tag{10}$$

B. The WKB approximation of the wave function

The probability current at infinity, the numerator of Eq. (8), is calculated by means of the WKB wave function [17,20–22]. According to our assumption, the dominant contribution to the probability current at infinity comes from the neighborhood of the x axis, that is from the region $y\approx 0$. In this region, the dominant contribution to the probability current at infinity comes from the classically forbidden region $x^2\approx\mu x^4$ [17,20–22]. To find an approximation to the wave function in the region of large $x\approx\mu^{-1/2}$ and small $y\approx 0$, we scale the coordinate x by means of the substitution $x=\mu^{-1/2}u$. Equation (6) then becomes

$$\left[\mu^2\frac{\partial^2}{\partial u^2}+\mu\omega\frac{\partial^2}{\partial y^2}\right]\psi$$
$$=\left[u^2-u^4+\mu\left(\omega y^2-\frac{\gamma}{\omega}u^2y^2-E_0\right)+\ \dots\ \right]\psi. \tag{11}$$

Here, the RSPT expansion of the real part of the energy $\mathrm{Re}\,E=E_0+\mu E_1+\mu^2E_2+\ \dots$ was used.

At this point, we would like to emphasize that the scaling of the variable x is the crucial idea for obtaining the multidimensional WKB approximation of the wave function. More detailed discussion follows.

Searching for the solution of Eq. (11) in the form of the WKB wave function taken at the zeroth order of μ

$$\psi^{(0)}_{\mathrm{WKB}}(u,y)=\exp\left[\frac{S_0(u,y)}{\mu}+S_1(u,y)\right] \tag{12}$$

and comparing the terms of the same power in μ we find in the minus first order of μ

$$\frac{\partial S_0(u,y)}{\partial y}=0. \tag{13}$$

Obviously, this equation has the solution

$$S_0(u,y)=S_0(u). \tag{14}$$

In the zeroth order of μ we find

$$\frac{dS_0}{du}=\pm\,u(1-u^2)^{1/2}, \tag{15}$$

where the other terms on the left-hand side of Eq. (11) vanish due to Eq. (13). Equation (15) can be easily integrated

$$S_0(u)=\frac{(1-u^2)^{3/2}}{3}-A_0. \tag{16}$$

Here, we chose the minus sign in Eq. (15) to get the exponentially decaying solution in the classically forbidden region corresponding to the particle going through the barrier to infinity. The integration constant was put equal to $-A_0$. This constant will be determined from the asymptotic matching of the functions, Eqs. (9) and (12). The eikonal term $S_0(u)$ gives the probability current along the x axis. Therefore, it is not surprising that it has the same form as for the one-dimensional potential $V(x)=x^2-\mu x^4$ [20].

At the first order of μ we get

$$2\frac{dS_0}{du}\frac{\partial S_1(u,y)}{\partial u}+\frac{d^2S_0}{du^2}+\omega\left[\frac{\partial^2S_1(u,y)}{\partial y^2}+\left(\frac{\partial S_1(u,y)}{\partial y}\right)^2\right]$$
$$=y^2\left(\omega-\frac{\gamma}{\omega}u^2\right)-E_0. \tag{17}$$

This is the equation for the transport term $S_1(u,y)$ which gives the probability current in the potential well in the vicinity of the x axis. The terms depending only on the variable u can be integrated as in the one-dimensional case [20]

$$S_1(u,y)=-\frac{1}{4}\ln(u^2-u^4)-\frac{E_0}{4}\ln\frac{1+(1-u^2)^{1/2}}{1-(1-u^2)^{1/2}}$$
$$+\phi(u,y)-A_1, \tag{18}$$

where the integration constant was put equal to $-A_1$.

Inserting Eq. (18) into Eq. (17) we see that the function $\phi(u,y)$ obeys the equation

$$-2u(1-u^2)^{1/2}\frac{\partial\phi(u,y)}{du}+\omega\left[\frac{\partial^2\phi(u,y)}{\partial y^2}+\left(\frac{\partial\phi(u,y)}{\partial y}\right)^2\right]$$
$$=y^2\left(\omega-\frac{\gamma}{\omega}u^2\right). \tag{19}$$

The solution of this equation is searched for in the form

$$\phi(u,y)=-\frac{f(u)}{2}y^2-\frac{\ln g(u)}{2}. \tag{20}$$

By inserting this ansatz into Eq. (19) and comparing the terms of the same power in y we obtain the equations for the functions $f(u)$ and $g(u)$

$$u(1-u^2)^{1/2}\frac{df(u)}{du}+\omega f(u)^2=\omega-\frac{\gamma}{\omega}u^2 \tag{21}$$

and

$$\frac{u(1-u^2)^{1/2}}{\omega}\,\frac{d\ln g(u)}{du}=f(u). \tag{22}$$

The functions $f(u)$ and $g(u)$ can be expressed in terms of the associate Legendre functions. The explicit form of these functions is given in the Appendix.

C. The asymptotic matching

To find the integration constants A_0 and A_1 in Eqs. (16) and (18) we require that for $u\to 0$ the RSPT and WKB functions in the zeroth order of μ (asymptotically) equal [20]

$$\frac{S_0(\mu^{1/2}x,y)}{\mu}+S_1(\mu^{1/2}x,y)=\ln\psi_0(x,y). \tag{23}$$

To get the left-hand side of Eq. (23) accurate in the zeroth order of μ, we take the expansion of the S_0 and S_1 functions near $u=0$ [20].

For $S_0(u)$ we take the first two terms of the expansion

$$S_0(u)=\frac{1}{3}-\frac{u^2}{2}+O(u^4). \tag{24}$$

Substituting $u=\mu^{1/2}x$ and dividing this equation by μ we get in the zeroth order of μ

$$\frac{S_0(\mu^{1/2}x)}{\mu}=\frac{1}{3\mu}-\frac{x^2}{2}. \tag{25}$$

To get the asymptotic expansion of $S_1(u,y)$ we take

$$-\frac{\ln(u^2-u^4)}{4}=-\frac{\ln u^2}{4}+O(u^2) \tag{26}$$

and

$$-\frac{E_0}{4}\ln\frac{1+(1-u^2)^{1/2}}{1-(1-u^2)^{1/2}}=-\frac{E_0}{4}\ln\frac{4}{u^2}+O(u^2). \tag{27}$$

By inserting the asymptotic expansion of the functions $f(u)$ and $g(u)$ for $u\to 0$, Eqs. (A3) and (A9) of the Appendix, into Eq. (20) we get also the expansion of the function $\phi(u,y)$

$$\phi(u,y)=-\frac{y^2}{2}+\frac{\omega}{4}\ln\frac{4}{u^2}+O(u^2). \tag{28}$$

By inserting these expansions, Eqs. (26), (27), and (28), into Eq. (18) and substituting $u=\mu^{1/2}x$ we get in the zeroth order of μ

$$S_1(\mu^{1/2}x,y)=\frac{E_0-\omega-1}{2}\ln x-\frac{y^2}{2}-\frac{E_0-\omega}{4}\ln\frac{4}{\mu}-\frac{\ln\mu}{4}. \tag{29}$$

By inserting Eqs. (25) and (29) and the ground state energy $E_0=1+\omega$ into the left-hand side of Eq. (23) and Eq. (9) into the right-hand side of Eq. (23) we obtain in the zeroth order of μ

$$\frac{1}{3\mu}-\frac{1}{4}\ln\frac{4}{\mu}-\frac{\ln\mu}{4}=\frac{A_0}{\mu}+A_1. \tag{30}$$

This is the equation for the integration constants A_0 and A_1 we searched for. Using this equation, the WKB and RSPT approximations have the same normalization.

We note that for the excited states with the unperturbed energies $E_0=2K_x+1+\omega(2K_y+1)$, where $K_x,K_y=0,1,2,\ldots$, it is not possible to find the overlap region of the mutual validity of the RSPT and WKB approximations. The asymptotics of the RSPT approximation in the zeroth order of μ reads for an arbitrary state

$$\ln\psi_0(x,y)\approx-\frac{x^2+y^2}{2}+K_x\ln x+K_y\ln y. \tag{31}$$

Comparing the multiplicative factors in front of the logarithmic terms in Eqs. (29) and (31) shows, quite generally, that the RSPT and WKB wave functions overlap only for the states with $K_y=0$. Analogously, taking the MPEP along the y axis we find that the RSPT and WKB approximations overlap only for the states with $K_x=0$. Obviously, our WKB approximation does not provide sufficient information about the wave function for large distances from the x or y axes. This approximation is able to describe the exponential but not the power dependence of the wave function in the direction perpendicular to that of the probability current. Therefore, it can be used for the ground state but not for a general excited state.

D. The final formula for Im E

Taking $u\to\infty$ in Eqs. (16), (18), and (20) we get the asymptotics of the WKB wave function

$$\psi^{(0)}_{\mathrm{WKB}}(x\to\infty,y)=\exp\left[-\sum_{i=0}^{1}A_i\mu^{i-1}\right]\times\frac{e^{i\mu^{1/2}x^3/3}(1+O(1/x^2))}{(-i)^{1/2}\mu^{1/2}x}\,\frac{e^{-f(\mu^{1/2}x)y^2/2}}{g(\mu^{1/2}x)^{1/2}}. \tag{32}$$

By inserting the last equation into Eq. (8) and using Eq. (30) for the constants A_0 and A_1 we find that

$$\mathrm{Im}\,E(\mu,\omega,\gamma)=-\frac{2}{\pi}\left(\frac{4}{\mu}\right)^{1/2}e^{-2/(3\mu)}T(\omega,\gamma)[1+O(\mu)], \tag{33}$$

where

$$T(\omega,\gamma)=\lim_{x\to\infty}\frac{\int_{-\infty}^{\infty}\exp[-\mathrm{Re}\,f(\mu^{1/2}x)y^2]dy}{|g(\mu^{1/2}x)|}. \tag{34}$$

The argument of the real functions $f(u)$ and $g(u)$ becomes purely imaginary for $u>1$ and is real for $u<1$. Therefore, the functions $f(u)$ and $g(u)$ become for $u>1$ purely imaginary, while for $u<1$ they are real [see the discussion after Eq. (A6) of the Appendix]. Thus, we can write

$$\lim_{x\to\infty}\mathrm{Re}\,f(\mu^{1/2}x)=\lim_{u\to\infty}\mathrm{Re}\,f(u)=f(u=1) \tag{35}$$

and

$$\lim_{x\to\infty}|g(\mu^{1/2}x)|=\lim_{u\to\infty}|g(u)|=g(u=1). \tag{36}$$

Hence, the function $T(\omega,\gamma)$ can be written in the form

$$T(\omega,\gamma)=\frac{\int_{-\infty}^{\infty}\exp[-f(u=1)y^2]dy}{g(u=1)}=\frac{\pi^{1/2}}{\sqrt{f(u=1)}g(u=1)}. \tag{37}$$

Using the explicit form of the functions $f(u)$ and $g(u)$ given in the Appendix the last equation can be rewritten in the form (see Appendix)

$$T(\omega,\gamma)=\frac{\omega^{1/2}\pi}{\Gamma(1+\omega)}\left\{-\sin[\pi(\nu-\omega)]\frac{\Gamma(1+\nu-\omega)}{\Gamma(1+\nu+\omega)}\right\}^{-1/2}, \tag{38}$$

where

$$\nu=-\frac{1}{2}\pm\frac{(1+4\gamma)^{1/2}}{2}. \tag{39}$$

The imaginary part of the energy, Eq. (33), was obtained as the product of three factors. The first one, $2/\pi$, corresponds to the norm of the two-dimensional wave function. The second one, the μ-dependent part, is the probability current for the one-dimensional potential $V(x)=x^2-\mu x^4$. The last one, $T(\omega,\gamma)$, is the probability current in the potential well in the vicinity of the x axis for $x^2\approx\mu x^4$. For the one-dimensional potential $V(x)=x^2-\mu x^4$ this term equals 1.

For $\gamma=\omega(\omega+1)$, the expression in the curly brackets in Eq. (38) equals zero and the function $T(\omega,\gamma)$ diverges at this point. For $\gamma>\omega(\omega+1)$ this expression becomes negative and the function $T(\omega,\gamma)$ is purely imaginary. Therefore, Eq. (33) can be used only for

$$\gamma<\omega(\omega+1). \tag{40}$$

When approaching the critical point $\gamma=\omega(\omega+1)$ from the left, Eq. (33) becomes inaccurate. It is obvious that for $\gamma\geqslant\omega(\omega+1)$ the assumption of the MPEP oriented along the x axis is not satisfied.

We note that for $\gamma<\omega(\omega+1)$ the function $T(\omega,\gamma)$ is monotonically decreasing with increasing ω for fixed γ and monotonically increasing with increasing γ for fixed ω.

For $\omega=1$, Eqs. (33) and (38) yield the formula given in [17,18].

Finally we note that Eq. (33) was obtained by performing calculations at the zeroth order of μ. Therefore, the error following from the use of this equation is of the order μ.

III. GENERALIZATION

In this section we discuss possible generalizations of the formula, Eq. (33).

A. MPEP along the y axis

In the preceding section we supposed that the MPEP was directed along the x axis. Here we show that, despite the asymmetry in the x and y variables for $\omega\neq1$, the case of the MPEP directed along the y axis can be treated in the same manner.

Dividing Eq. (6) by ω we get

$$\left[-\frac{\partial^2}{\partial y^2}+y^2+\frac{1}{\omega}\left(-\frac{\partial^2}{\partial x^2}+x^2\right)-\frac{\mu\delta}{\omega^3}\left(y^4+\frac{\gamma\omega}{\delta}x^2y^2+\frac{\omega^2}{\delta}x^4\right)\right]\psi=\frac{E}{\omega}\psi. \tag{41}$$

Thus, performing the substitutions $\omega\to\tilde{\omega}=1/\omega$, $\mu\to\tilde{\mu}=\mu\delta/\omega^3$, $E\to\tilde{E}=E/\omega$, $\gamma\to\tilde{\gamma}=\gamma/\delta$, and $\delta\to\tilde{\delta}=1/\delta$ we can also use Eqs. (33) and (38) for the imaginary part of the energy given by the probability current along the y axis

$$\operatorname{Im}\tilde{E}(\tilde{\mu},\tilde{\omega},\tilde{\gamma})=\omega\operatorname{Im}E\left(\frac{\mu\delta}{\omega^3},\frac{1}{\omega},\frac{\gamma}{\delta}\right). \tag{42}$$

The condition for applicability of Eq. (38), $\tilde{\gamma}<\tilde{\omega}(1+\tilde{\omega})$, reads in terms of the original parameters

$$\gamma<\frac{\delta}{\omega^3}\omega(1+\omega). \tag{43}$$

It means that the assumption of the MPEP directed along the y axis is justified if the parameter γ satisfies condition (43).

Summarizing, our method can be used for the potentials Eq. (1) if the parameter γ obeys inequalities Eqs. (40) or (43).

B. Formula for an arbitrary number of space dimensions

The suggested method was also applied to the simplest nonseparable model of the D-dimensional coupled oscillators with the MPEP oriented along one of the coordinate axes

$$\left[\sum_{i=1}^{D}-\frac{\partial^2}{\partial x_i^2}+x_1^2+\sum_{i=2}^{D}\omega_i^2x_i^2-\mu\left(x_1^4+x_1^2\sum_{i=2}^{D}\gamma_ix_i^2\right)\right]\psi=E\psi, \tag{44}$$

where inequalities

$$\gamma_i<\omega_i(\omega_i+1),\quad i=2,3,\ldots,D \tag{45}$$

are assumed. Proceeding along the same lines as in the two-dimensional case, we easily generalize formula (33) to an arbitrary number of dimensions

$$\operatorname{Im}E(\mu,\omega_2,\ldots,\omega_D,\gamma_2,\ldots,\gamma_D)=-\frac{2}{\pi^{D/2}}\left(\frac{4}{\mu}\right)^{1/2}e^{-2/(3\mu)}\Pi_{i=2}^{D}T(\omega_i,\gamma_i)[1+O(\mu)]. \tag{46}$$

The individual terms in this formula have interpretation analogous to that in Eq. (33). The first one, $2/\pi^{D/2}$, corresponds to the norm of the D-dimensional wave function, the second one, the μ-dependent part, gives the probability current along the x_1 axis and the last one, the product of the functions $T(\omega_i,\gamma_i)$ gives the probability current in the $D-1$ dimensional well in the neighborhood of the x_1 axis.

C. Hénon-Heiles Hamiltonian

The suggested method can be also applied to the case of the Hénon-Heiles Hamiltonian

$$\left[-\frac{\partial^2}{\partial x^2}-\frac{\partial^2}{\partial y^2}+x^2+\omega'^2y^2-\mu'(x^3+\gamma'xy^2)\right]\psi=E\psi, \tag{47}$$

which differs from the problem Eq. (1) in the power dependence of the variable x in the interaction potential.

Proceeding similarly as in the Sec. II we obtain

$$\mathrm{Im}\,E(\mu',\omega',\gamma')=-\frac{1}{\pi}\frac{4}{\mu'}e^{-8/(15\mu'^2)}T(2\omega',4\gamma')\times[1+O(\mu'^2)], \tag{48}$$

where the function $T(2\omega',4\gamma')$ is given by Eq. (38) for $\omega=2\omega'$ and $\gamma=4\gamma'$. Formula (48) can be used for γ' satisfying the inequality

$$\gamma'<\omega'(\omega'+1/2). \tag{49}$$

Analogously to Eq. (33), the first factor in Eq. (48), $1/\pi$, corresponds to the norm of the wave function. This term is twice smaller than that for the problem, Eq. (1). This is due to the fact that the perturbation potential in Eq. (47) is an odd function of x, while in Eq. (1) it is an even function. Thus, while for the problem Eq. (1), there is a nonzero probability current both at the $x\to\infty$ and $x\to-\infty$ limits, the probability current vanishes for the problem Eq. (47) at $x\to-\infty$. The second (μ'-dependent) term in Eq. (48) is the same as for the one-dimensional potential $V(x)=x^2-\mu' x^3$ [23] and gives the probability current along the x axis. The last term, $T(2\omega',4\gamma')$, gives the probability current in the well in the vicinity of the x axis for $x^2\approx\mu' x^3$.

IV. NUMERICAL CALCULATIONS

In this section we describe numerical tests of the analytic formulas found above. This is done in two ways: using the dispersion relation technique and by direct numerical calculation.

A. Dispersion relation

The coefficients of the perturbation coefficients of the energy

$$E=\sum_{n=0}^{\infty}E_n\beta^n \tag{50}$$

for the bound state potentials $V(x,y)=P(x,y)+\beta Q(x,y)$, $\beta>0$ can be at large orders calculated via the dispersion relation [17,21,22,24]

$$E_n=-\frac{1}{\pi}\int_{-\infty}^{0}\frac{\mathrm{Im}\,E(\tilde{\beta})}{\tilde{\beta}^{n+1}}d\tilde{\beta}. \tag{51}$$

The dominant contribution to the integral Eq. (51) for $n\to\infty$ comes from the region $\mu\to 0$, $\mu=-\tilde{\beta}$.

Thus, we can calculate perturbation coefficients for the energy of the bound state problems either directly from the perturbation theory or by inserting expression for $\mathrm{Im}\,E$, Eq. (33), into Eq. (51). This method of verification of the formulas for $\mathrm{Im}\,E$ can be, however, used only for the potentials in Eq. (1) that have bound states for $\mu=-\beta$. In the following paragraph we find the conditions for the parameters in Eq. (1) following from this requirement.

The existence of the bound states for the potential $V(x,y)=P(x,y)+\beta Q(x,y)$ in Eq. (1) for $x=0$ requires $\delta>0$. Since the term x^2y^2 reaches its maximum value for $x=y$ and $x=-y$ we rotate the coordinate axes about the right angle

$$\tilde{x}=\frac{x+y}{\sqrt{2}}, \tag{52}$$

$$\tilde{y}=\frac{x-y}{\sqrt{2}} \tag{53}$$

and get from Eq. (1) an equivalent equation

$$\left\{-\frac{\partial^2}{\partial\tilde{x}^2}-\frac{\partial^2}{\partial\tilde{y}^2}+\frac{1+\omega^2}{2}(\tilde{x}^2+\tilde{y}^2)+(1-\omega^2)\tilde{x}\tilde{y}+\frac{\beta}{4}[(\tilde{x}+\tilde{y})^4+\gamma(\tilde{x}^2-\tilde{y}^2)^2+\delta(\tilde{x}-\tilde{y})^4]\right\}\psi=E\psi. \tag{54}$$

The stability of the potential in this equation for $\tilde{x}=0$ or $\tilde{y}=0$ requires that $\gamma>-(1+\delta)$. Thus, the dispersion relation Eq. (51) can be used only for the potentials Eq. (1) satisfying the conditions

$$\delta>0,\gamma>-(1+\delta). \tag{55}$$

These conditions are, however, the conditions restricting the use of the dispersion relation Eq. (51), not the use of Eq. (33).

For μ going to zero, behavior of $\mathrm{Im}\,E$ described by Eq. (33) is given by behavior of the μ-dependent part $\mu^{-1/2}e^{-2/(3\mu)}$. Therefore, for $\delta<\omega^3$ leading to $\mu>\tilde{\mu}$ [see Eq. (42)], the dominant contribution to the probability current at infinity comes from the x axis, for $\delta>\omega^3$ ($\mu<\tilde{\mu}$) from the y axis, and for $\delta=\omega^3$ ($\mu=\tilde{\mu}$) we have to sum the contributions from both MPEP's.

Hence, by inserting Eq. (33) with $\mu=-\tilde{\beta}$ into Eq. (51) we obtain the large-order behavior of the series Eq. (50) for the problem Eq. (1)

$$E_n=\frac{4}{\pi^2}T(\omega,\gamma)(-1)^{n+1}\left(\frac{3}{2}\right)^{n+1/2}\Gamma(n+1/2)\times[1+O(1/n)],\quad \delta<\omega^3, \tag{56}$$

$$E_n=\frac{4\omega}{\pi^2}T(1/\omega,\gamma/\delta)\sqrt{\frac{3}{2}}(-1)^{n+1}\left(\frac{3\delta}{2\omega^3}\right)^{n}\Gamma(n+1/2)\times[1+O(1/n)],\quad \delta>\omega^3, \tag{57}$$

and

$$E_n=\frac{4}{\pi^2}[T(\omega,\gamma)+\omega T(1/\omega,\gamma/\delta)](-1)^{n+1}\left(\frac{3}{2}\right)^{n+1/2}\times\Gamma(n+1/2)[1+O(1/n)],\quad \delta=\omega^3. \tag{58}$$

TABLE I. The numerical test of the formula Eq. (33) by means of the dispersion relation technique. The values of the multiplicative constant in Eqs. (56), (57), and (58) obtained numerically by [5,5] Thiele-Padé extrapolation of the ratio $E_n/[(-1)^{n+1}(\frac{3}{2})^{n+1/2}\Gamma(n+1/2)]$ from the interval n from 40 to 50 are compared with the functions $(4/\pi^2)T(\omega,\gamma)$ for $\delta<\omega^3$, $(4/\pi^2)[T(\omega,\gamma)+\omega T(1/\omega,\gamma/\delta)]$ for $\delta=\omega^3$, and $(4\omega/\pi^2)T(1/\omega,\gamma/\delta)$ for $\delta>\omega^3$ (denoted as WKB). Δ denotes the difference of the analytic and extrapolated values.

ω	γ	δ	Extrapolation	WKB	Δ
2	16/3	0	5.870 083 062 7	5.874 998 385 2	0.491×10^{-2}
2	4	0	2.570 547 036 1	2.570 547 387 8	0.351×10^{-6}
2	3	0	1.728 278 668 5	1.728 278 681 5	0.130×10^{-7}
2	2	0	1.244 216 074 0	1.244 216 079 6	0.557×10^{-8}
2	-1	0	0.564 598 208 5	0.564 598 210 4	0.191×10^{-8}
3	3	0	1.222 077 569 9	1.222 077 575 5	0.557×10^{-8}
5	5	0	1.205 852 575 0	1.205 852 580 6	0.556×10^{-8}
11	11	0	1.193 691 669 9	1.193 691 675 5	0.553×10^{-8}
2	4	18/5	2.570 547 370 9	2.570 547 387 8	0.168×10^{-7}
2	4	4	2.570 547 369 6	2.570 547 387 8	0.181×10^{-7}
2	4	22/5	2.570 547 364 2	2.570 547 387 8	0.235×10^{-7}
2	4	16/3	2.570 547 325 6	2.570 547 387 8	0.621×10^{-7}
2	4	6	2.570 641 847 9	2.570 547 387 8	-0.944×10^{-4}
2	4	20/3	2.569 103 774 6	2.570 547 387 8	0.144×10^{-2}
2	4	8	5.529 205 877 0	5.528 620 757 0	-0.585×10^{-3}
3	6	27	5.589 645 087 9	5.589 665 089 7	0.200×10^{-4}
4	8	64	6.069 189 272 2	6.069 174 352 0	-0.149×10^{-4}
10	20	1000	10.039 074 161 9	10.039 075 275 2	0.111×10^{-5}
2	4	32/3	2.310 262 074 2	2.310 226 605 8	-0.354×10^{-4}
2	4	12	2.159 849 893 7	2.159 850 698 3	0.804×10^{-6}
2	4	20	1.795 059 117 6	1.795 059 125 6	0.794×10^{-8}
2	4	40	1.595 941 057 4	1.595 941 063 9	0.655×10^{-8}

Using MAPLE we calculated the first 50 coefficients E_n in the form of the rational numbers for different values of ω, γ, and δ satisfying conditions (40) or (43) and (55) by the difference equation method described in [17]. Extrapolating the ratio of the exact E_n coefficients and those given by Eqs. (56), (57), and (58) for n from 40 to 50 by means of the [5,5] Thiele-Padé approximants (see e.g., [25]) we obtained results shown in Table I. It is seen that for γ far from the critical value $\omega(\omega+1)$ the accuracy of Eqs. (56), (57), and (58) is about eight significant digits. When approaching the critical value, the accuracy of the formulas goes down as expected. Furthermore, it is seen that for δ approaching the value ω^3, the contribution of both MPEP's has to be taken into account.

By inserting Eq. (46) for $D=3$ into Eq. (51) we obtain the large-order behavior of the series Eq. (50) for the problem Eq. (44)

$$E_n=\frac{4}{\pi^{5/2}}T(\omega_2,\gamma_2)T(\omega_3,\gamma_3)(-1)^{n+1}\left(\frac{3}{2}\right)^{n+1/2}\times\Gamma(n+1/2)[1+O(1/n)]. \tag{59}$$

Using MAPLE we calculated the first 50 E_n coefficients. Numerical verification of Eq. (59) is shown in Table II.

The numerical analysis described above indicates that Eqs. (56), (57), (58), and (59) are exact for n going to infinity. This implies that Eqs. (33), (42), and (46) are exact for μ going to zero.

B. Direct numerical solution

Formula (48) was compared for some definite values of μ with the numerical results obtained via the complex scaling method (see e.g., [23,26–28]).

It is seen from Table III that for finite values of the coupling constant μ' the WKB approximation provides for $\gamma \ll \omega(\omega+1/2)$ good results close to the exact value. As it can be expected, the agreement between direct numerical solution and the WKB method goes down with increasing value of the coupling constant μ' and for fixed ω with increasing γ. Particularly, it is seen that for $\omega=3$, the WKB method provides for μ' between 0.17 and 0.19, good results only for γ smaller than 2, i.e., only for γ sufficiently far from the critical value 10.5.

Generally speaking, the WKB method is better, the smaller the value of $\mathrm{Im}\,E$ is. Particularly, for negative values

TABLE II. The numerical test of the formula Eq. (46) for $D=3$ by means of the dispersion relation technique. The values of the multiplicative constant in Eq. (59) obtained numerically by [5,5] Thiele-Padé extrapolation of the ratio $E_n/[(-1)^{n+1}(\frac{3}{2})^{n+1/2}\Gamma(n+1/2)]$ from the interval n from 40 to 50 are compared with the function $(4/\pi^5/2)T(\omega_2,\gamma_2)T(\omega_3,\gamma_3)$ for fixed $\omega_2=2$, $\gamma_2=2$ and varying ω_3, γ_3. Δ denotes the difference of the analytic and extrapolated values.

ω_3	$\gamma_3/(2\omega_3)$	Extrapolation	$4T(2,2)T(\omega_3,\gamma_3)/\pi^{5/2}$	Δ
2	1	4.452 317 804 3	4.452 318 678 9	0.874×10^{-6}
3	1	3.934 556 738 0	3.934 556 713 0	-0.250×10^{-7}
5	1	3.661 541 187 0	3.661 541 139 6	-0.474×10^{-7}
5	2	13.966 288 546 8	13.966 290 855 1	0.230×10^{-5}
5	1/2	2.088 597 929 7	2.088 597 936 0	0.631×10^{-8}

TABLE III. Comparison of the imaginary part of the energy $\mathrm{Im}\,E$ obtained via the complex scaling method (denoted as CS) and WKB approximation for the Hénon-Heiles Hamiltonian Eq. (47). The last number is rounded. The numbers in the parentheses give the percentage error of the WKB approximation with respect to the complex scaling method.

μ'	ω'	γ'	CS	WKB [error (%)]
0.15	$\sqrt{2}$	-1	0.380×10^{-9}	0.395×10^{-9} (4.2)
0.15	$\sqrt{2}$	1	0.152×10^{-8}	0.167×10^{-8} (9.9)
0.15	2	1	0.119×10^{-8}	0.129×10^{-8} (8.4)
0.15	2	2	0.207×10^{-8}	0.230×10^{-8} (11.)
0.15	2	3	0.391×10^{-8}	0.452×10^{-8} (16.)
0.17	1	1/2	0.199×10^{-6}	0.222×10^{-6} (11.6)
0.17	3	1/2	0.138×10^{-6}	0.152×10^{-6} (10.1)
0.17	10	1/2	0.124×10^{-6}	0.135×10^{-6} (8.9)
0.17	50	1/2	0.119×10^{-6}	0.130×10^{-6} (9.2)
0.17	3	7	0.159×10^{-5}	0.212×10^{-5} (33)
0.17	3	6	0.103×10^{-5}	0.130×10^{-5} (26)
0.17	3	2	0.228×10^{-6}	0.257×10^{-6} (12.7)
0.17	3	1/3	0.131×10^{-6}	0.144×10^{-6} (9.9)
0.17	3	-5	0.266×10^{-7}	0.275×10^{-7} (3.4)
0.18	1	1/2	0.136×10^{-5}	0.154×10^{-5} (13.2)
0.18	3	1/2	0.947×10^{-6}	0.106×10^{-5} (11.9)
0.18	10	1/2	0.847×10^{-6}	0.936×10^{-6} (10.5)
0.18	50	1/2	0.815×10^{-6}	$0.899\ 10^{-6}$ (10.3)
0.18	3	7	0.106×10^{-4}	0.147×10^{-4} (39)
0.18	3	6	0.691×10^{-5}	0.900×10^{-5} (30)
0.18	3	2	0.156×10^{-5}	0.178×10^{-5} (14.1)
0.18	3	1/3	0.898×10^{-6}	0.995×10^{-6} (10.8)
0.18	3	-5	0.183×10^{-6}	0.191×10^{-6} (4.4)
0.19	1	1/2	0.683×10^{-5}	0.789×10^{-5} (15.5)
0.19	3	1/2	0.478×10^{-5}	0.539×10^{-5} (12.8)
0.19	10	1/2	0.428×10^{-5}	0.479×10^{-5} (11.9)
0.19	50	1/2	0.412×10^{-5}	0.460×10^{-5} (11.6)
0.19	3	7	0.519×10^{-4}	0.751×10^{-4} (48)
0.19	3	6	0.341×10^{-4}	0.461×10^{-4} (35)
0.19	3	2	0.781×10^{-5}	0.912×10^{-5} (17)
0.19	3	1/3	0.453×10^{-5}	0.509×10^{-5} (12.4)
0.19	3	-5	0.934×10^{-6}	0.977×10^{-6} (4.6)

of γ, the method provides very good results in the wide range of the coupling constant μ' from 0 to about decimals. This can be easily understood, because in the case of the negative values of γ, the assumption of the MPEP directed along the x axis is fully justified.

V. CONCLUSIONS

An alternative WKB approach for calculating the lifetime of the ground state of the coupled oscillators was suggested. Assuming that the dominant contribution to the outgoing probability current comes from that along one of the coordinate axes we derived an alternative *analytic* formula for the imaginary part of the energy. This formula extends the known result in the case of the same frequencies to the case of arbitrary frequencies of the oscillators. This formula was further generalized for an *arbitrary number of space dimensions* and verified via extensive numerical calculations. It was shown that for the states having a long lifetime, the suggested method provides very accurate results.

The proposed WKB method yields very good results for the ground-state energy. For the excited states, however, the proposed approximations seem to be inadequate. For these states it is not possible to find the overlap region of the mutual validity of the RSPT and WKB approximations and hence guarantee the same normalization of these functions. For a general excited state we obviously also need information about the wave function at larger distances from the x or y axes than can be achieved by our WKB approximation.

If the parameter γ is so large that none of the conditions, Eqs. (40) and (43), is satisfied, the suggested method cannot be used as well. This is because the function $T(\omega,\gamma)$ Eq. (38) appearing in the final formula for $\mathrm{Im}\,E$ Eq. (33) becomes purely imaginary. In this case the dominant contribution to the imaginary part of the energy comes from the lines $y=x$ and $y=-x$. At a glance, this case can be treated by introducing new variables, Eqs. (52) and (53), and applying our method to Eq. (54) for $\beta=-\mu$. However, for $\omega\neq1$ a new coupling term $\tilde{x}\tilde{y}(1-\omega^2)$ appears in the unperturbed part of the Hamiltonian. This term prohibits our method from being used for $\omega\neq1$ and $\gamma>\omega(1+\omega)$ and $\gamma>\delta\omega(1+\omega)/\omega^3$. The physical reason for this is that our method, at least in the present form, can deal only with straight line MPEP's, while the discussed case presents the problem of the curved MPEP's [17]. The extension of our method to

these problems will be subject of further investigations.

Since the function $T(\omega,\gamma)$ diverges at the point $\gamma=\omega(\omega+1)$, the proposed method also does not provide reliable results for the values of γ satisfying conditions (40) and (43) but too close to this critical point.

In this paper we considered only the simplest case of the interaction potential, however, for the case of the straight line MPEP's, the extension to the more complex polynomial potentials seems to be straightforward [17].

From the mathematical point of view, the arguments given in this paper are rather heuristic. Nevertheless, on the basis of agreement of analytical and numerical approaches we believe that the results of this paper are correct. Thus, from a mathematical point of view these results represent conjectures that should be rigorously proven, namely the following ones. First, the agreement of the complex scaling method and the WKB approximation seems to confirm the conjecture made in [23], that the complex scaling method works for all potentials, not only for dilation analytic ones [29]. Second, one should get rigorous proof of the formula Eq. (33), as it was also done for the Avron formula [30] describing the Zeeman effect in the hydrogen atom in [31,32]. Since the latter problem can be transformed to a problem similar to the one considered in this paper, namely to the problem of four coupled oscillators with internal $O(2)\times O(2)$ symmetry [33], this could be relatively easy. The last and probably the most difficult problem is to find the connection between the theory of pseudodifferential operators based on the Weyl quantitization scheme (see e.g., [31,34,35]) and the approach suggested in this paper. Such a connection has to exist, because our formulation of the WKB method gives essentially the same results as the usual semiclassical one.

The main result of this paper is that the WKB method can be easily extended to the problems with an arbitrary number of space dimensions (see also [17]) for the polynomial potentials with the straight line MPEP's (or for the potentials that can be well approximated by these potentials). This is not valid for any numerical method and from this point of view, the analytic WKB method is preferable to the numerical ones.

Until now, the multidimensional WKB calculation of the lifetime of the ground state of the coupled oscillators has been restricted to the case of the same oscillators frequencies only. Since the method suggested in this paper generalizes it to a wide class of the potentials with arbitrary frequencies of the oscillators, we believe that it is of much interest.

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APPENDIX

In this appendix we derive the explicit form of the functions $f(u)$ and $g(u)$ and their properties used in Sec. II.

Introducing the variable $w=(1-u^2)^{1/2}$ and inserting Eq. (22) into Eq. (21) after some manipulation we get

$$(1-w^2)\frac{d^2g[(1-w^2)^{1/2}]}{dw^2}-2w\frac{dg[(1-w^2)^{1/2}]}{dw}+\left(\gamma-\frac{\omega^2}{1-w^2}\right)g[(1-w^2)^{1/2}]=0 \tag{A1}$$

and

$$f[(1-w^2)^{1/2}]=\frac{w^2-1}{\omega}\,\frac{d\ln g[(1-w^2)^{1/2}]}{dw}. \tag{A2}$$

Equation (A1) is the equation for the associated Legendre functions on the cut $-1<w<1$ [36]. Let us note that Eqs. (A1) and (A2) are for $\omega=1$ identical to Eqs. (4.17) and (4.18) of [17]. However, they are derived in a different way here.

The physically relevant solution of Eqs. (A2) and (A1) can be found from the requirement that the overlap region of mutual validity of the RSPT and WKB approximations exists. To satisfy Eq. (23), we have to get on the left-hand side of this equation the term $-y^2/2$ appearing in $\ln\psi_0(x,y)$ on the right-hand side of this equation [see Eq. (9)]. Therefore, $f(u)$ in Eq. (20) has to approach 1 for $u\to 0$, i.e.,

$$f(u)=1+O(u^2) \tag{A3}$$

and $g(u)$ has for $u\to 0$ behaved in such a way that all the terms proportional to $\ln x$ on the left-hand side of Eq. (23) cancel. The solution of Eq. (A1) satisfying these conditions is

$$g[(1-w^2)^{1/2}]=\Gamma(1+\omega)P_\nu^{-\omega}(w), \tag{A4}$$

where $P_\nu^{-\omega}(w)$ denotes the associate Legendre function of the first kind [36]

$$P_\nu^{-\omega}(w)=\frac{1}{\Gamma(1+\omega)}\left(\frac{1-w}{1+w}\right)^{\omega/2}F\left(-\nu,\nu+1,1+\omega,\frac{1-w}{2}\right). \tag{A5}$$

Here, ν is the solution of the quadratic equation

$$\nu(\nu+1)=\gamma \tag{A6}$$

and $F(-\nu,\nu+1,1+\omega,(1-w)/2)$ is the hypergeometric function [36].

At this point it will be useful to comment the last two equations. First, we note that the function $P_\nu^{-\omega}(w)$ is a real function of generally complex variable $w=(1-u^2)^{1/2}$. This is due to the fact that ν, although generally complex, appears in the series defining the hypergeometric function in the form of the product $\nu(\nu+1)$ only [36]. Now, since w is real for $u<1$ and purely imaginary for $u>1$, the function $P_\nu^{-\omega}(w)$ has real values for $u<1$ and purely imaginary values for $u>1$. From Eqs. (A4) and (A2) we easily see that the same

holds also for the functions $g(u)$ and $f(u)$. This fact is used in Eqs. (35) and (36) of Sec. II.

Second, there is a question which of the solution of Eq. (A6)

$$\nu=-\frac{1}{2}\pm\frac{(1+4\gamma)^{1/2}}{2} \tag{A7}$$

is physically relevant. It is seen, however, that due to the symmetry [36]

$$P_{\nu}^{-\omega}(w)=P_{-\nu-1}^{-\omega}(w), \tag{A8}$$

the two solutions given by Eq. (A7) are physically equivalent. For this reason, an arbitrary of these solutions can be taken.

Now we derive the asymptotic expansion of the function $g(u)$ for $u\to 0$. The hypergeometric function $F(-\nu,\nu+1,1+\omega,(1-w)/2)$ in Eq. (A5) goes to 1 for $u\to 0$ $(w\to 1)$. Therefore, we get from Eqs. (A4) and (A5) that the function $g(u)$ behaves for $u\to 0$ $(w\to 1)$ as

$$\begin{aligned} g(u)&=\left(\frac{1-(1-u^2)^{1/2}}{1+(1-u^2)^{1/2}}\right)^{\omega/2}[1+O(u^2)]\\ &=\left(\frac{u^2}{4}+O(u^2)\right)^{\omega/2}[1+O(u^2)]. \end{aligned} \tag{A9}$$

Finally, we derive the explicit form of the function $T(\omega,\gamma)$ needed in the final formula Eq. (33) for $\mathrm{Im}\,E$

$$T(\omega,\gamma)=\frac{\pi^{1/2}}{\sqrt{f(u=1)}g(u=1)}. \tag{A10}$$

Using Eqs. (A2) and (A4) at the point $w=0$ corresponding to the point $u=1$ we can rewrite the last equation in the form

$$\begin{aligned} T(\omega,\gamma)&=\frac{\pi^{1/2}\omega^{1/2}}{\sqrt{-\frac{dg((1-w^2)^{1/2})}{dw}\Big|_{w=0}g(w=0)}}\\ &=\frac{\pi^{1/2}\omega^{1/2}}{\Gamma(1+\omega)}\left(-P_{\nu}^{-\omega}(w=0)\frac{dP_{\nu}^{-\omega}(w)}{dw}\Bigg|_{w=0}\right)^{-1/2}. \end{aligned} \tag{A11}$$

Taking into account the properties of the associate Legendre functions and the Gamma function [36]

$$P_{\nu}^{-\omega}(w=0)=\frac{2^{-\omega}}{\sqrt{\pi}}\cos\left[\frac{\pi}{2}(\nu-\omega)\right]\frac{\Gamma\left(\frac{1+\nu-\omega}{2}\right)}{\Gamma\left(1+\frac{\nu+\omega}{2}\right)}, \tag{A12}$$

$$\frac{dP_{\nu}^{-\omega}(w)}{dw}\Big|_{w=0}=\frac{2^{-\omega+1}}{\sqrt{\pi}}\sin\left[\frac{\pi}{2}(\nu-\omega)\right]\frac{\Gamma\left(1+\frac{\nu-\omega}{2}\right)}{\Gamma\left(\frac{1+\nu+\omega}{2}\right)}, \tag{A13}$$

and

$$\Gamma(2z)=(2\pi)^{-1/2}2^{2z-1/2}\Gamma(z)\Gamma(z+1/2), \tag{A14}$$

the formula for the function $T(\omega,\gamma)$ can be further simplified to the form identical to Eq. (38) of Sec. II

$$T(\omega,\gamma)=\frac{\omega^{1/2}\pi}{\Gamma(1+\omega)}\left\{-\sin[\pi(\nu-\omega)]\frac{\Gamma(1+\nu-\omega)}{\Gamma(1+\nu+\omega)}\right\}^{-1/2}. \tag{A15}$$

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