Nonadiabatic transmission: Exact quantum-mechanical solution for a special case of the two-state exponential model

V. I. Osherov* and V. G. Ushakov†
Institute of Problems of Chemical Physics, Russian Academy of Sciences, 142432 Chernogolovka, Russia
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The exact quantum-mechanical solution of the two-state exponential model with one flat diabatic potential has been found for a specific energy below the higher threshold. The *N* matrix has been derived in the adiabatic representation and the closed analytical expression for the transmission coefficient has been obtained. The results reveal the influence of the closed channel on the nonadiabatic transmission.

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I. INTRODUCTION

Nonadiabatic transmission is a well-known quantum-mechanical problem of two-state dynamics. It has been discussed extensively in the literature over the three last decades and reviewed in monographs [1–3]. The most comprehensive description of this phenomenon based on an exact relation between the Stokes constants for linear potentials is given in Ref. [3]. Analytical studies of the nonadiabatic behavior of systems with nonlinear potentials have been mostly restricted to the exponential model in the semiclassical approximation [4–6]. Only recently have some exact quantum-mechanical results for the exponential model been deduced relating to the Demkov model [7], the special model of Nikitin [8,9], and a model with asymptotic degeneration [10]. The results obtained have increased the understanding of the nonadiabatic transmission significantly. However, they cannot treat cases with an adiabatic barrier in the lower state and, in particular, are unable to describe nonadiabatic tunneling.

In this paper we consider an exponential model that involves tunneling and reveals the role of the closed channel in the dynamics of the nonadiabatic transmission. The paper is organized as follows. In Sec. II, a general exponential model is formulated in terms of the Bessel representation. In Sec. III, using the Heun equation, we derive a special model and find its solution. The asymptotic behavior and the matching procedure are described in Secs. IV and V. The *N* matrix is obtained in Sec. VI. The results are discussed in the concluding section.

II. FORMULATION OF THE PROBLEM: BESSEL REPRESENTATION

In the diabatic representation, the Schrödinger equation for the general exponential model has the form

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\begin{pmatrix}U_1-V_1e^{-\alpha x}, Ve^{-\alpha x}\\ Ve^{-\alpha x}, U_2-V_2e^{-\alpha x}\end{pmatrix}\right]\Psi=E\Psi. \qquad (1)$$

For definiteness we assume $U_1>U_2$ and $V>0$. The transformation to adiabatic vectors Φ is performed by the rotation R,

$$\Phi=R\Psi,\quad \Phi=\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix},\quad \Psi=\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}. \qquad (2)$$

The matrix R diagonalizes the potential of Eq. (1) and is given by the expression

$$R=\begin{pmatrix}\cos g, & -\sin g\\ \sin g, & \cos g\end{pmatrix}, \qquad (3)$$

where

$$\tan 2g=\frac{2Ve^{-\alpha x}}{U_2-U_1-(V_2-V_1)e^{-\alpha x}}. \qquad (4)$$

The asymptotic amplitudes of the normalized incoming and outgoing adiabatic waves are related by the *N* matrix.

As in Ref. [4] we substitute the variable

$$\rho^2=\frac{8mV}{(\hbar\alpha)^2}e^{-\alpha x}, \qquad (5)$$

and obtain the system of coupled equations

$$\begin{aligned}\left(\rho^2\frac{d^2}{d\rho^2}+\rho\frac{d}{d\rho}+\nu^2+\beta_1\rho^2\right)\psi_1&=\rho^2\psi_2,\\ \left(\rho^2\frac{d^2}{d\rho^2}+\rho\frac{d}{d\rho}+\mu^2+\beta_2\rho^2\right)\psi_2&=\rho^2\psi_1,\end{aligned} \qquad (6)$$

where the following notations are used:

$$\nu^2=\frac{8m}{(\hbar\alpha)^2}(E-U_1),\quad \mu^2=\frac{8m}{(\hbar\alpha)^2}(E-U_2),\quad \beta_i=\frac{V_i}{V}. \qquad (7)$$

The contour Bessel transformation that is determined by the formulaes

$$\psi_{1,2}=\oint_L pF_{1,2}(p)Z_{i\nu}(p\rho)dp,$$

$$\left[\left(\varrho\frac{d}{d\varrho}\right)^2+\varrho^2+\nu^2\right]Z_{i\nu}(\varrho)=0 \qquad (8)$$

results in the amplitudes

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*Electronic address: osherov@icp.ac.ru
†Electronic address: uvg@icp.ac.ru

$$F_1(p) = \frac{f(p)}{p^{1/2}(p^2 - a_1)(p^2 - a_2)}, \quad F_2 = (\beta_1 - p^2)F_1(p), \tag{9}$$

and the principal equation

$$\left(\frac{d^2}{dp^2} + \frac{1+4\mu^2}{4}\frac{p^4 - 4\varepsilon p^2 + \lambda}{p^2(p^2-a_1)(p^2-a_2)}\right)f = 0 \tag{10}$$

with the parameters

$$\varepsilon = \frac{\frac{1}{4}(\beta_1+\beta_2) + (\beta_1\mu^2 + \beta_2\nu^2)}{1+4\mu^2}, \quad \lambda = \frac{(\beta_1\beta_2 - 1)(1+4\nu^2)}{1+4\mu^2}. \tag{11}$$

The finite singular points of Eq. (10) are given by the expression

$$a_{1,2} = \frac{\beta_1+\beta_2}{2} \mp \sqrt{\left(\frac{\beta_1-\beta_2}{2}\right)^2 + 1}. \tag{12}$$

The integrals (8) must converge and the contours L must be chosen so that the increment conditions

$$F_i(p)\frac{dZ_{i\nu}(p\rho)}{dp}p^n\bigg|_L = 0, \qquad \frac{d}{dp}[F_i(p)p^n]Z_{i\nu}(p\rho)\bigg|_L = 0, \quad n = 1\text{–}3,$$

$$F_i(p)p^n Z_{i\nu}(p\rho)\big|_L = 0, \quad n = 0,2 \tag{13}$$

are satisfied.

III. HEUN EQUATION: SOLUTION OF A SPECIAL CASE

We will consider the systems where the first potential is flat:

$$\beta_1 = 0. \tag{14}$$

The substitution of the variable and the function

$$\varsigma = \frac{p^2}{a_2}, \quad \phi = p^{-1/2+i\nu}f \tag{15}$$

transforms Eq. (10) to the standard Heun equation

$$\frac{d^2\phi}{d\varsigma^2} + \frac{1-i\nu}{\varsigma}\frac{d\phi}{d\varsigma} + \frac{\mu^2-\nu^2}{4}\frac{1}{(\varsigma-1)(\varsigma-a_1/a_2)}\phi = 0 \tag{16}$$

with four singularities in the points $\varsigma = 0, 1, a_1/a_2, \infty$. In the special case

$$\nu = -i \tag{17}$$

the singularity $\varsigma = 0$ disappears and Eq. (16) is reduced to the normal Gauss form

$$z(1-z)\frac{d^2\phi}{dz^2} + [c - (a+b+1)z]\frac{d\phi}{dz} - ab\phi = 0 \tag{18}$$

with the following variable and parameters:

$$z = \frac{p^2 - a_2}{a_1 - a_2}, \quad a = -\frac{1}{2} + \frac{i\mu}{2}, \quad b = -\frac{1}{2} - \frac{i\mu}{2}, \quad c = 0. \tag{19}$$

The parameters of the physical model take the form

$$\mu^2 = \frac{8m}{(\hbar\alpha)^2}(U_1 - U_2) - 1, \quad a_{1,2} = \frac{\beta}{2} \mp \sqrt{\frac{\beta^2}{4} + 1},$$

$$\beta = \beta_2 = \frac{V_2}{V}. \tag{20}$$

Thus we restrict our treatment of these systems to the flat diabatic potential $V_1 = 0$ and fixed energy

$$E = U_1 - \frac{(\hbar\alpha)^2}{8m} \tag{21}$$

when this channel is closed. Below we consider $E > U_2$ which means that the second channel is open.

As the solution for ϕ we choose the Kummer series w_5, which is one of two fundamental solutions of the Gauss hypergeometric equation (18) in the neighborhood of infinity ($z = \infty$)

$$\phi(p) = w_5 = (z^{-1}e^{i\pi})^a \, {}_2F_1(a, a+1, a+1-b, z^{-1}). \tag{22}$$

We choose also the following contours and the Hankel functions for Z_1:

$$L_1 = (\sqrt{a_2} + i\infty, \sqrt{a_2}+, \sqrt{a_2} + i\infty), \quad Z_1 = H_1^{(1)}, \quad \text{(I)},$$

$$L_2 = (i\infty, i\sqrt{-a_1}+, i\infty), \quad Z_1 = H_1^{(1)}, \quad \text{(II)},$$

$$L_3 = (\sqrt{a_2} - i\infty, \sqrt{a_2}+, \sqrt{a_2} - i\infty), \quad Z_1 = H_1^{(2)}, \quad \text{(III)}. \tag{23}$$

The integrals in Eq. (8) converge on these contours because the Hankel functions dominate in the integrand and exponentially decrease in the upper ($H_1^{(1)}$) and lower ($H_1^{(2)}$) complex half p plane. The conditions (13) are also satisfied by solutions given in Eqs. (22) and (23).

For further consideration we thus take only the three solutions to system (6). We will see below that these solutions are finite at $\rho \to \infty$. Thus, these solutions satisfy the physical boundary conditions at $x \to -\infty$, and they are linearly independent (see below). Therefore these solutions are the basis set to the problem under consideration.

The contours (23) are going along the sides of three corresponding cuts of the complex p plane and they wind around the points $p=i\sqrt{-a_1}$ and $\sqrt{a_2}$, which are the singularities of the solution w_5 corresponding to branch points $z=1$ and 0. Analytical continuation of w_5 is given by [11]

$$w_5(z) = V(z) = \frac{\Gamma(1+a-b)}{\Gamma(1-b)\Gamma(1+a)} + \frac{ze^{-i\pi}\Gamma(1+a-b)}{\Gamma(-b)\Gamma(a)}\left([\ln(ze^{-i\pi}) + Q^0]\, {}_2F_1(1+a,1+b,2,z) + \sum_{k=0}^{\infty} Q_k^0 z^k \right) \tag{24}$$

for contours I and III, and

$$w_5(z) = U(z) = \frac{\Gamma(1+a-b)e^{i\pi a}}{\Gamma(1-b)\Gamma(1+a)} + \frac{(1-z)\Gamma(1+a-b)e^{i\pi(1+a)}}{\Gamma(a)\Gamma(-b)}\left([\ln(1-z)e^{i\pi} + Q^1]\, {}_2F_1(1+a,1+b,2,1-z) + \sum_{k=0}^{\infty} Q_k^1 (1-z)^k \right) \tag{25}$$

for contour II. In these expressions $Q^{0,1}$ and $Q_k^{0,1}$ are constants.

Contributions to the integrals of Eq. (8) from terms proportional to $Q^{0,1}$ and $Q_k^{0,1}$ cancel out at the integration along the cut sides. Using the relation [11]

$${}_2F_1(a,b,c,z) = (1-z)^{c-a-b}\, {}_2F_1(c-a,c-b,c,z) \tag{26}$$

we get the following representation for the limited physical basis set of the problem:

$$\Psi^{(\mathrm{I})} = \frac{C_1}{i\pi}\begin{pmatrix} \oint_{L_1} \left(\frac{1}{z(1-z)} + ab \ln z\, {}_2F_1(1-a,1-b,2,z) \right) H_1^{(1)}(p\rho)dp \\ -\oint_{L_1} p^2 \left(\frac{1}{z(1-z)} + ab \ln z\, {}_2F_1(1-a,1-b,2,z) \right) H_1^{(1)}(p\rho)dp \end{pmatrix}, \tag{27}$$

$$\Psi^{(\mathrm{II})} = \frac{C_2}{i\pi}\begin{pmatrix} \oint_{L_2} \left(\frac{1}{z(1-z)} + ab \ln(1-z)\, {}_2F_1(1-a,1-b,2,1-z) \right) H_1^{(1)}(p\rho)dp \\ -\oint_{L_2} p^2 \left(\frac{1}{z(1-z)} + ab \ln(1-z)\, {}_2F_1(1-a,1-b,2,1-z) H_1^{(1)}(p\rho) \right) dp \end{pmatrix}, \tag{28}$$

$$\Psi^{(\mathrm{III})} = \frac{C_3}{i\pi}\begin{pmatrix} \oint_{L_3} \left(\frac{1}{z(1-z)} + ab \ln z\, {}_2F_1(1-a,1-b,2,z) \right) H_1^{(2)}(p\rho)dp \\ -\oint_{L_3} p^2 \left(\frac{1}{z(1-z)} + ab \ln z\, {}_2F_1(1-a,1-b,2,z) \right) H_1^{(2)}(p\rho)dp \end{pmatrix}, \tag{29}$$

where the constants C_{1-3} can be chosen arbitrarily. The contributions of the singular terms are calculated by the residues. The values of $\ln z$ and $\ln(1-z)$ differ by $2i\pi$ on cut sides and the corresponding integrals are reduced to the integrals along one side of the cuts. After that, for the solutions I and III, it is possible to displace the integration contour to the real axis. Taking appropriate values of the constants C_{1-3} for further convenience we get the final expression of the basis set in the form

$$\Psi^{(\mathrm{I})} = \pi^2(a_2 - a_1)\begin{pmatrix} -\frac{H_1^{(1)}(\sqrt{a_2}\rho)}{\sqrt{a_2}} + \frac{2ab}{a_2-a_1}\int_{\sqrt{a_2}}^{\infty} {}_2F_1\left(1-a,1-b,2,-\frac{p^2-a_2}{a_2-a_1}\right) H_1^{(1)}(p\rho)dp \\ \sqrt{a_2}H_1^{(1)}(\sqrt{a_2}\rho) - \frac{2ab}{a_2-a_1}\int_{\sqrt{a_2}}^{\infty} p^2\, {}_2F_1\left(1-a,1-b,2,-\frac{p^2-a_2}{a_2-a_1}\right) H_1^{(1)}(p\rho)dp \end{pmatrix}, \tag{30}$$

$$\Psi^{(\mathrm{II})} = i\pi^2(a_2 - a_1)\begin{pmatrix} -\frac{H_1^{(1)}(i\sqrt{-a_1}\rho)}{i\sqrt{-a_1}} - \frac{2ab}{a_2-a_1}\int_{i\sqrt{-a_1}}^{i\infty} {}_2F_1\left(1-a,1-b,2,\frac{p^2-a_1}{a_2-a_1}\right) H_1^{(1)}(p\rho)dp \\ i\sqrt{-a_1}H_1^{(1)}(i\sqrt{-a_1}\rho) + \frac{2ab}{a_2-a_1}\int_{i\sqrt{-a_1}}^{i\infty} p^2\, {}_2F_1\left(1-a,1-b,2,\frac{p^2-a_1}{a_2-a_1}\right) H_1^{(1)}(p\rho)dp \end{pmatrix}, \tag{31}$$

$$\Psi^{(\mathrm{III})}=\pi^2(a_2-a_1)\begin{pmatrix} -\dfrac{H_1^{(2)}(\sqrt{a_2}\rho)}{\sqrt{a_2}}+\dfrac{2ab}{a_2-a_1}\displaystyle\int_{\sqrt{a_2}}^{\infty}{}_2F_1\left(1-a,1-b,2,-\dfrac{p^2-a_2}{a_2-a_1}\right)H_1^{(2)}(p\rho)dp \\ \sqrt{a_2}H_1^{(2)}(\sqrt{a_2}\rho)-\dfrac{2ab}{a_2-a_1}\displaystyle\int_{\sqrt{a_2}}^{\infty}p^2\,{}_2F_1\left(1-a,1-b,2,-\dfrac{p^2-a_2}{a_2-a_1}\right)H_1^{(2)}(p\rho)dp \end{pmatrix}. \tag{32}$$

The solutions (30)–(32) cannot be expressed in terms of the known higher transcendental functions. However for the N-matrix calculation it is sufficient to know only its asymptotic behavior at $\rho\to\infty$ and $\rho\to 0$.

IV. BASIS-SET ASYMPTOTIC BEHAVIOR

The asymptotic form of the basis set at $\rho\to\infty$ follows from Eqs. (30)–(32) immediately as

$$\Psi^{(\mathrm{I})}(\rho\to\infty)=(2\pi)^{3/2}\begin{pmatrix} \dfrac{a_2-a_1}{2a_2}\sqrt{\dfrac{\sqrt{a_2}}{\rho}}e^{i(\sqrt{a_2}\rho+\pi/4)} \\ \dfrac{a_1-a_2}{2}\sqrt{\dfrac{\sqrt{a_2}}{\rho}}e^{i(\sqrt{a_2}\rho+\pi/4)} \end{pmatrix}, \tag{33}$$

$$\Psi^{(\mathrm{II})}(\rho\to\infty)=(2\pi)^{3/2}\begin{pmatrix} \dfrac{a_1-a_2}{2a_1}\sqrt{\dfrac{\sqrt{-a_1}}{\rho}}e^{-\sqrt{-a_1}\rho} \\ \dfrac{a_2-a_1}{2}\sqrt{\dfrac{\sqrt{-a_1}}{\rho}}e^{-\sqrt{-a_1}\rho} \end{pmatrix}, \tag{34}$$

$$\Psi^{(\mathrm{III})}(\rho\to\infty)=(2\pi)^{3/2}\begin{pmatrix} \dfrac{a_2-a_1}{2a_2}\sqrt{\dfrac{\sqrt{a_2}}{\rho}}e^{-i(\sqrt{a_2}\rho+\pi/4)} \\ \dfrac{a_1-a_2}{2}\sqrt{\dfrac{\sqrt{a_2}}{\rho}}e^{-i(\sqrt{a_2}\rho+\pi/4)} \end{pmatrix}. \tag{35}$$

In particular it demonstrates that the functions (30)–(32) are linearly independent.

The basis set under consideration corresponds to the system with $\nu^2=-1$, i.e., at $E<U_1$, the first channel is closed and in the general case at $\rho\to 0$ the solutions I–III have to include singular terms with the asymptotic behavior $\sim\rho^{-1}$. These terms appear from the isolation of the Hankel function singularity:

$$H_{1r}^{(1,2)}(p\rho)=H_1^{(1,2)}(p\rho)\pm\frac{2i}{\pi p\rho}. \tag{36}$$

This creates the partition

$$\psi_{1,2}^{(1,2)}(\rho\to 0)=\psi_{1,2s}^{(1,2)}+\psi_{1,2r}^{(1,2)}, \tag{37}$$

and one gets

$$\Psi_s^{(\mathrm{I})}=\frac{2\pi i}{\rho}\begin{pmatrix} \dfrac{a_2-a_1}{a_2}-2ab\displaystyle\int_{\sqrt{a_2}}^{\infty}{}_2F_1\left(1-a,1-b,2,-\dfrac{p^2-a_2}{a_2-a_1}\right)\dfrac{1}{p}dp \\ a_1-a_2+2ab\displaystyle\int_{\sqrt{a_2}}^{\infty}{}_2F_1\left(1-a,1-b,2,-\dfrac{p^2-a_2}{a_2-a_1}\right)p\,dp \end{pmatrix}, \tag{38}$$

$$\Psi_s^{(\mathrm{II})}=\frac{2\pi}{\rho}\begin{pmatrix} \dfrac{a_1-a_2}{a_1}-2ab\displaystyle\int_{\sqrt{-a_1}}^{\infty}{}_2F_1\left(1-a,1-b,2,-\dfrac{p^2+a_1}{a_2-a_1}\right)\dfrac{1}{p}dp \\ a_2-a_1-2ab\displaystyle\int_{\sqrt{-a_1}}^{\infty}{}_2F_1\left(1-a,1-b,2,-\dfrac{p^2+a_1}{a_2-a_1}\right)p\,dp \end{pmatrix}, \tag{39}$$

$$\Psi_s^{(\mathrm{III})}=\frac{2\pi i}{\rho}\begin{pmatrix} \dfrac{a_1-a_2}{a_2}+2ab\displaystyle\int_{\sqrt{a_2}}^{\infty}{}_2F_1\left(1-a,1-b,2,-\dfrac{p^2-a_2}{a_2-a_1}\right)\dfrac{1}{p}dp \\ a_2-a_1-2ab\displaystyle\int_{\sqrt{a_2}}^{\infty}{}_2F_1\left(1-a,1-b,2,-\dfrac{p^2-a_2}{a_2-a_1}\right)p\,dp \end{pmatrix}. \tag{40}$$

The integration variable substitution results in the following intermediate form:

$$\Psi_s^{(\mathrm{I})} = \frac{2\pi i}{\rho}\begin{pmatrix} \dfrac{a_2-a_1}{a_2}ab\displaystyle\int_0^\infty \frac{\zeta}{\zeta+a_2/(a_2-a_1)}\, {}_2F_1(1-a,1-b,2,-\zeta)d\zeta \\ (a_1-a_2)\left(1-ab\displaystyle\int_0^\infty {}_2F_1(1-a,1-b,2,-\zeta)d\zeta\right) \end{pmatrix}, \tag{41}$$

$$\Psi_s^{(\mathrm{II})} = \frac{2\pi}{\rho}\begin{pmatrix} \dfrac{a_1-a_2}{a_1}ab\displaystyle\int_0^\infty \frac{\zeta}{\zeta+a_1/(a_1-a_2)}\, {}_2F_1(1-a,1-b,2,-\zeta)d\zeta \\ (a_2-a_1)\left(1-ab\displaystyle\int_0^\infty {}_2F_1(1-a,1-b,2,-\zeta)d\zeta\right) \end{pmatrix}, \tag{42}$$

$$\Psi_s^{(\mathrm{III})} = \frac{2\pi i}{\rho}\begin{pmatrix} \dfrac{a_1-a_2}{a_2}ab\displaystyle\int_0^\infty \frac{\zeta}{\zeta+a_2/(a_2-a_1)}\, {}_2F_1(1-a,1-b,2,-\zeta)d\zeta \\ (a_2-a_1)\left(1-ab\displaystyle\int_0^\infty {}_2F_1(1-a,1-b,2,-\zeta)d\zeta\right) \end{pmatrix}. \tag{43}$$

The final asymptotic representation for the singular part of the basis set at $\rho\to 0$ is then obtained as

$$\Psi_s^{(\mathrm{I})} = \begin{pmatrix} iD_1\dfrac{4}{\rho} \\ 0 \end{pmatrix}, \tag{44}$$

$$\Psi_s^{(\mathrm{II})} = \begin{pmatrix} D_2\dfrac{4}{\rho} \\ 0 \end{pmatrix}, \tag{45}$$

$$\Psi_s^{(\mathrm{III})} = \begin{pmatrix} -iD_3\dfrac{4}{\rho} \\ 0 \end{pmatrix}, \tag{46}$$

where

$$D_1 = D_3 = \frac{\pi(a_2-a_1)}{2a_2}ab\Gamma(-a)\Gamma(-b)\, {}_2F_1\left(-a,-b,2,\frac{a_1}{a_1-a_2}\right),$$

$$D_2 = \frac{\pi(a_1-a_2)}{2a_1}ab\Gamma(-a)\Gamma(-b)\, {}_2F_1\left(-a,-b,2,\frac{a_2}{a_2-a_1}\right). \tag{47}$$

The regular part of the basis set at $\rho\to 0$ has the form

$$\Psi_r^{(\mathrm{I})} = \begin{pmatrix} 0 \\ -\dfrac{\pi^2 ab}{\rho^3}\displaystyle\int_0^\infty \zeta^{1/2}{}_2F_1\left(1-a,1-b,2,-\frac{\zeta}{\rho^2(a_2-a_1)}\right)H_{1r}^{(1)}(\zeta^{1/2})d\zeta \end{pmatrix}, \tag{48}$$

$$\Psi_r^{(\mathrm{II})} = \begin{pmatrix} 0 \\ \dfrac{\pi^2 ab}{\rho^3}\displaystyle\int_0^\infty \zeta^{1/2}\, {}_2F_1\left(1-a,1-b,2,-\frac{\zeta}{\rho^2(a_2-a_1)}\right)H_{1r}^{(1)}(i\zeta^{1/2})d\zeta \end{pmatrix}, \tag{49}$$

$$\Psi_r^{(\mathrm{III})} = \begin{pmatrix} 0 \\ -\dfrac{\pi^2 ab}{\rho^3}\displaystyle\int_0^\infty \zeta^{1/2}\, {}_2F_1\left(1-a,1-b,2,-\frac{\zeta}{\rho^2(a_2-a_1)}\right)H_{1r}^{(2)}(\zeta^{1/2})d\zeta \end{pmatrix}. \tag{50}$$

The second component of each vector is indeed regular. That becomes clear after substitution of the asymptotic expression for the hypergeometric function ${}_2F_1$ [11]. Because of the limiting behavior of the Hankel functions $H_{1r}^{(1,2)}(\zeta^{1/2})$ the integrals converge. We represent the result in the form

$$\Psi_r^{(\mathrm{I})}=\begin{pmatrix}0\\ -\left(\frac{a_2-a_1}{2}\right)^{3/2}\left[A_1\left(\frac{\rho}{4}\right)^{i\mu}+B_1\left(\frac{\rho}{4}\right)^{-i\mu}\right]\end{pmatrix}, \quad (51)$$

$$\Psi_r^{(\mathrm{II})}=\begin{pmatrix}0\\ \left(\frac{a_2-a_1}{2}\right)^{3/2}\left[A_2\left(\frac{\rho}{4}\right)^{i\mu}+B_2\left(\frac{\rho}{4}\right)^{-i\mu}\right]\end{pmatrix}, \quad (52)$$

$$\Psi_r^{(\mathrm{III})}=\begin{pmatrix}0\\ -\left(\frac{a_2-a_1}{2}\right)^{3/2}\left[A_3\left(\frac{\rho}{4}\right)^{i\mu}+B_3\left(\frac{\rho}{4}\right)^{-i\mu}\right]\end{pmatrix}, \quad (53)$$

where

$$A_{1,2,3}=A'_{1,2,3}(\mu)\left(\frac{a_2-a_1}{2}\right)^{i\mu/2},$$

$$B_{1,2,3}=B'_{1,2,3}(\mu)\left(\frac{a_2-a_1}{2}\right)^{-i\mu/2}, \quad (54)$$

and the coefficients $A'_{1,2,3}$ and $B'_{1,2,3}$ are functions of μ only. Here we do not evaluate the integrals over ζ. The coefficients $A'_{1,2,3}$ and $B'_{1,2,3}$ will be found by matching to the Demkov model in the next section.

V. MATCHING TO THE DEMKOV MODEL

The problem under consideration at $\beta=0$ ($\beta_1=\beta_2=0$) transforms into the three-channel Demkov problem, which has an exact quantum-mechanical solution (see Ref. [12]). The basis set of the Demkov problem is represented in terms of the Meijer functions:

$$\Psi_0^{(\mathrm{I})}=\begin{pmatrix}G_{04}^{40}\left[e^{-2\pi i}\left(\frac{\rho}{4}\right)^4\middle| b_q\right]\\ -G_{04}^{40}\left[e^{-2\pi i}\left(\frac{\rho}{4}\right)^4\middle| b'_q\right]\end{pmatrix}, \quad (55)$$

$$\Psi_0^{(\mathrm{II})}=\begin{pmatrix}G_{04}^{40}\left[\left(\frac{\rho}{4}\right)^4\middle| b_q\right]\\ G_{04}^{40}\left[\left(\frac{\rho}{4}\right)^4\middle| b'_q\right]\end{pmatrix}, \quad (56)$$

$$\Psi_0^{(\mathrm{III})}=\begin{pmatrix}G_{04}^{40}\left[e^{2\pi i}\left(\frac{\rho}{4}\right)^4\middle| b_q\right]\\ -G_{04}^{40}\left[e^{2\pi i}\left(\frac{\rho}{4}\right)^4\middle| b'_q\right]\end{pmatrix}, \quad (57)$$

with the parameters

$$b_{1,2}=\pm\frac{1}{4}, \quad b_{3,4}=\frac{1}{2}\pm\frac{1}{4}i\mu, \quad b'_{1,2}=\pm\frac{1}{4}i\mu, \quad b'_{3,4}=\frac{3}{4},\frac{1}{4}. \quad (58)$$

Using the asymptotic behavior of the Meijer functions [11] we write the asymptotic behavior of this basis set at $\rho\to\infty$ as

$$\Psi_0^{(\mathrm{I})}(\rho\to\infty)=(2\pi)^{3/2}\begin{pmatrix}\sqrt{\frac{1}{\rho}}e^{i(\rho+\pi/4)}\\ -\sqrt{\frac{1}{\rho}}e^{i(\rho+\pi/4)}\end{pmatrix}, \quad (59)$$

$$\Psi_0^{(\mathrm{II})}(\rho\to\infty)=(2\pi)^{3/2}\begin{pmatrix}\sqrt{\frac{1}{\rho}}e^{-\rho}\\ \sqrt{\frac{1}{\rho}}e^{-\rho}\end{pmatrix}, \quad (60)$$

$$\Psi_0^{(\mathrm{III})}(\rho\to\infty)=(2\pi)^{3/2}\begin{pmatrix}\sqrt{\frac{1}{\rho}}e^{-i(\rho+\pi/4)}\\ -\sqrt{\frac{1}{\rho}}e^{-i(\rho+\pi/4)}\end{pmatrix}, \quad (61)$$

and at $\rho\to 0$ as

$$\Psi_0^{(\mathrm{I})}(\rho\to 0)=\begin{pmatrix}iD_1^0\frac{4}{\rho}\\ -\left[A_1^0\left(\frac{\rho}{4}\right)^{i\mu}+B_1^0\left(\frac{\rho}{4}\right)^{-i\mu}\right]\end{pmatrix}, \quad (62)$$

$$\Psi_0^{(\mathrm{II})}(\rho\to 0)=\begin{pmatrix}D_2^0\frac{4}{\rho}\\ A_2^0\left(\frac{\rho}{4}\right)^{i\mu}+B_2^0\left(\frac{\rho}{4}\right)^{-i\mu}\end{pmatrix}, \quad (63)$$

$$\Psi_0^{(\mathrm{III})}(\rho\to 0)=\begin{pmatrix}-iD_3^0\frac{4}{\rho}\\ -\left[A_3^0\left(\frac{\rho}{4}\right)^{i\mu}+B_3^0\left(\frac{\rho}{4}\right)^{-i\mu}\right]\end{pmatrix} \quad (64)$$

with

$$A_1^0=e^{\pi\mu/2}A^0, \quad A_2^0=A^0, \quad A_3^0=e^{-\pi\mu/2}A^0,$$

$$B_1^0=e^{-\pi\mu/2}B^0, \quad B_2^0=B^0, \quad B_3^0=e^{\pi\mu/2}B^0, \quad (65)$$

and

$$A^0=\Gamma\left(-\tfrac{1}{2}i\mu\right)\Gamma\left(\tfrac{3}{4}-\tfrac{1}{4}i\mu\right)\Gamma\left(\tfrac{1}{4}-\tfrac{1}{4}i\mu\right),$$

$$B^0=\Gamma\left(\tfrac{1}{2}i\mu\right)\Gamma\left(\tfrac{3}{4}+\tfrac{1}{4}i\mu\right)\Gamma\left(\tfrac{1}{4}+\tfrac{1}{4}i\mu\right). \quad (66)$$

Note that here (1) the basis sets $\Psi^{(\mathrm{I-III})}(a_2=1,a_1=-1)$ and $\Psi_0^{(\mathrm{I-III})}$ satisfy the same equation, (2) their asymptotic behavior at $\rho\to\infty$ coincide, and (3) their singular asymptotic behaviors at $\rho\to 0$ also coincide owing to the equality

$$D_{1,2,3}(a_2=1,a_1=-1)=\pi ab\Gamma(-a)\Gamma(-b)\ {}_2F_1\left(-a,-b,2,\tfrac{1}{2}\right) =\Gamma\left(\tfrac{1}{2}\right)\Gamma\left(\tfrac{3}{4}+\tfrac{1}{4}i\mu\right)\Gamma\left(\tfrac{3}{4}-\tfrac{1}{4}i\mu\right)=D^0_{1,2,3}, \quad (67)$$

which is the consequence of the quadratic transformation of the Kummer functions and the relation between contiguous hypergeometric functions. It means that the set $\Psi^{(\text{I–III})}(a_2=1,a_1=-1)$ is matched to the set $\Psi_0^{(\text{I–III})}$ and leads unavoidably to the principal identity

$$\Psi^{(\text{I–III})}(a_2=1,a_1=-1)=\Psi_0^{(\text{I–III})}. \quad (68)$$

Therefore, we finally get

$$A'_{1,2,3}=A^0_{1,2,3}, \quad B'_{1,2,3}=B^0_{1,2,3}. \quad (69)$$

VI. *N*-MATRIX CALCULATION

The general solution to the problem (6) decreasing at $\rho\to\infty$ and satisfying the conditions (14) and (17) can be represented in the form

$$\Psi=\left(\frac{2}{a_2-a_1}\right)^{3/2}(c_1\Psi^{(\text{I})}+c_2\Psi^{(\text{II})}+c_3\Psi^{(\text{III})}) \quad (70)$$

where c_{1-3} are arbitrary constants. The physical solutions must be regular, i.e., satisfy the condition

$$\Psi_s=0, \quad \to iD_1c_1+D_2c_2-iD_3c_3=0. \quad (71)$$

This condition leads to the general physical solution by eliminating one of the constants in Eq. (70) (below it is c_2).

To calculate now the N matrix we transfer to the adiabatic basis set by the rotation R, which has the following limiting forms:

$$R=1, \quad \rho\to 0; \quad R=(a_2-a_1)^{-1/2}\begin{pmatrix} a_2^{1/2}, & (-a_1)^{1/2} \\ -(-a_1)^{1/2}, & a_2^{1/2}\end{pmatrix}, \quad \rho\to\infty. \quad (72)$$

We obtain

$$\Phi(\rho\to 0)=-\begin{pmatrix} 0 \\ c^+A(\rho/4)^{i\mu}+c^-B(\rho/4)^{-i\mu}\end{pmatrix} \quad (73)$$

with

$$A=A^0\left(\frac{a_2-a_1}{2}\right)^{i\mu/2}, \quad B=B^0\left(\frac{a_2-a_1}{2}\right)^{-i\mu/2} \quad (74)$$

and

$$c^+=c_1\exp(\pi\mu/2)+i(c_1-c_3)\delta+c_3\exp(-\pi\mu/2),$$

$$c^-=c_1\exp(-\pi\mu/2)+i(c_1-c_3)\delta+c_3\exp(\pi\mu/2), \quad (75)$$

where the new principal parameter δ arises:

$$\delta=\frac{D_1}{D_2}=-\frac{a_1\ {}_2F_1\left(-a,-b,2,\dfrac{a_1}{a_1-a_2}\right)}{a_2\ {}_2F_1\left(-a,-b,2,\dfrac{a_2}{a_2-a_1}\right)}. \quad (76)$$

At $\rho\to\infty$,

$$\Phi(\rho\to\infty)=-\begin{pmatrix} 0 \\ c_1 4\pi^{3/2}\sqrt{\dfrac{1}{\sqrt{a_2}\rho}}e^{i(\sqrt{a_2}\rho+\pi/4)}+c_3 4\pi^{3/2}\sqrt{\dfrac{1}{\sqrt{a_2}\rho}}e^{-i(\sqrt{a_2}\rho+\pi/4)}\end{pmatrix}. \quad (77)$$

As it should be expected, only the wave function of the open adiabatic channel is asymptotically not equal to zero.

We introduce asymptotic waves normalized by the unit flow:

$$E_1^{\pm}=\sqrt{\frac{1}{\sqrt{a_2}\rho}}e^{\pm i\left(\sqrt{a_2}\rho+\pi/4\right)}, \quad E_2^{\pm}=\frac{1}{\sqrt{\mu}}\left(\frac{\rho}{4}\right)^{\pm i\mu}. \quad (78)$$

In these terms the asymptotes of two linearly independent solutions corresponding to the choice $(n=1)$ $c_1=-1,c_3=0$ and $(n=2)$ $c_1=0,c_3=-1$ take the forms

$$\phi_2^{(n)}(\rho\to\infty)=U_1^{(n)}E_1^++W_1^{(n)}E_1^-,$$

$$\phi_2^{(n)}(\rho\to 0)=U_2^{(n)}E_2^-+W_2^{(n)}E_2^+, \quad (79)$$

where

$$U_1^{(1)}=W_1^{(2)}=4\pi^{3/2}, \quad W_1^{(1)}=U_1^{(2)}=0,$$

$$U_2^{(1)}=\sqrt{\mu}B(e^{-\pi\mu/2}+i\delta), \quad W_2^{(1)}=\sqrt{\mu}A(e^{\pi\mu/2}+i\delta),$$

$$U_2^{(2)}=\sqrt{\mu}B(e^{\pi\mu/2}-i\delta), \quad W_2^{(2)}=\sqrt{\mu}A(e^{-\pi\mu/2}-i\delta). \quad (80)$$

The definition

$$U^{(n)}=NW^{(n)} \quad (81)$$

is the system of equations for the elements N_{ik}. The N matrix obtained is symmetric and unitary,

$$N_{12}=N_{21}, \quad NN^+=1, \quad (82)$$

and has the form

$$N = e^{i(\vartheta_0-\vartheta_2)}\begin{pmatrix} -\sqrt{1-T}e^{-i(\vartheta_0+\vartheta_1)}, \sqrt{T} \\ \sqrt{T}, \quad \sqrt{1-T}e^{i(\vartheta_0+\vartheta_1)} \end{pmatrix} \quad (83)$$

where

$$\vartheta_0 = -\frac{\mu}{2}\ln\frac{a_2-a_1}{2} - \frac{3\mu}{2}\ln 2 + \arg\Gamma(i\mu),$$

$$\vartheta_1 = \arctan\,\delta e^{\pi\mu/2}, \quad \vartheta_2 = \arctan\,\delta e^{-\pi\mu/2}. \quad (84)$$

The value T is the nonadiabatic transmission coefficient

$$T = \frac{1-e^{-2\pi\mu}}{1+\delta^2 e^{-\pi\mu}}. \quad (85)$$

It has the following limiting behavior:

$$\lim_{\beta\to\infty} T = 1 - e^{-2\pi\mu},$$

$$\lim_{\beta\to 0} T = 1 - e^{-\pi\mu},$$

$$\lim_{\beta\to -\infty} T = \varkappa\beta^{-4}, \quad (86)$$

where

$$\varkappa = \frac{\pi^2}{4}(\mu^2+1)^2\tanh\,\pi\mu.$$

The first limit in Eq. (86) describes the nonadiabatic transmission for uncoupled diabatic potentials. The second one is the transmission for the Demkov model. The third expression demonstrates the transmission at the avoided crossing of adiabatic potentials for small static coupling V. This expression coincides rigorously with the result of perturbation theory if the part of the potential that is proportional to $e^{-\alpha x}$ is diagonalized beforehand. At large finite μ it differs from the adiabatic transmission coefficient squared, which can be evaluated in this case semiclassically, by the factor $4\pi^2 e^{-4} < 1$. This inequality generalizes the well-known claim for the linear model [1–3] that the nonadiabatic transmission is smaller than the adiabatic one.

VII. CONCLUSION

The main result of this work is given in Eq. (85), which represents the exact quantum-mechanical expression for the transmission coefficient in a special exponential model at an energy below the threshold of the excited state. This formula extends the results for the exponential models [7–10] to systems with a different form of the potential matrix. It reproduces situations both with and without intersection of the diabatic potentials, in particular, the situation with the barrier in the lower adiabatic state. The latter permits treating the tunneling in the presence of the closed channel, which was lacking in the models of Refs. [7–10], and estimating the effect of virtual transitions.

The model investigated is restricted due to a special choice of the system's energy in the domain below the excitation threshold. However, we hope to relax this condition in the future by finding solutions for different values of this parameter. To this end we can use the method of Ref. [13], where some solutions to the Heun equation are constructed as linear combinations of the hypergeometric functions. In this case, the derivation of the asymptotes and the N matrix for the problem under investigation can be based on matching with the asymptotes of the solutions of the special comparison equations, as performed in Sec. V for the specific case considered here.

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