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Interferences in adiabatic transition probabilities mediated by Stokes lines

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We consider the transition probability for two-level quantum-mechanical systems in the adiabatic limit when the Hamiltonian is analytic. We give a general formula for the leading term of the transition probability when it is governed by N complex eigenvalue crossings. This leading term is equal to a decreasing exponential times an oscillating function of the adiabaticity parameter. The oscillating function comes from an interference phenomenon between the contributions from each complex eigenvalue crossing, and when $N = 1$, it reduces to the geometric prefactor recently studied.

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I. INTRODUCTION

Two-level systems in quantum mechanics have always played an important role. This is not only because they provide the simplest nontrivial quantum-mechanical systems but mostly because many interesting phenomena in physics can be reduced to the study of such systems. In particular, the adiabatic limit for time-dependent two-level systems has been studied for a long time [1–3] and is still the object of recent investigations on the theoretical, as well as on the experimental sides [4]. The study of the adiabatic regime for two-level systems is relevant in atomic and molecular physics and particularly in the theory of slow atomic collisions, for example. Indeed, by using the Born-Oppenheimer approximation, the motion of the electrons in the field created by the slowly moving nuclei can sometimes be reduced to the study of a two-level system driven by a slowly varying time-reversal real Hamiltonian (see, e.g., the monograph by Nikitin and Umanskii [5]). In this paper we are concerned with the asymptotic behavior of the transition probability $P(T)$ in the adiabatic limit characterized by $T \to \infty$, where T is the typical time scale of the Hamiltonian. It is well known [1, 6, 7] that $P(T)$ decreases exponentially fast to zero, with exponential decay rate given by the so-called Dykhne formula, when the Hamiltonian is real symmetric and depends analytically on time. It has been shown recently [8–10] under "generic" hypotheses that the Dykhne formula must be completed by a geometrical prefactor when the Hamiltonian is Hermitian and analytic. A careful analysis of this formula, as well as a purely geometric interpretation of it is given in [9]. The geometrical prefactor has been measured successfully by Zwanziger, Rucker, and Chingas [11] in a spin experiment. Nevertheless, as they emphasize in the conclusion of their paper, realistic systems are not necessarily "generic" in the sense described below. This is precisely this aspect of the problem that we address here. Our analysis of these nongeneric cases shows that the leading term of $P(T)$ is not given anymore by an exponential times a constant geometric prefactor but by an exponential times an oscillatory function of T [see Eq. (1.12)]. This oscillatory behavior is the result of some interference phenomenon between different contributions to the transition probability. These features are present in particular in the theory of atomic collisions. The transition probability for such systems is described by an approximate formula, motivated by the treatment given in Landau and Lifschitz [12], which displays this oscillatory behavior (paragraph 7.3.3 in [5]). In the present paper we make a thorough investigation of the nongeneric situations, resuming and generalizing the work of Davis and Pechukas [13] to the case of complex Hermitian Hamiltonians. Our main result is formula (1.12) which gives the leading term of the transition probability when $T \to \infty$. To our knowledge, this formula does not appear in the literature. An example borrowed from the theory of atomic collisions, studied by Nikitin [14], will illustrate our results as well as a family of examples which will provide the different possible behaviors of the transition probability (see Sec. VIII). In particular, these examples will show the importance of the global features of the problem.

Similar rapid oscillations in the exponentially decreasing transition probability also appear in the exactly soluble model of Rosen and Zener [2] although their origin is different.

Let us state precisely our results: We consider the two-level system defined by

$$H(t) = \mathbf{B}(t)\cdot\mathbf{s} \equiv B_1(t)\frac{1}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} + B_2(t)\frac{1}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} + B_3(t)\frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} \quad (1.1)$$

with the following properties for the magnetic field.

(i) *Analyticity*: the functions B_k are analytic in a strip $S_a = \{z = t + is \in \mathbb{C} | \; |s| \leq a\}$ and we also assume the following technical condition.

(ii) *Behavior at infinity*: there exist two nonzero limiting fields $\mathbf{B}(+)$ and $\mathbf{B}(-)$ such that

$$\lim_{t\to\pm\infty} \sup_{|s|\leq a} |B_k(t+is) - B_k(\pm)| \, |t|^{1+\alpha} = 0$$

for some positive α, $k = 1, 2, 3$. Moreover we have the following.

(iii) *Separation of the spectrum*: for each $t \in \mathbb{R}$ the spectrum of $H(t)$ consists of two separated eigenvalues $e_1(t)$ and $e_2(t)$ such that $e_2(t) - e_1(t) \geq \delta$, $\delta > 0$.

The eigenvalues on the real axis are

$$e_j(t) = (-1)^j \tfrac{1}{2}\sqrt{\rho(t)}, \quad j = 1, 2, \tag{1.2}$$

where

$$\rho(t) = B_1^2(t) + B_2^2(t) + B_3^2(t) \tag{1.3}$$

is strictly positive. By convention we choose in (1.2) the branch of the square root which is positive on the positive real axis. The corresponding eigenprojections are

$$P_j(t) = \tfrac{1}{2}\, \mathbb{I} + (-1)^j \frac{\mathbf{B}(t)\cdot \mathbf{s}}{\sqrt{\rho(t)}}, \quad j = 1, 2 \; . \tag{1.4}$$

The eigenvalues and eigenprojections on S_a are defined by the analytic continuations of (1.2) and (1.4). They are multivalued and singular at the eigenvalue crossings which coincide with the zeros of the analytic continuation $\rho(z)$ of $\rho(t)$ in S_a. Notice that $\rho(z)$ is single-valued in S_a. We suppose furthermore the following.

(iv) *Eigenvalue crossings*: the set X of zeros of $\rho(z)$ in S_a consists of $2n$ interior points $z_1, \bar{z}_1, \ldots, z_n, \bar{z}_n$ and each zero is simple. By convention $\text{Im} z_k > 0$, $k = 1, \ldots, n$.

Let ψ_T be a normalized solution of the Schrödinger equation (with $\hbar = 1$)

$$i\frac{\partial}{\partial t}\psi_T(t) = TH(t)\psi_T(t) \tag{1.5}$$

satisfying the boundary condition

$$\lim_{t\to-\infty} ||P_1(t)\psi_T(t)|| = 1 \tag{1.6}$$

or equivalently

$$\lim_{t\to-\infty} ||P_2(t)\psi_T(t)|| = 0 \; . \tag{1.7}$$

The transition probability P is thus given by the expression

$$P = \lim_{t\to\infty} ||P_2(t)\psi_T(t)||^2 \; . \tag{1.8}$$

In this problem, the Stokes lines play an important role (as in any WKB analysis). These lines are defined as follows: Let $\Delta_{12}(z)$ be the analytic continuation of the function

$$\Delta_{12}(t) = \int_0^t [e_1(s) - e_2(s)]ds$$
$$= -\int_0^t \sqrt{\rho(s)}ds \; . \tag{1.9}$$

$\Delta_{12}(z)$ is a multivalued function in S_a with branch points at the points of X and $\Delta_{12}(z_j)$ is defined by continuity, when $z_j \in X$. The level lines $\text{Im}\Delta_{12}(z) = \text{Im}\Delta_{12}(z_j) =$ const constitute the set of the *Stokes lines* of the problem. For the whole analysis of this paper, as well as in our previous papers, it is essential that there exists a Stokes line (hereafter called infinite Stokes line) going from $-\infty$ to $+\infty$ which is entirely contained in the strip S_a. Such an hypothesis is not always explicitly stated but it is always implicitly used at some point. In [9] and [10], we considered the generic situation where the infinite Stokes line passes through exactly one eigenvalue crossing. This eigenvalue crossing is then the one which governs the asymptotic behavior of P. This is the reason why it is an important issue to determine this Stokes line when there are several eigenvalue crossings in the problem. (See the examples and discussion of this point in [9].) In this paper we analyze nongeneric situations satisfying the following hypothesis.

(v) *Existence of an infinite Stokes line through N eigenvalue crossings*: there exist N eigenvalue crossings $z_1, \ldots, z_N$ and a Stokes line $t \mapsto \gamma(t)$, $t \in \mathbb{R}$ in S_a, passing through $z_1, \ldots, z_{N-1}$ and z_N such that $\lim_{t\to\pm\infty} \text{Re}\gamma(t) = \pm\infty$ and $|\text{Im}\gamma(t)| < a$ for large enough $|t|$.

Although we call the above situation nongeneric, we expect that it will occur for time-reversal Hamiltonians, as a consequence of this symmetry. When the infinite Stokes line passes through one eigenvalue crossing only, we have the result [9]

$$P = \left|\exp(-i\theta_1)\exp\left(-iT\int_{\eta_1} e_1(z)dz\right)[1 + O(1/T)]\right|^2 , \tag{1.10}$$

where η_1 is a loop in the complex plane, based at the origin, encircling the eigenvalue crossing z_1 clockwise and $\int_{\eta_1} e_1(z)dz$ is the integral over η_1 of the analytic continuation of e_1 along η_1. The prefactor $e^{-i\theta_1}$ is of geometric nature and is an analogue of the Berry phase. Indeed, there exists a particular choice of multivalued analytic eigenvectors $\varphi_1(z)$ and $\varphi_2(z)$ of $H(z)$, associated with $e_1(z)$ and $e_2(z)$ such that the analytic continuation of $\varphi_1(z)$ along η_1, noted $\tilde{\varphi}_1(0)$, is given by

$$\tilde{\varphi}_1(0) = e^{-i\theta_1}\varphi_2(0) \; . \tag{1.11}$$

The phase θ_1 is in general complex and its imaginary part has been measured by Zwanziger, Rucker, and Chingas [11] in their spin experiment. The analysis of Sec. VII shows that when hypotheses (i)–(v) hold, the transition probability is given by

$$P = \Bigg| \sum_{j=1}^{N} \exp(-i\theta_j) \exp\left(-iT \int_{\eta_j} e_1(z)dz\right) + O\left(\exp\left(T \,\mathrm{Im} \int_{\eta_1} e_1(z)dz\right) \Big/ T^{1/5}\right)\Bigg|^2 , \quad (1.12)$$

where θ_j and η_j are defined in analogy with (1.10).

Notice that the transition probability is independent of the location of the basis of the loops η_j on the real axis. Indeed, if we replace all integrals from 0 to z_j by integrals from c to z_j, $c \in I\!R$, the expression for P is unaffected. There exists an entirely geometric formulation of the transition probability which reads

$$P = \exp\left[-2Td_\rho(z_1, I\!R)\right]\left[\sum_{j=1}^{N} \exp(2\,\mathrm{Im}\theta_j) + 2\sum_{k<j}^{N} \exp[\mathrm{Im}(\theta_k + \theta_j)] \cos\left[Td_\rho(z_k, z_j) + \mathrm{Re}(\theta_k - \theta_j)\right] + O\left(\frac{1}{T^{1/5}}\right)\right], \quad (1.13)$$

where d_ρ is a distance dependent of ρ (see [9]). As $d_\rho(z_k, z_j) > 0$ if $k \neq j$, the interference phenomenon is always present when $N \geq 2$.

II. PRELIMINARIES

Let us consider the normalized solution $\psi_T(t)$ of (1.5) satisfying the boundary condition (1.6). It is convenient to expand this solution on a normalized basis of instantaneous eigenvectors of $H(t)$. There are several ways to choose them. We define the eigenvectors by requiring that

$$H(t)\varphi_k(t) = e_k(t)\varphi_k(t), \quad k = 1,2 \quad (2.1)$$

and

$$\left\langle \varphi_k(t) \middle| \frac{d}{dt}\varphi_k(t) \right\rangle = 0, \quad k = 1,2 \quad (2.2)$$

where $\langle\,|\,\rangle$ is the usual scalar product in $\mathbb{C}^2$. The vectors defined by (2.2) coincide with those defined by means of the solution of the equation (see, e.g., Kato [15], Chap. II.4)

$$\frac{d}{dt}U(t) = K(t)U(t), \quad U(0) = \underline{I} \quad (2.3)$$

where

$$K(t) = P_1'(t)P_1(t) + P_2'(t)P_2(t) = i\frac{\mathbf{B}(t) \times \mathbf{B}'(t)}{\rho(t)} \cdot \mathrm{s} \quad (2.4)$$

and $\mathbf{B} \times \mathbf{B}'$ denotes the vector product of $\mathbf{B}$ and $\mathbf{B}'$. We have $\varphi_k(t) = U(t)\varphi_k(0)$. The solution $\psi_T(t)$ of (1.5) has an analytic extension on S_a, $\psi_T(z)$, which is a single-valued function satisfying the differential equation

$$i\psi_T'(z) = TH(z)\psi_T(z) \,. \quad (2.5)$$

Here, and throughout the paper, a prime denotes d/dz, z complex. The operator K has a single-valued meromorphic extension in S_a with poles at the points of X. Thus U and the eigenvectors φ_k have multivalued analytic extensions in S_a, with singularities at the points of X. In order to deal with single-valued functions, we construct a simply connected domain Ω, with no eigenvalue crossing in its interior, in the following way: Let Ω be the simply connected domain whose borders are the real axis and the infinite Stokes line of condition (v). It can be shown along the lines of [9] that there is no eigenvalue crossing inside Ω. Thus, from now on, we shall restrict all analytic functions to Ω, in which they are single valued. The image of Ω by Δ_{12} is the strip $\mathrm{Im}\Delta_{12}(z_1) \leq \mathrm{Im}\xi \leq 0$ and this map is one-to-one. In particular the infinite Stokes line is mapped onto the horizontal line $\mathrm{Im}\xi = \mathrm{Im}\Delta_{12}(z_1) < 0$. As a consequence of condition (ii) there exist two operators $U(+)$ and $U(-)$ such that

$$\lim_{t\to\pm\infty} \sup_{|s|<a} \|U(t+is) - U(\pm)\| = 0 \,. \quad (2.6)$$

These limiting operators do not depend on s. Let

$$\lambda_k(z) = \int_0^z e_k(z')dz', \quad k = 1,2 \quad (2.7)$$

and

$$\Delta_{ij}(z) = \lambda_i(z) - \lambda_j(z), \quad i \neq j, \quad (2.8)$$

where in (2.7) the integral is over any path in Ω starting at 0 and ending at z. We expand the analytic continuation of $\psi_T(t)$ in Ω as follows :

$$\psi_T(z) = \sum_{j=1}^{2} c_j(z)e^{-iT\lambda_j(z)}\varphi_j(z). \quad (2.9)$$

By inserting (2.9) in (2.5) we obtain a differential equation for the coefficients c_j which reads

$$c_k'(z) = \sum_{j=1}^{2} a_{kj}(z)e^{iT\Delta kj}c_j(z), \quad j \neq k \quad (2.10)$$

where

$$a_{kj}(z) = -\langle\varphi_k(0)|U(z)^{-1}\varphi_j'(z)\rangle = -\langle\varphi_k(0)|U(z)^{-1}K(z)U(z)\varphi_j(0)\rangle. \quad (2.11)$$

Again, it follows from condition (ii) that the coefficients $c_j(t+is)$ have well-defined s-independent limits $c_j(\pm\infty)$ as $t \to \pm\infty$:

$$\lim_{|t|\to\infty} |c_j(t+is) - c_j(\pm\infty)| = 0, \quad j = 1,2. \quad (2.12)$$

In particular, the boundary condition (1.6) reads

$$\lim_{t\to-\infty}|c_1(t)| = |c_1(-\infty)| = 1,$$
$$\lim_{t\to-\infty}|c_2(t)| = |c_2(-\infty)| = 0, \tag{2.13}$$

and the transition probability P is equal to

$$P = |c_2(+\infty)|^2 . \tag{2.14}$$

We refer the reader to [9] for more details on this analysis.

Let us outline briefly the strategy we shall follow for the case $N = 2$. We shall use formula (2.12) in order to compute P. This formula allows the differential equation (2.10) to be solved along a path which follows the infinite Stokes line except in the neighborhoods of the crossing points, which are singular points for the differential equation.

We control the solution of Eq. (2.10) from $-\infty$ to a point z_1^- in a T-dependent neighborhood of z_1 (see Fig. 1) along the infinite Stokes line. We use the fact that along this line $\mathrm{Im}\Delta_{12}$ is constant so that we control the solution by performing an integration by parts in the equivalent integral equation.

We then determine the singularity of the coefficients a_{kj} in the T-dependent neighborhood of z_1. This is done by analytically continuing an explicit expression for them from the real axis to this neighborhood.

Retaining the dominant terms of the differential equation near z_1, we define a comparison equation which can be solved explicitly.

We use this equation to go from z_1^- to z_1^+ in the T-dependent neighborhood of z_1 and by a standard streching and matching procedure, we get an estimate of the solution of (2.10) at z_1^+.

We iterate the whole procedure.

III. STUDY OF THE SINGULARITIES

In this section we first determine the singularities of Eq. (2.10). Let z^* be one of the eigenvalue crossings located on the infinite Stokes line. In order to study these singularities we need an explicit form for the eigenvectors $\varphi_j(z)$ defined by (2.2). We show in the Appendix the following lemma by an explicit analytic continuation. The proof is rather technical.

Lemma 3.1. Let z^* be a simple zero of $\rho(z)$ such that $B_3(z^*) \neq 0$. Let γ be a path from some fixed point of $\mathbb{R}$ to z, in the neighborhood of z^* such that $B_1^2(u)+B_2^2(u) \neq 0$ $\forall u \in \gamma$. Then

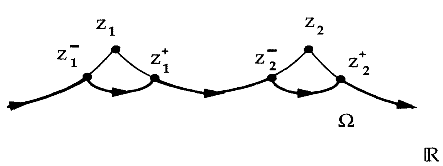

FIG. 1. The integration path for $N = 2$.

$$a_{kj}(z) = -\left[\exp\left((-1)^j i \int_0^z \frac{\varphi(z')}{\sqrt{\rho(z')}}dz'\right) \Big/ \rho(z)\right] \times[(-1)^j\alpha_1(z) + \sqrt{\rho(z)}\alpha_2(z)] , \tag{3.1}$$

where $\varphi(z)$, $\alpha_1(z)$, and $\alpha_2(z)$ are analytic around z^*, $\alpha_1(z^*) \neq 0$, and are given by

$$\varphi(z) = \frac{B_3(z)[B_1(z)B_2'(z) - B_2(z)B_1'(z)]}{B_1^2(z) + B_2^2(z)} , \tag{3.2}$$

$$\alpha_1(z) = \frac{B_3(z)\rho'(z)}{4\sqrt{B_1^2(z) + B_2^2(z)}} - \frac{B_3'(z)\rho(z)}{2\sqrt{B_1^2(z) + B_2^2(z)}} , \tag{3.3}$$

$$\alpha_2(z) = \frac{i[B_1(z)B_2'(z) - B_2(z)B_1'(z)]}{2\sqrt{B_1^2(z) + B_2^2(z)}} . \tag{3.4}$$

(The integration and analytic continuations are along γ.)

Remarks.

(1) If $B_3(z^*) = 0$, then $B_1(z^*)$ or $B_2(z^*)$ is nonzero because z^* is a simple zero of ρ. In such a case the lemma holds with a suitable permutation of the indices (see the Appendix).

(2) Notice that $a_{kj}(z^*)$ is independent of the choice of γ but this is not true for α_1, α_2 and the exponent in (3.1).

By denoting the exponent in (3.1) by $\Phi(z)$ we can write, in the vicinity of z^*,

$$a_{kj}(z) = -\exp[(-1)^j i\Phi(z^*) + O((z - z^*)^{1/2})] \times (-1)^j \frac{\alpha_1(z^*)}{\rho'(z^*)}\left(\frac{1}{z - z^*} + O((z - z^*)^{-1/2})\right), \tag{3.5}$$

where we have used hypothesis (iv) to write $\rho(z) = \rho'(z^*)(z-z^*)+O((z-z^*)^2)$. By similar computations we obtain the following approximation for a_{kj}' in the same neighborhood,

$$a_{kj}'(z) = \exp[(-1)^j i\Phi(z^*) + O((z - z^*)^{1/2})] \times (-1)^j \frac{\alpha_1(z^*)}{\rho'(z^*)}\left(\frac{1}{(z - z^*)^2} + O((z - z^*)^{-3/2})\right) . \tag{3.6}$$

Let $t \mapsto \gamma(t)$ be a parametrization of the infinite Stokes line. We control the solutions of (2.10) along a segment $s_1 \leq t \leq s_2$ of the Stokes line, which does not contain any singularity of Eqs. (2.10), so that s_1 and s_2 are either such that $\gamma(s_1) = z_j^+ \equiv \gamma(t_j^+)$ and $\gamma(s_2) = z_{j+1}^- \equiv \gamma(t_{j+1}^-)$ (see Fig. 1) or $s_1 = -\infty$ and $\gamma(s_2) = z_1^- \equiv \gamma(t_1^-)$ or $s_2 = +\infty$ and $\gamma(s_1) = z_N^+ \equiv \gamma(t_N^+)$. We follow [9] and write $\dot\gamma(t)$ for

$(d/dt)\gamma(t)$, $f(t)$ for $f(\gamma(t))$, and so on. Equations (2.10) are equivalent to the integral equations

$$c_1(t) = c_1(s_1) + \int_{s_1}^{t} ds\, \dot\gamma(s) a_{12}(s) e^{iT\Delta_{12}}(s) c_2(s),$$
$$c_2(t) = c_2(s_1) + \int_{s_1}^{t} ds\, \dot\gamma(s) a_{21}(s) e^{iT\Delta_{21}}(s) c_1(s), \tag{3.7}$$
$$s_1 \le t \le s_2 .$$

We perform an integration by parts and write the result in terms of the new variables,

$$\widehat{c}_1(s) \equiv c_1(s) ,$$
$$\widehat{c}_2(s) \equiv \exp[-T\,\mathrm{Im}\Delta_{12}(s)] c_2(s) ; \tag{3.8}$$

we get

$$\widehat{c}_1(t) = \widehat{c}_1(s_1) + \frac{1}{iT\Delta'_{12}(s)} \exp[iT\,\mathrm{Re}\Delta_{12}(s)] a_{12}(s)\widehat{c}_2(s)\Big|_{s_1}^{t} - \frac{1}{iT}\int_{s_1}^{t} ds\,\dot\gamma(s) \exp[iT\,\mathrm{Re}\Delta_{12}(s)] \left(\frac{a_{12}}{\Delta'_{12}}\right)'(s)\widehat{c}_2(s) - \frac{1}{iT}\int_{s_1}^{t} ds\,\dot\gamma(s)\frac{a_{12}(s)a_{21}(s)}{\Delta'_{12}(s)}\widehat{c}_1(s) , \tag{3.9}$$

$$\widehat{c}_2(t) = \widehat{c}_2(s_1) - \frac{1}{iT\Delta'_{12}(s)} \exp[-iT\,\mathrm{Re}\Delta_{12}(s)] a_{21}(s)\widehat{c}_1(s)\Big|_{s_1}^{t} + \frac{1}{iT}\int_{s_1}^{t} ds\,\dot\gamma(s) \exp[-iT\,\mathrm{Re}\Delta_{12}(s)] \left(\frac{a_{21}}{\Delta'_{12}}\right)'(s)\widehat{c}_1(s) + \frac{1}{iT}\int_{s_1}^{t} ds\,\dot\gamma(s)\frac{a_{12}(s)a_{21}(s)}{\Delta'_{12}(s)}\widehat{c}_2(s), \quad s_1 \le t \le s_2 .$$

If $\gamma(t_j) = z_j$ denotes the eigenvalue crossing z_j, it follows from (3.5) and (3.6) that we can find a constant independent of j and s such that, for all j and s,

$$\left|\frac{a_{ij}(s)}{\Delta'_{12}(s)}\right| \le \text{const} \times |\gamma(s) - \gamma(t_j)|^{-3/2} ,$$
$$\left|\frac{a_{12}(s)a_{21}(s)}{\Delta'_{12}(s)}\right| \le \text{const} \times |\gamma(s) - \gamma(t_j)|^{-5/2} , \tag{3.10}$$
$$\left|\left(\frac{a_{ij}}{\Delta'_{12}}(s)\right)'\right| \le \text{const} \times |\gamma(s) - \gamma(t_j)|^{-5/2} .$$

Let $\epsilon > 0$. We suppose that $|\gamma(s) - \gamma(t_j)| \ge \epsilon$ for all s and we define $\|\widehat{c}_k\| = \sup_{s_1 \le t \le s_2} |\widehat{c}_k(t)|$. We have

$$|\widehat{c}_1(t)| \le |\widehat{c}_1(s_1)| + \frac{\text{const} \times (\|\widehat{c}_1\| + \|\widehat{c}_2\|)}{T}(1 + \epsilon^{-3/2}) \tag{3.11}$$

and

$$|\widehat{c}_2(t)| \le |\widehat{c}_2(s_1)| + \frac{\text{const} \times (\|\widehat{c}_1\| + \|\widehat{c}_2\|)}{T}(1 + \epsilon^{-3/2}) . \tag{3.12}$$

Let T be large enough so that $\text{const} \times (1 + \epsilon^{-3/2})/T \le \frac{1}{2}$. Summing the inequalities above and taking the supremum over t we get

$$\|\widehat{c}_1\| + \|\widehat{c}_2\| \le 2[|\widehat{c}_1(s_1)| + |\widehat{c}_2(s_1)|] . \tag{3.13}$$

Coming back to (3.9) we obtain under the same condition

$$|\widehat{c}_k(t) - \widehat{c}_k(s_1)| \le \frac{\text{const} \times [|\widehat{c}_1(s_1)| + |\widehat{c}_2(s_1)|]}{T} \times (1 + \epsilon^{-3/2}) \tag{3.14}$$

for $s_1 \le t \le s_2$ and $k = 1, 2$.

IV. COMPARISON EQUATION

The c_k's satisfy

$$c'_1(z) = a_{12}(z) e^{iT\Delta_{12}(z)} c_2(z) ,$$
$$c'_2(z) = a_{21}(z) e^{-iT\Delta_{12}(z)} c_1(z) . \tag{4.1}$$

To study this equation close to a crossing point z_j, we introduce the new variable

$$x \equiv T[\Delta_{12}(z) - \Delta_{12}(z_j)] = -T\int_{z_j}^{z} dz' \sqrt{\rho(z')} . \tag{4.2}$$

This change of variable is locally well defined everywhere in a neighborhood in Ω of the crossing point. Note that x depends on T and j and that on the infinite Stokes line x is real and $x = 0$ when $z = z_j$. In terms of this new variable, Eq. (4.1) reads

$$\frac{d}{dx} c_1(z(x)) = -\frac{a_{12}(z(x))}{T\sqrt{\rho(z(x))}} \times \exp\{i[x + T\Delta_{12}(z_j)]\} c_2(z(x)) , \tag{4.3}$$

$$\frac{d}{dx} c_2(z(x)) = -\frac{a_{21}(z(x))}{T\sqrt{\rho(z(x))}} \times \exp\{-i[x + T\Delta_{12}(z_j)]\} c_1(z(x)) .$$

We retain in this expression the dominant terms when $|z - z_j|$ is small and express the result in terms of the new variable x, which behaves as

$$x = -T\tfrac{2}{3}\sqrt{\rho'(z_j)}(z - z_j)^{3/2}[1 + O(z - z_j)] . \quad (4.4)$$

Thus, reversing the formula,

$$z - z_j = O\left(\left(\frac{x}{T}\right)^{2/3}\right) . \quad (4.5)$$

Hence, by using (3.5),

$$-\frac{a_{kj}(z(x))}{T\sqrt{\rho(z(x))}}\exp\{(-1)^j i[x + T\Delta_{12}(z_j)]\}$$

$$= -\exp\left\{(-1)^j i\left[\Phi(z_j) + T\Delta_{12}(z_j) + x\right]\right\}$$

$$\times (-1)^j \frac{2\alpha_1(z_j)}{3\rho'(z_j)}\left[\frac{1}{x} + \frac{1}{T}O\left(\left(\frac{T}{x}\right)^{2/3}\right)\right] , \quad (4.6)$$

where

$$\frac{2\alpha_1(z_j)}{3\rho'(z_j)} = \frac{B_3(z_j)}{6\sqrt{B_1^2(z_j) + B_2^2(z_j)}}$$

$$= \frac{B_3(z_j)}{6\sqrt{-B_3^2(z_j)}} \equiv \epsilon(z_j)\frac{i}{6} . \quad (4.7)$$

The factor $\epsilon(z_j) = \pm 1$ depends on the analytic continuation of $B_1^2(z_j) + B_2^2(z_j)$ along the path γ of lemma 3.1. See the remarks following the lemma.

We define the comparison equation by

$$\frac{d}{dx}c_1^A(x) = -\frac{i\epsilon(z_j)}{6}\exp\left[i\Phi(z_j) + iT\Delta_{12}(z_j)\right] \times \frac{e^{ix}}{x}c_2^A(x) ,$$

$$\frac{d}{dx}c_2^A(x) = +\frac{i\epsilon(z_j)}{6}\exp\left[-i\Phi(z_j) - iT\Delta_{12}(z_j)\right] \times \frac{e^{-ix}}{x}c_1^A(x) . \quad (4.8)$$

In order to absorb the exponentials in the constant coefficients, we consider the equivalent equation

$$\frac{d}{dx}\widetilde{\mathbf{c}}^A(x) = \begin{pmatrix} 0 & -\frac{i\epsilon(z_j)}{6}\frac{e^{ix}}{x} \\ \frac{i\epsilon(z_j)}{6}\frac{e^{-ix}}{x} & 0 \end{pmatrix}\widetilde{\mathbf{c}}^A(x)$$

$$\equiv A(x)\widetilde{\mathbf{c}}^A(x) \quad (4.9)$$

with

$$\widetilde{c}_1^A(x) \equiv c_1^A(x),$$

$$\widetilde{c}_2^A(x) \equiv \exp\left[i\Phi(z_j) + iT\Delta_{12}(z_j)\right]c_2^A(x) . \quad (4.10)$$

Similarly, we introduce

$$\widetilde{c}_1(x) \equiv c_1(z(x)) ,$$

$$\widetilde{c}_2(x) \equiv \exp\left[i\Phi(z_j) + iT\Delta_{12}(z_j)\right]c_2(z(x)) = \widehat{c}_2(z(x))\exp\left[i\Phi(z_j) + iT\,\mathrm{Re}\Delta_{12}(z_j)\right] , \quad (4.11)$$

satisfying an equation which is equivalent to (4.3),

$$\frac{d}{dx}\widetilde{\mathbf{c}}(x) = [A(x) + B(x,T)]\widetilde{\mathbf{c}}(x) , \quad (4.12)$$

where $B(x,T)$ is defined by

$$A(x) + B(x,T) \equiv \begin{pmatrix} 0 & -\frac{a_{12}(z(x))}{T\sqrt{\rho(z(x))}}e^{-i\Phi(z_j)}e^{ix} \\ -\frac{a_{21}(z(x))}{T\sqrt{\rho(z(x))}}e^{i\Phi(z_j)}e^{-ix} & 0 \end{pmatrix} . \quad (4.13)$$

It follows from the foregoing that

$$||B(x,T)|| \le \frac{\text{const} \times e^{|\mathrm{Im}x|}}{T(|x|/T)^{2/3}}$$

and (4.14)

$$||A(x)|| \le \frac{e^{|\mathrm{Im}x|}}{6|x|} \text{ if } \left|\frac{x}{T}\right| \ll 1 .$$

The bounds obtained in the preceding section on the integration of $\widehat{c}_j$ along the arcs of Stokes line between successive eigenvalue crossings give accuracies of order $1/(T\epsilon^{3/2}) \equiv O(1/T|z_j^{\pm} - z_j|^{3/2})$, where $z_j^{\pm}$ are defined as in Fig. 1. In terms of the variable x, this means accuracies of order $1/|x^{\pm}|$ if $x(z_j^{\pm}) \equiv x^{\pm}$. Thus we already see that the scaling limit will be such that $|x| \to \infty$ and $|x|/T \to 0$.

We postpone the determination of the adequate scaling limit to a subsequent section and turn to the resolution of the comparison equation.

V. SOLUTION OF THE COMPARISON EQUATION

We first go from the two coupled first-order differential equations (4.9) to a second-order differential equation for $\widetilde{c}_1^A(x) = c_1^A(x)$. This coefficient satisfies

$$f''(x) + \left(\frac{1}{x} - i\right) f'(x) - \frac{d^2}{x^2} f(x) = 0 \ , \tag{5.1}$$

where

$$d^2 = -\left(\frac{i\epsilon(z_j)}{6}\right)^2 = \frac{1}{36} \ . \tag{5.2}$$

By introducing the auxiliary function $v(x)$ such that

$$f(x) = \exp(ix + d \ln x) v(x) \tag{5.3}$$

we are led to

$$v''(x) + \left(i + \frac{2d+1}{x}\right) v'(x) + \frac{i(d+1)}{x} v(x) = 0 \tag{5.4}$$

which reduces to the Kummer's equation for w,

$$y w''(y) + (b - y) w'(y) - a w(y) = 0, \tag{5.5}$$

where $y = -ix$, $w(y) = v(iy)$, $a = d + 1 = \frac{7}{6}$, and $b = 2d + 1 = \frac{4}{3}$. This last equation has been extensively studied and its solutions are well known (see, for example, [16], p. 268).

Two linearly independent solutions of (5.5) are given by $w_1(a,b,y) = M(a,b,y)$ and $w_2(a,b,y) = y^{1-b} M(a - b + 1, 2 - b, y)$ where

$$M(a,b,y) = \frac{\Gamma(b)}{\Gamma(a)} \sum_{n=0}^{\infty} \frac{\Gamma(a+n)}{\Gamma(b+n)} \frac{y^n}{n!} \tag{5.6}$$

is single valued and is called the Kummer's or confluent hypergeometric function. The asymptotic behaviors of w_1 and w_2 for large arguments are given by

$$\begin{aligned} w_1(a,b,y) &= e^{-i\pi a} \frac{\Gamma(b)}{\Gamma(b-a)} w_1^{\infty}(a,b,y) \\ &\quad + \frac{\Gamma(b)}{\Gamma(a)} w_2^{\infty}(a,b,y) \ , \\ w_2(a,b,y) &= e^{-i\pi(a-b+1)} \frac{\Gamma(2-b)}{\Gamma(1-a)} w_1^{\infty}(a,b,y) \\ &\quad + \frac{\Gamma(2-b)}{\Gamma(a-b+1)} w_2^{\infty}(a,b,y) \ , \end{aligned} \tag{5.7}$$

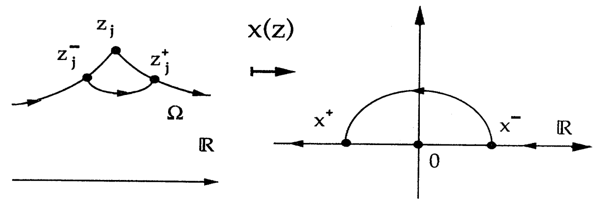

FIG. 2. The image of a neighborhood in Ω of z_j by $x(z)$.

where

$$\begin{aligned} w_1^{\infty}(a,b,y) &= y^{-a}\left(1 - a(a-b+1)\frac{1}{y} + O(y^{-2})\right) \ , \\ w_2^{\infty}(a,b,y) &= y^{a-b} e^{y}\left(1 + (b-a)(1-a)\frac{1}{y} + O(y^{-2})\right) \ , \end{aligned} \tag{5.8}$$

when $|y| \to \infty$ with $-3\pi/2 < \arg y < \pi/2$.

Thanks to these solutions we can write

$$\widetilde{c}_1^A(x) = e^{ix} x^{1/6} [p w_1(\tfrac{7}{6}, \tfrac{4}{3}, -ix) + q w_2(\tfrac{7}{6}, \tfrac{4}{3}, -ix)] \ , \tag{5.9}$$

where p and q are constants and

$$\widetilde{c}_2^A = \frac{x e^{-ix}}{\gamma} \frac{d}{dx} \widetilde{c}_1^A(x), \quad \gamma = -\frac{i\epsilon(z_j)}{6} \ . \tag{5.10}$$

Using the relations ([16], p. 264)

$$\begin{aligned} \frac{d}{dy} w_1(a,b,y) &= \frac{a}{b} w_1(a+1, b+1, y) \ , \\ \frac{d}{dy} w_2(a,b,y) &= \frac{d}{dy}[y^{1-b} M(a-b+1, 2-b, y)] \\ &= \frac{1-b}{y} w_2(a,b,y) \\ &\quad + \frac{a-b+1}{y(2-b)} w_2(a, b-1, y) \ , \end{aligned} \tag{5.11}$$

we obtain from (5.10) the explicit expression

$$\begin{aligned} \widetilde{c}_2^A(x) = {} & \frac{p}{\gamma}[i x^{7/6} w_1(\tfrac{7}{6}, \tfrac{4}{3}, -ix) + \tfrac{1}{6} x^{1/6} w_1(\tfrac{7}{6}, \tfrac{4}{3}, -ix) - i\tfrac{7}{8} x^{7/6} w_1(\tfrac{13}{6}, \tfrac{7}{3}, -ix)] \\ & + \frac{q}{\gamma}[i x^{7/6} w_2(\tfrac{7}{6}, \tfrac{4}{3}, -ix) - \tfrac{1}{6} x^{1/6} w_2(\tfrac{7}{6}, \tfrac{4}{3}, -ix) + \tfrac{5}{4} x^{1/6} w_2(\tfrac{7}{6}, \tfrac{1}{3}, -ix)] \ . \end{aligned} \tag{5.12}$$

On the arc of the Stokes line linking z_{j-1} and z_j, the variable x defined by (4.2) is real and positive. Indeed, $\mathrm{Re}\Delta_{12}(z) \to \infty$ when $\mathrm{Re} z \to -\infty$, $|\mathrm{Im} z| < a$ [see (2.8) and condition (ii)] and $\mathrm{Re}\Delta_{12}$ is strictly monotone along the infinite Stokes line of condition (vi), as $\Delta_{12}' \neq 0$ there. Thus on the arc of Stokes line between z_j and z_{j+1}, x is real negative, and the passage from x positive to x negative is such that $0 < x \mapsto e^{i\pi} x$ if $z(x)$ is constrained to stay in Ω (see Fig. 2). The asymptotic behaviors of $\widetilde{c}_1^A$ and $\widetilde{c}_2^A$ for x large and positive are computed with the help of (5.7) and (5.8) since $\arg(-ix) = -\pi/2$. It is straightforward to obtain from these formulas and the property $\Gamma(z+1) = z\Gamma(z)$ the following expansions:

$$\tilde{c}_1^A(x) = e^{i\pi/12}\left[p\left(\frac{\Gamma(\frac{4}{3})}{\Gamma(\frac{7}{6})} + O(x^{-1})\right) + q\left(\frac{\Gamma(\frac{2}{3})}{\Gamma(\frac{5}{6})} + O(x^{-1})\right)\right] ,$$

$$\tilde{c}_2^A(x) = \frac{ie^{-i7\pi/12}}{6\gamma}\left[p\left(\frac{\Gamma(\frac{4}{3})}{\Gamma(\frac{7}{6})} + O(x^{-1})\right) - e^{i\pi/3}q\left(\frac{\Gamma(\frac{2}{3})}{\Gamma(\frac{5}{6})} + O(x^{-1})\right)\right] \tag{5.13}$$

as $x \to \infty$. We also need $\tilde{\mathbf{c}}^A(xe^{i\pi})$ as $x \to \infty$ but the asymptotic formulas (5.8) are not valid in this case since $\arg(-ixe^{i\pi}) = \pi/2$ if $x > 0$. Hence we use the following symmetry relation ([16], p. 267):

$$M(a,b,y) = e^y M(b-a,b,-y) \tag{5.14}$$

from which we deduce

$$w_1(a,b,e^{i\pi}y) = e^{-y}w_1(b-a,b,y) , \quad w_2(a,b,e^{i\pi}y) = e^{i\pi(1-b)}e^{-y}w_2(b-a,b,y) . \tag{5.15}$$

Now we can write

$$\tilde{c}_1^A(xe^{i\pi}) = e^{i\pi/6}x^{1/6}[pw_1(\tfrac{1}{6},\tfrac{4}{3},-ix) + e^{-i\pi/3}qw_2(\tfrac{1}{6},\tfrac{4}{3},-ix)] ,$$

$$\tilde{c}_2^A(xe^{i\pi}) = e^{i\pi/6}e^{ix}\Bigg(\frac{p}{\gamma}[-ix^{7/6}w_1(\tfrac{1}{6},\tfrac{4}{3},-ix) + \tfrac{1}{6}x^{1/6}w_1(\tfrac{1}{6},\tfrac{4}{3},-ix) + i\tfrac{7}{8}x^{7/6}w_1(\tfrac{1}{6},\tfrac{7}{3},-ix)]$$
$$+e^{-i\pi/3}\frac{q}{\gamma}[-ix^{7/6}w_2(\tfrac{1}{6},\tfrac{4}{3},-ix) - \tfrac{1}{6}x^{1/6}w_2(\tfrac{1}{6},\tfrac{4}{3},-ix) - \tfrac{5}{4}x^{1/6}w_2(-\tfrac{5}{6},\tfrac{1}{3},-ix)]\Bigg) , \tag{5.16}$$

with $x > 0$ and we can apply formulas (5.8) to compute the asymptotic behaviors. By a direct computation we obtain

$$\tilde{c}_1^A(xe^{i\pi}) = e^{i\pi/12}\left[p\left(\frac{\Gamma(\frac{4}{3})}{\Gamma(\frac{7}{6})} + O(x^{-1})\right) + q\left(\frac{\Gamma(\frac{2}{3})}{\Gamma(\frac{5}{6})} + O(x^{-1})\right)\right] ,$$

$$\tilde{c}_2^A(xe^{i\pi}) = \frac{ie^{-i7\pi/12}}{6\gamma}\left[e^{i\pi/3}p\left(\frac{\Gamma(\frac{4}{3})}{\Gamma(\frac{7}{6})} + O(x^{-1})\right) - q\left(\frac{\Gamma(\frac{2}{3})}{\Gamma(\frac{5}{6})} + O(x^{-1})\right)\right] , \tag{5.17}$$

as $x \to \infty$.

Lemma 5.1. Let $\tilde{\mathbf{c}}^A(x)$ be a vector solution of (4.9) whose asymptotic behavior is given by

$$\tilde{\mathbf{c}}^A(x) = \begin{pmatrix} a \\ b \end{pmatrix} + O(x^{-1}) \quad \text{as } x \to \infty .$$

Then

$$\tilde{\mathbf{c}}^A(xe^{i\pi}) = Y(z_j)\begin{pmatrix} a \\ b \end{pmatrix} + O(x^{-1}) \quad \text{as } x \to \infty$$

where

$$Y(z_j) = \begin{pmatrix} 1 & 0 \\ -\epsilon(z_j) & 1 \end{pmatrix}$$

and $\epsilon(z_j) = 6i\gamma = \pm 1$.

Proof. The hypothesis and (5.13) lead to the relation

$$\begin{pmatrix} a \\ b \end{pmatrix} + O(x^{-1}) = W(x)\begin{pmatrix} p \\ q \end{pmatrix} , \tag{5.18}$$

where

$$W(x) = W^+ + O(x^{-1}),$$

$$W^+ = \begin{pmatrix} e^{i\pi/12}\dfrac{\Gamma(\frac{4}{3})}{\Gamma(\frac{7}{6})} & e^{i\pi/12}\dfrac{\Gamma(\frac{2}{3})}{\Gamma(\frac{5}{6})} \\ \dfrac{ie^{-i7\pi/12}}{6\gamma}\dfrac{\Gamma(\frac{4}{3})}{\Gamma(\frac{7}{6})} & -\dfrac{ie^{-i7\pi/12}}{6\gamma}e^{i\pi/3}\dfrac{\Gamma(\frac{2}{3})}{\Gamma(\frac{5}{6})} \end{pmatrix} . \tag{5.19}$$

From (5.17) we can write

$$W(xe^{i\pi}) = W^- + O(x^{-1}) \; , \qquad (5.20)$$

$$W^- = \begin{pmatrix} e^{i\pi/12}\dfrac{\Gamma(\frac{4}{3})}{\Gamma(\frac{7}{6})} & e^{i\pi/12}\dfrac{\Gamma(\frac{2}{3})}{\Gamma(\frac{5}{6})} \\ \dfrac{ie^{-i7\pi/12}}{6\gamma}e^{i\pi/3}\dfrac{\Gamma(\frac{4}{3})}{\Gamma(\frac{7}{6})} & -\dfrac{ie^{-i7\pi/12}}{6\gamma}\dfrac{\Gamma(\frac{2}{3})}{\Gamma(\frac{5}{6})} \end{pmatrix} .$$

Thus

$$W(xe^{i\pi})\begin{pmatrix} p \\ q \end{pmatrix} = W(xe^{i\pi})W^{-1}(x)\left[\begin{pmatrix} a \\ b \end{pmatrix} + O(x^{-1})\right] \qquad (5.21)$$

$$= W^-(W^+)^{-1}\begin{pmatrix} a \\ b \end{pmatrix} + O(x^{-1}) \qquad (5.22)$$

and we compute $W^-(W^+)^{-1} = Y(z_j)$.

VI. ASYMPTOTIC MATCHING

In this section we estimate the difference between the solution of (4.12) and the solution of the comparison equation (4.9). This estimation will define the scaling limit for the asymptotic matching of these solutions.

Let $U_A(x,x_0)$ and $U(x,x_0)$ be the associated propagators such that

$$U_A'(x,x_0) = A(x)U_A(x,x_0), \quad U_A(x_0,x_0) = \underline{I} \; ,$$
$$U'(x,x_0) = [A(x) + B(x,T)]U(x_0,x_0), \quad U(x_0,x_0) = \underline{I} \; . \qquad (6.1)$$

We can evaluate their difference by means of the differential equation

$$\frac{d}{dx}\left[U(x,x_0) - U_A(x,x_0)\right] = A(x)\left[U(x,x_0) - U_A(x,x_0)\right] + B(x,T)U(x,x_0) \qquad (6.2)$$

and $U(x_0,x_0) - U_A(x_0,x_0) = 0$. Hence, by the method of variation of constants,

$$U(x,x_0) - U_A(x,x_0) = U_A(x,x_0)\int_{x_0}^{x} ds\, U_A^{-1}(s,x_0)B(s,T)U(s,x_0)$$
$$= \int_{x_0}^{x} ds\, U_A(x,s)B(s,T)U(s,x_0) \; . \qquad (6.3)$$

Now we consider the path consisting in the three following parts: a rectilinear path from x_0 to 1, $x_0 > 1$; a semicircular path from 1 to -1, in the upper half-plane; a rectilinear path from -1 to $-x_0$. We want to evaluate $U(-x_0,x_0) - U_A(-x_0,x_0)$ integrated along the path described above. We can write

$$\begin{aligned} U(-x_0,x_0) - U_A(-x_0,x_0) &= U(-x_0,-1)U(-1,1)U(1,x_0) - U_A(-x_0,-1)U_A(-1,1)U_A(1,x_0) \\ &= \left[U(-x_0,-1) - U_A(-x_0,-1)\right]U_A(-1,1)U_A(1,x_0) \\ &\quad + U(-x_0,-1)\left[U(-1,1) - U_A(-1,1)\right]U_A(1,x_0) \\ &\quad + U(-x_0,-1)U(-1,1)\left[U(1,x_0) - U_A(1,x_0)\right] \end{aligned} \qquad (6.4)$$

and bound each term separately. Let us consider (6.3) for x_0 and x on the same arc of Stokes line ($xx_0 > 0$). In this case x, x_0, and the integration variable s are all real, so that, by (4.14)

$$\|B(s,T)\| \le \frac{\text{const}}{T(|s|/T)^{2/3}} \quad \text{and} \quad \|A(s)\| \le \frac{1}{6|s|} \quad \text{for} \quad \left|\frac{s}{T}\right| \ll 1 \; . \qquad (6.5)$$

By standard estimates on (6.3) we get

$$\|U(x,x_0) - U_A(x,x_0)\| \le e^{|\ln(x/x_0)|/6} \times \text{const} \times \left(\left|\frac{x}{T}\right|^{1/3} + \left|\frac{x_0}{T}\right|^{1/3}\right) \quad \text{for} \quad \left|\frac{x}{T}\right| \text{ and } \left|\frac{x_0}{T}\right| \ll 1 \qquad (6.6)$$

for any x and $x_0 \in I\!R$ such that $xx_0 > 0$. Similarly along the circular path $x(\theta) = \exp(i\theta)$, $\theta \in [0,\pi]$ we have

$$\|A(e^{i\theta})\| \le \frac{e}{6}, \quad \|B(e^{i\theta},T)\| \le \frac{\text{const}\times e}{T^{1/3}} \tag{6.7}$$

and therefore

$$\|U(e^{i\pi},1) - U_A(e^{i\pi},1)\| \le \frac{\text{const}}{T^{1/3}} \text{ as } T \to \infty \tag{6.8}$$

for a constant independent of T. Gathering together these estimates we get

$$\|U(-x_0,x_0) - U_A(-x_0,x_0)\| \le \text{const}\times x_0^{1/3}\left[\left(\frac{x_0}{T}\right)^{1/3} + \frac{1}{T^{1/3}}\right] + \text{const}\times\left(\frac{x_0}{T}\right)^{1/3} + \text{const}\times x_0^{1/3}\left[\left(\frac{x_0}{T}\right)^{1/3} + \frac{1}{T^{1/3}}\right] \quad \text{when } \frac{x_0}{T} \ll 1 \text{ and } T \gg 1\,. \tag{6.9}$$

Since we shall take $x_0 \gg 1$, we can write

$$\|U(-x_0,x_0) - U_A(-x_0,x_0)\| \le \text{const}\times x_0^{1/3}\left(\frac{x_0}{T}\right)^{1/3} \tag{6.10}$$

when

$$\frac{x_0}{T} \ll 1 \text{ and } x_0\,,\; T \gg 1\,. \tag{6.11}$$

We are now in a position allowing the right scaling limit to be determined. Let us consider the arc of the Stokes line leading from $-\infty$ to z_1, the first eigenvalue crossing of condition (v). According to (2.13) we choose initial conditions for $\hat{\mathbf{c}}(t)$,

$$\hat{\mathbf{c}}(-\infty) = \begin{pmatrix}1\\0\end{pmatrix}\,. \tag{6.12}$$

From the bounds (3.9) we have

$$\left\|\hat{\mathbf{c}}(t_1^-) - \begin{pmatrix}1\\0\end{pmatrix}\right\| \le \text{const}\times\left(\frac{1}{T|z_1^- - z_1|^{3/2}} + \frac{1}{T}\right) \tag{6.13}$$

with $s_1 = -\infty$, $\gamma(s_2) = z_1^- = \gamma(t_1^-)$. In terms of the real positive x and of $\tilde{\mathbf{c}}$ [see (4.11)] this last estimate reads, with $x_1 = T[\Delta_{12}(\gamma(t_1^-)) - \Delta_{12}(\gamma(z_1))]$,

$$\left\|\tilde{\mathbf{c}}(x_1) - \begin{pmatrix}1\\0\end{pmatrix}\right\| \le \text{const}\times\left(\frac{1}{x_1} + \frac{1}{T}\right) \le \text{const}\times\frac{1}{x_1} \quad \text{when } \frac{1}{x_1}, \frac{1}{T} \text{ and } \frac{x_1}{T} \ll 1 \tag{6.14}$$

since $\tilde{c}_j(x) = O(\hat{c}_j(x))$ for $j = 1,2$. Then, from x_1 to $e^{i\pi}x_1$, we use $U_A(e^{i\pi}x_1, x_1)$ instead of $U(e^{i\pi}x_1, x_1)$ to continue the solution. That is we consider $\tilde{\mathbf{c}}^A(x)$ such that

$$\tilde{\mathbf{c}}^A(x_1) = \tilde{\mathbf{c}}(x_1) = \begin{pmatrix}1\\0\end{pmatrix} + O\left(\frac{1}{x_1}\right) \tag{6.15}$$

and we are interested in $\tilde{\mathbf{c}}^A(e^{i\pi}x_1)$ which is an approximation of $\tilde{\mathbf{c}}(e^{i\pi}x_1)$. We can apply lemma 5.1 to obtain

$$\begin{aligned}\tilde{\mathbf{c}}^A(e^{i\pi}x_1) &= Y(z_1)\begin{pmatrix}1\\0\end{pmatrix} + O\left(\frac{1}{x_1}\right)\\ &= \begin{pmatrix}1\\-\epsilon(z_1)\end{pmatrix} + O\left(\frac{1}{x_1}\right)\,.\end{aligned} \tag{6.16}$$

Now, using the bound (6.10), we have that

$$\begin{aligned}\tilde{\mathbf{c}}(e^{i\pi}x_1) &= \tilde{\mathbf{c}}^A(e^{i\pi}x_1) + O\left(x_1^{1/3}\left(\frac{x_1}{T}\right)^{1/3}\right)\\ &= Y(z_1)\begin{pmatrix}1\\0\end{pmatrix} + O\left(\frac{1}{x_1}\right)\\ &\quad + O\left(x_1^{1/3}\left(\frac{x_1}{T}\right)^{1/3}\right).\end{aligned} \tag{6.17}$$

At this point we impose the conditions

$$\frac{x_1}{T} \ll 1, \quad \frac{1}{x_1} \ll 1, \quad \text{and } x_1^{1/3}\left(\frac{x_1}{T}\right)^{1/3} = \frac{1}{x_1} \tag{6.18}$$

so that we can write

$$\tilde{\mathbf{c}}(e^{i\pi}x_1) = Y(z_1)\begin{pmatrix}1\\0\end{pmatrix} + O\left(\frac{1}{x_1}\right)\,. \tag{6.19}$$

Coming back to the variable t and to $\hat{c}_j(t)$, this last equation reads

$$\hat{\mathbf{c}}(t_1^+) = X(z_1)\begin{pmatrix}1\\0\end{pmatrix} + O\left(\frac{1}{T|z_1^+ - z_1|^{3/2}}\right)\,, \tag{6.20}$$

where $e^{i\pi}x_1 = T[\Delta_{12}(\gamma(t_1^+)) - \Delta_{12}(\gamma(z_1))]$ and

$$X(z_1) = \begin{pmatrix}1 & 0\\ -\epsilon(z_1)\exp[-i\Phi(z_1) - iT\,\mathrm{Re}\Delta_{12}(\gamma(z_1))] & 1\end{pmatrix}\,. \tag{6.21}$$

Note that $\|X(z_1)\| = O(1)$ so that $\hat{c}_j(t_1^+) = O(1)$. We are now exactly in the same situation as we were in at the beginning of the computation. This shows that provided conditions (6.18) are satisfied, we can iterate this procedure as many times as there are eigenvalue crossings on the Stokes line, by choosing $x_j = T[\Delta_{12}(\gamma(t_j^-)) - \Delta_{12}(\gamma(z_j))] = x_1$

$\forall j = 1, \ldots, N$ in the analysis close to z_j.

Let us give the scaling explicitly: We set $x_1 = T^\kappa$ with $\kappa > 0$ to be determined. Thus

$$\frac{x_1}{T} = \frac{1}{T^{1-\kappa}} \quad \text{and } x_1^{1/3}\left(\frac{x_1}{T}\right)^{1/3} = \frac{1}{T^{(1-2\kappa)/3}} \,. \tag{6.22}$$

Condition (6.18) implies

$$\frac{1-2\kappa}{3} = \kappa, \quad \text{i.e., } \kappa = \frac{1}{5} \,, \tag{6.23}$$

and actually have with this κ,

$$x_1 = T^{1/5} \to \infty \text{ and } \frac{x_1}{T} = \frac{1}{T^{4/5}} \to 0 \text{ as } T \to \infty \tag{6.24}$$

as required throughout the above analysis. We have proven the following lemma.

Lemma 6.1. Let $\widehat{c}_1(t)$ and $\widehat{c}_2(t)$ be defined by (3.8) and (6.12). Then

$$\widehat{c}(+\infty) = \begin{pmatrix} a \\ b \end{pmatrix} + O\left(\frac{1}{T^{1/5}}\right) \,,$$

where

$$\begin{pmatrix} a \\ b \end{pmatrix} = X(z_N)X(z_{N-1})\cdots X(z_1)\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
$$= \begin{pmatrix} 1 \\ -\sum_{j=1}^{N}\epsilon(z_j)\exp[-i\Phi(z_j) - iT\,\mathrm{Re}\Delta_{12}(\gamma(z_j))] \end{pmatrix} .$$

VII. TRANSITION PROBABILITY

The preceding lemma is actually the main result of this paper since all the results concerning the transition probability in the adiabatic limit are direct consequences of this lemma. Let us first see how we can recover the case treated in [9]. We assume that conditions (i)–(v) hold with $N = 1$. By lemma 6.1 and (2.12),

$$\lim_{t\to\infty} c_2(t) = \exp[T\,\mathrm{Im}\Delta_{12}(z_1)]\left[-\epsilon(z_1)\exp[-i\Phi(z_1) - iT\,\mathrm{Re}\Delta_{12}(z_1)] + O\left(\frac{1}{T^{1/5}}\right)\right]$$
$$= -\epsilon(z_1)\exp[-i\Phi(z_1) - iT\Delta_{12}(z_1)]\left[1 + O\left(\frac{1}{T^{1/5}}\right)\right] \,. \tag{7.1}$$

From [9] we have [see Eq. (1.10)]

$$c_2(\infty) = \exp\left(-i\theta_1 - iT\int_{\eta_1} e_1(z)dz\right)\left[1 + O\left(\frac{1}{T}\right)\right] \,. \tag{7.2}$$

As

$$\int_{\eta_1} e_1(z)dz = \int_0^{z_1}[e_1(z) - e_2(z)]dz = \Delta_{12}(z_1),$$

where the second integral is over any path in Ω leading from 0 to z_1, we obtain by comparison

$$e^{-i\theta_1} \equiv -\epsilon(z_1)e^{-i\Phi(z_1)} \,. \tag{7.3}$$

Remark. The method used in this paper is less accurate than the one designed in [7]. We have an explicit formula for $e^{-i\theta_1}$ [under the hypothesis $B_3(z_1) \neq 0$] which reads

$$e^{-i\theta_1} = e^{-ik_1\pi}\exp\left(-i\int_{\gamma_1}\frac{B_3(z)[B_1(z)B_2'(z) - B_2(z)B_1'(z)]}{2\sqrt{\rho(z)}[B_1^2(z) + B_2^2(z)]}dz\right) \,, \tag{7.4}$$

where $e^{-ik_1\pi} = -\epsilon(z_1)$ and γ_1 is a loop based at the origin which is homotopic to η_1 and encloses neither singularities nor zeros of $(B_1 - iB_2)/(B_1 + iB_2)$. Moreover, (7.3) is valid for any eigenvalue crossing z_j since both quantities are defined independently of the differential equations and asymptotic relations studied here. This gives to the expression $-\epsilon(z_1)e^{-i\Phi(z_1)}$ a geometric status since $e^{-i\theta_j}$ is geometric in nature. For a proof of this formula, see the Appendix of [9]. (Notice that in the last line $\pi/2$ should be replaced by $-k\pi$.)

Theorem 7.1. Let $H(z) = B_1(z)s_1 + B_2(z)s_2 + B_3(z)s_3$ be a 2×2 matrix which satisfies conditions (i)–(v). Let ψ_T be a normalized solution of the Schrödinger equation $i\psi_T' = TH\psi_T$ such that $\lim_{t\to-\infty} \|P_1(t)\psi_T(t)\| = 1$. Then

$$\lim_{t\to\infty} \|P_2(t)\psi_T(t)\|^2 = \left| \sum_{j=1}^{N} e^{-i\theta_j} \exp\left(-iT\int_{\eta_j} e_1(z)dz\right) + O\left(\frac{\exp\left(T\,\mathrm{Im}\int_{\eta_1} e_1(z)dz\right)}{T^{1/5}}\right)\right|^2$$
$$= \exp\left(2T\,\mathrm{Im}\int_{\eta_1} e_1(z)dz\right)\left[\left|\sum_{j=1}^{N} e^{-i\theta_j}\exp\left(-iT\,\mathrm{Re}\int_{\eta_j} e_1(z)dz\right)\right|^2 + O\left(\frac{1}{T^{1/5}}\right)\right] . \quad (7.5)$$

Remark. In the case of a real symmetric Hamiltonian on the real axis, the preceding formula reduces to

$$\lim_{t\to\infty} \|P_2(t)\psi_T(t)\|^2 = \exp\left(2T\,\mathrm{Im}\int_{\eta_1} e_1(z)dz\right)\left[\left|\sum_{j=1}^{N} \epsilon(z_j)\exp\left(-iT\,\mathrm{Re}\int_{\eta_j} e_1(z)dz\right)\right|^2 + O\left(\frac{1}{T^{1/5}}\right)\right] , \quad (7.6)$$

where $\epsilon(z_j) = \pm 1$.

Using the geometric notions introduced in [9] we can give a geometric formulation of this theorem.

Theorem 7.2. Under the hypothesis of theorem 7.1 we have

$$\lim_{t\to\infty} \|P_2(t)\psi_T(t)\|^2 = e^{-2Td_\rho(z_1,\mathbb{R})}\left[\sum_{j=1}^{N} e^{2\,\mathrm{Im}\theta_j} + 2\sum_{j>k}^{N} e^{\mathrm{Im}(\theta_j+\theta_k)}\cos\left[Td_\rho(z_j,z_k) + \mathrm{Re}(\theta_j-\theta_k)\right] + O\left(\frac{1}{T^{1/5}}\right)\right] .$$

Remarks.

(1) Theorems 7.1 and 7.2 have been obtained under the boundary conditions $c_2(-\infty) = 0$ and $c_1(\infty) = 1$. Nevertheless, if these boundary conditions are reversed, the theorems still hold (with P_1 in place of P_2). Indeed, if $(c_1(x), c_2(x))$ are solutions of (2.10) for $x \in \mathbb{R}$ with the above boundary conditions, then $(-\overline{c_2}(x), \overline{c_1}(x))$ satisfy the same equation with reversed boundary conditions, $x \in \mathbb{R}$. Now the transition probability is given by $|c_2(\infty)|^2$ in the first case, and by $|-\overline{c_2(\infty)}|^2 = |c_2(\infty)|^2$ in the second one, showing that they are equal.

(2) If we replace the oscillating function of T in front of the exponential by its mean value and denote by $\overline{P(T)}$ the result, we get

$$\overline{P(T)} = \exp\left(2T\,\mathrm{Im}\int_{\eta_1} e_1(z)dz\right) \times \left[\sum_{j=1}^{N} e^{2\,\mathrm{Im}\theta_j} + O\left(\frac{1}{T^{1/5}}\right)\right] , \quad (7.7)$$

where the mean prefactor is equal to the sum of the individual geometric prefactors.

VIII. EXAMPLES

The first example comes from a model designed by Nikitin [14]. The physical process is the following: one excited atom A^* moves along a straight line with velocity $v \ll 1$. It passes near a second atom B with impact parameter b'. We want to compute the probability of the reaction $A^* + B \to A + B + \Delta\epsilon$ when the interaction between the atoms is of the dipole-dipole type. This is one of the processes which can be studied with the help of a 2×2 real symmetric Hamiltonian. In this case the Hamiltonian reads (see [5], paragraph 9.3.2 and [14])

$$H(R) = \begin{pmatrix} \frac{\Delta\epsilon}{2} & \frac{C}{R^3} \\ \frac{C}{R^3} & -\frac{\Delta\epsilon}{2} \end{pmatrix} , \quad (8.1)$$

where $\Delta\epsilon$ and C are constants and $R = R(\tau) = \sqrt{b'^2 + \tau^2 v^2}$ is the distance between the atoms at time τ. We also introduce the quantity $d = (2C/\Delta\epsilon)^{1/3}$, which is the typical interaction distance of the problem. The probability of the reaction is then equal to the transition probability, $|c_1(\infty)|^2$ with boundary conditions $c_1(-\infty) = 0$ and $c_2(-\infty) = 1$ in the adiabatic limit $v \to 0$. It is given by the formulas of theorems 7.1 and 7.2 (see the remark after the theorems). By introducing the rescaled dimensionless time $t = v\tau/d$, and the ratio $b = b'/d$, where d is fixed, the time-dependent Hamiltonian reads

$$H(t) = \frac{\Delta\epsilon}{2}\begin{pmatrix} 1 & \frac{1}{(b^2+t^2)^{3/2}} \\ \frac{1}{(b^2+t^2)^{3/2}} & -1 \end{pmatrix} . \quad (8.2)$$

It is easily verified that this Hamiltonian satisfies hypotheses (i)–(iv). The function $\rho(z)$ is given by

$$\rho(z) = \Delta\epsilon^2 \left(1 + \frac{1}{(b^2+z^2)^3}\right) \tag{8.3}$$

and its zeros are

$$\begin{aligned} z_2 &= (1+b^4-\sqrt{3}b^2)^{1/4} e^{i\varphi}, \\ z_1 &= (1+b^4-\sqrt{3}b^2)^{1/4} e^{i(\pi-\varphi)}, \\ \varphi &= \frac{1}{2}\arg\left(\frac{1}{2}-b^2+i\frac{\sqrt{3}}{2}\right) < \frac{\pi}{2}, \\ z_3 &= (1+b^2)^{1/2} e^{i\pi}, \end{aligned} \tag{8.4}$$

and their complex conjugates.

We have computed numerically the level lines $\mathrm{Im}\Delta_{12}(z) = \mathrm{Im}\Delta_{12}(z_1)$ for different values of the parameter b. In all cases, they display the same general features represented on Fig. 3, where they are given for $b = 1$.

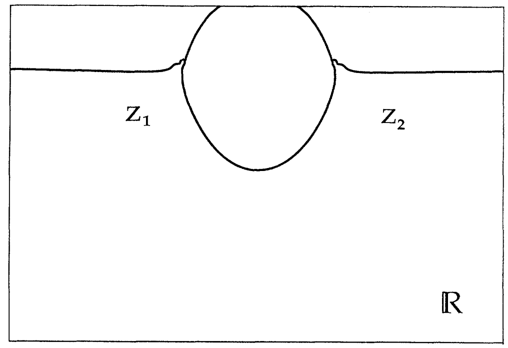

FIG. 3. The Stokes lines of example 1.

The main point is that they pass through z_1 and z_2. We also have computed that $\epsilon(z_1) = \epsilon(z_2) = -1$, thus by theorem 7.1, we have, with $T = d/v$,

$$\begin{aligned} |c_1(\infty)|^2 &= e^{2T\,\mathrm{Im}\Delta_{12}(z_1)} 2\left[1 + \cos\{T\,\mathrm{Re}[\Delta_{12}(z_1) - \Delta_{12}(z_2)]\} + O\left(\frac{1}{T^{1/5}}\right)\right] \\ &= \exp\left(-2T\,\mathrm{Im}\int_0^{z_1}\sqrt{\rho(z)}dz\right) 4\left[\cos^2\left(T\int_{z_1}^{z_2}\sqrt{\rho(z)}dz/2\right) + O\left(\frac{1}{T^{1/5}}\right)\right] . \end{aligned} \tag{8.5}$$

Let us now turn to a family of examples which will provide a wide variety of behaviors in the leading term of the asymptotic transition probability, as well as emphasize the global character of condition (v). Let $H(t) = \mathbf{B}(t)\cdot\mathbf{s}$ be defined by

$$\mathbf{B}(t) = \left(\frac{t^3+\alpha' t}{\sqrt{t^6+d^6}}, \frac{\beta' t}{\sqrt{t^6+d^6}}, \frac{\gamma'}{\sqrt{t^6+d^6}}\right) , \tag{8.6}$$

where α', β', and γ' are constants to be determined later and d is a large constant. Again, hypotheses (i)–(iii) are easily verified. The function $\rho(z)$ is

$$\begin{aligned} \rho(z) &= \frac{z^6 + 2\alpha' z^4 + (\alpha'^2+\beta'^2)z^2 + \gamma'^2}{z^6+d^6} \\ &\equiv \frac{z^6+\alpha z^4+\beta z^2+\gamma}{z^6+d^6} \end{aligned} \tag{8.7}$$

and we choose the constants appearing in (8.7) in such a way that the simple zeros of $\rho(z)$ are $z_1 = b+ic$, $z_2 = ia$, $z_3 = -b+ic$ and their complex conjugates. Thus we must have

$$\rho(z) = \frac{(z-z_1)(z-\overline{z_1})(z-z_2)(z-\overline{z_2})(z-z_3)(z-\overline{z_3})}{z^6+d^6} \tag{8.8}$$

and by expanding and comparing the coefficients of the powers of z we obtain

$$\begin{aligned} \alpha &= 2\alpha' = a^2 + 2(c^2-b^2) , \\ \beta &= \alpha'^2+\beta'^2 = (b^2+c^2)^2 + 2a^2(c^2-b^2) , \\ \gamma &= \gamma'^2 = a^2(b^2+c^2)^2 . \end{aligned} \tag{8.9}$$

Then the magnetic field $\mathbf{B}(t)$ is completely determined with

$$\alpha' = \frac{\alpha}{2} , \quad \beta' = \pm\sqrt{\beta-\alpha^2/4} , \quad \gamma' = \pm\sqrt{\gamma} . \tag{8.10}$$

In order to have a real magnetic field for real values of z, we have to impose

$$\beta - \frac{\alpha^2}{4} \geq 0 \tag{8.11}$$

which in terms of a, b, and c reads $2c \geq a$. We choose the

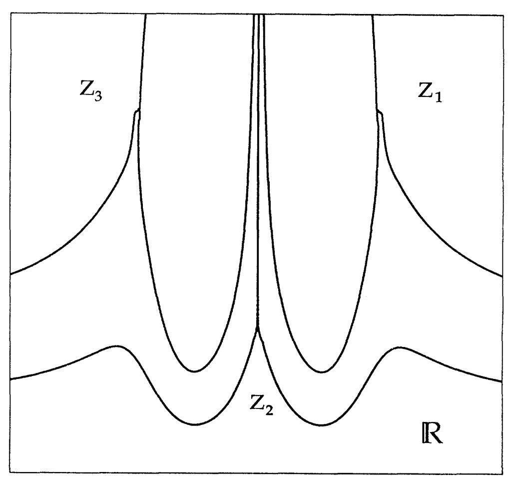

FIG. 4. The Stokes lines for $b = b_1 = 3$.

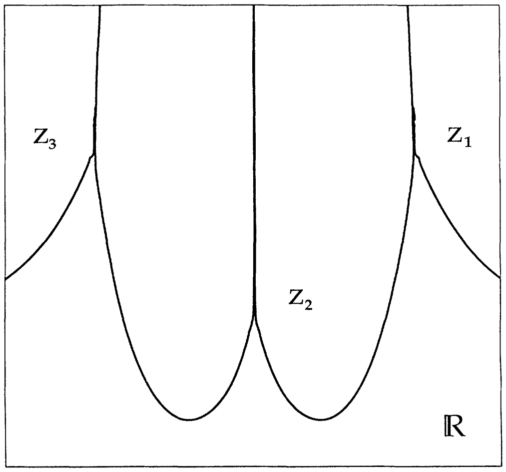

FIG. 5. The Stokes lines for $b = b_0 \simeq 3.88$.

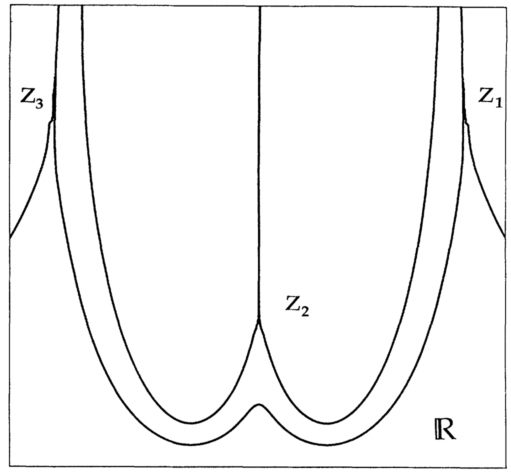

FIG. 6. The Stokes lines for $b = b_2 = 5$.

values $a = \frac{1}{2}$, $c = 1$, and $d = 2$ and keep b as a parameter of the model. By analyzing the model we can see that there are two different regimes characterized by $b \ll 1$ and $b \gg 1$ separated by a limiting case. By a numerical investigation we have obtained for three values of b: $b_1 = 3$, $b_0 \simeq 3.88$, $b_2 = 5$, the Stokes lines displayed in Figs. 4, 5, and 6. These figures lead to the following conclusions about the leading term of the transition probability.

In the case $b = b_1$, there is an infinite Stokes line passing through z_2 only, the closest eigenvalue crossing to the real axis in the Euclidean and the ρ metric (see [9]). Thus the leading term of the transition probability can be computed by means of the analysis given in [9].

In the case $b = b_0$, there is an infinite Stokes line passing through z_1, z_2 and z_3, and the analysis developed in this paper is necessary. Note that the Euclidean distance between the real axis and z_1 (or z_3) is greater than between z_2 and the real axis, although we have in the ρ distance $d_\rho(z_1, \mathbb{R}) = d_\rho(z_2, \mathbb{R}) = d_\rho(z_3, \mathbb{R})$. Thus the leading term of the transition probability will display the interference phenomenon described above.

In the case $b = b_2$, there is an infinite Stokes line passing through z_1 and z_3 only, showing that $d_\rho(z_1, \mathbb{R}) = d_\rho(z_3, \mathbb{R}) < d_\rho(z_2, \mathbb{R})$ although the contrary is true in the Euclidean metric. In this case too, an interference phenomenon, governed by z_1 and z_3, will take place in the leading term of the transition probability.

We have also computed the values of $e^{-i\theta_j}$ numerically and plotted the leading terms of the transition probability in the different cases considered:

$$P(T) \simeq e^{2T\,\mathrm{Im}\Delta_{12}(z_2)} \quad \text{if } b = b_1 = 3 \tag{8.12}$$

(see Fig. 7),

$$\begin{aligned} P(T) \simeq e^{2T\,\mathrm{Im}\Delta_{12}(z_1)}\, \big(& e^{2\,\mathrm{Im}\Phi(z_1)} + e^{-2\,\mathrm{Im}\Phi(z_1)} + 1 \\ &+ 2e^{2\,\mathrm{Im}\Phi(z_1)} \cos\{T\,\mathrm{Re}[\Delta_{12}(z_2) - \Delta_{12}(z_1)] + \mathrm{Re}[\Phi(z_2) - \Phi(z_1)]\} \\ &+ 2e^{-2\,\mathrm{Im}\Phi(z_1)} \cos\{T\,\mathrm{Re}[\Delta_{12}(z_1) + \Delta_{12}(z_2)] + \mathrm{Re}[\Phi(z_1) + \Phi(z_2)]\} + 2\cos[2T\,\mathrm{Re}\Delta_{12}(z_1)]\big) \end{aligned} \tag{8.13}$$

if $b = b_0 \simeq 3.88$ (see Fig. 8), and

$$\begin{aligned} P(T) \simeq e^{2T\,\mathrm{Im}\Delta_{12}(z_1)}\{ & e^{2\,\mathrm{Im}\Phi(z_1)} + e^{-2\,\mathrm{Im}\Phi(z_1)} \\ & + 2\cos[2T\,\mathrm{Re}\Delta_{12}(z_1)]\} \end{aligned} \tag{8.14}$$

if $b = b_2 = 5$ (see Fig. 9).

Note added in proof. It is possible by using other methods to show that all error terms of the form $O(1/T^{1/5})$ in the final results can be replaced by $O(1/T)$.

ACKNOWLEDGMENT

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APPENDIX

In this appendix we prove lemma 3.1. It is shown in the Appendix of [9] that the vectors defined by (2.2) are given by

$$\varphi_j(z) = e^{-i\delta_j(z)}\psi_j(z) \tag{A1}$$

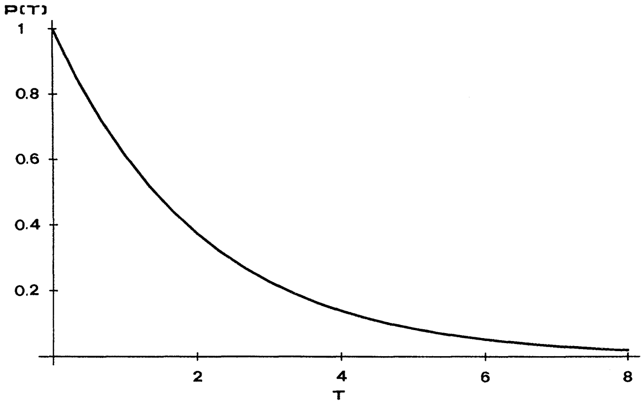

FIG. 7. $P(T)$ for $b = b_1 = 3$.

where

$$\psi_j(z) = (B_3(z) + (-1)^j \sqrt{\rho(z)}, B_1(z) + iB_2(z)) \tag{A2}$$

and

$$i\delta_j'(z) = \frac{1}{2}\frac{d}{dz}\ln\{2\sqrt{\rho(z)}[\sqrt{\rho(z)} + (-1)^j B_3(z)]\} + i\frac{B_1(z)B_2'(z) - B_2(z)B_1'(z)}{2\sqrt{\rho(z)}[\sqrt{\rho(z)} + (-1)^j B_3(z)]} \tag{A3}$$

with the choice

$$\psi_j(0) = \|\psi_j(0)\|\varphi_j(0) = e^{i\delta_j(0)}\varphi_j(0) \tag{A4}$$

we have

$$i\delta_j(0) = \tfrac{1}{2}\ln\{2\sqrt{\rho(0)}[\sqrt{\rho(0)} + (-1)^j B_3(0)]\} . \tag{A5}$$

This representation is valid as long as $\sqrt{\rho(z)} \neq \pm B_3(z)$, which is equivalent to $B_1^2(z) + B_2^2(z) \neq 0$. In particular we suppose that $B_3(z^*) \neq 0$. This restriction will be lifted later.

We first compute a_{kj} on the real axis and then analytically continue the result in the complex plane up to z^*:

$$\begin{aligned} a_{kj}(x) &= -\langle\varphi_k(0)|U(x)^{-1}\varphi_j'(x)\rangle \\ &= -\langle\varphi_k(x)|\varphi_j'(x)\rangle . \end{aligned} \tag{A6}$$

By (A1)

$$\varphi_j'(z) = -i\delta_j'(z)\varphi_j(z) + e^{-i\delta_j(z)}\psi_j'(z) \tag{A7}$$

and

$$\langle\varphi_k(x)|\varphi_j'(x)\rangle = \exp\{\overline{[-i\delta_k(x)]} - i\delta_j(x)\} \times\langle\psi_k(x)|\psi_j'(x)\rangle . \tag{A8}$$

An explicit computation yields

$$\langle\psi_k(x)|\psi_j'(x)\rangle = i[B_1(x)B_2'(x) - B_2(x)B_1'(x)] + (-1)^j\left(\frac{B_3(x)\rho'(x)}{2\sqrt{\rho(x)}} - B_3'(x)\sqrt{\rho(x)}\right) \tag{A9}$$

and on the real axis we have

$$\begin{aligned} \overline{i\delta_k(x)} + i\delta_j(x) &= \tfrac{1}{2}\ln\{4\rho(x)[\sqrt{\rho(x)} - (-1)^j B_3(x)][\sqrt{\rho(x)} + (-1)^j B_3(x)]\} \\ &\quad - i\int_0^x \frac{B_1(x')B_2'(x') - B_2(x')B_1'(x')}{2\sqrt{\rho(x')}} \\ &\quad \times\left(\frac{1}{\sqrt{\rho(x)} - (-1)^j B_3(x')} - \frac{1}{\sqrt{\rho(x')} + (-1)^j B_3(x')}\right)dx' \\ &= \tfrac{1}{2}\ln\{4\rho(x)[B_1^2(x) + B_2^2(x)]\} - i(-1)^j\int_0^x \frac{B_3(x')[B_1(x')B_2'(x') - B_2(x')B_1'(x')]}{\sqrt{\rho(x')}[B_1^2(x') + B_2^2(x')]}dx' . \end{aligned} \tag{A10}$$

These formulas lead to the following expression for $a_{kj}(x)$, $x \in \mathbb{R}$:

$$\begin{aligned} a_{kj}(x) = &-\frac{\exp\left(i(-1)^j\int_0^x \frac{B_3(x')[B_1(x')B_2'(x') - B_2(x')B_1'(x')]}{\sqrt{\rho(x')}[B_1^2(x') + B_2^2(x')]}dx'\right)}{2\sqrt{\rho(x)}\sqrt{(B_1^2(x) + B_2^2(x)]}} \\ &\times\left[(-1)^j\left(\frac{B_3(x)\rho'(x)}{2\sqrt{\rho(x)}} - B_3'(x)\sqrt{\rho(x)}\right) + i[B_1(x)B_2'(x) - B_2(x)B_1'(x)]\right] . \end{aligned} \tag{A11}$$

By assumption (i), the functions $B_j(x)$ have analytic extensions S_a so that the analytic continuation of a_{kj} from x to z in Ω is obtained by analytically continuing the expression (A11) along a path γ from x to z such that $\sqrt{\rho(u)} \neq \pm B_3(u)$ or, equivalently, $B_1^2(u) + B_2^2(u) \neq 0\ \forall u \in \gamma$. This leads to the formulas of lemma 3.1.

We now consider formula (3.1) when $B_3(z^*) = 0$. Condition (iv) implies then that one of the $B_j(z^*) \neq 0$,

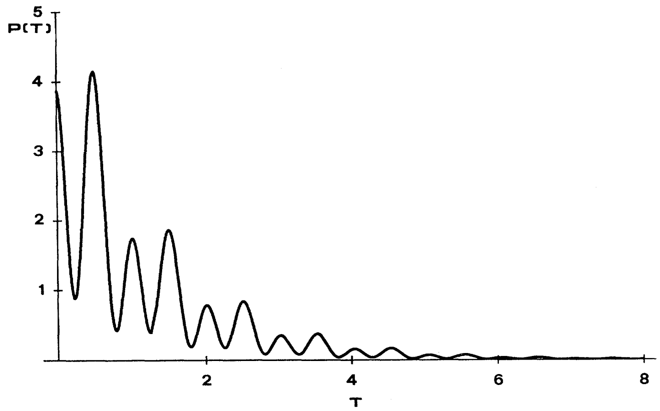

FIG. 8. $P(T)$ for $b = b_0 \simeq 3.88$.

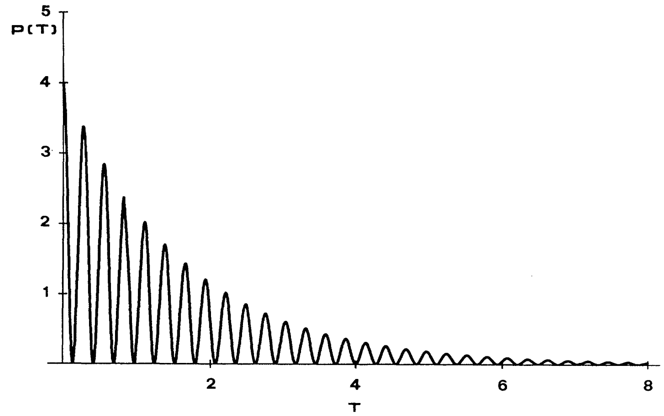

FIG. 9. $P(T)$ for $b = b_2 = 5$.

$k = 1, 2$ must be nonzero; say $B_1(z^*) \neq 0$. In this case we perform a change of axis, generated by a z-independent unitary operator S such that the axis $\mathbf{e}_j$ exchange their labels in the following way:

$$\mathbf{e}_1 \mapsto \mathbf{e}_3, \quad \mathbf{e}_2 \mapsto \mathbf{e}_1, \quad \mathbf{e}_3 \mapsto \mathbf{e}_2 \ . \tag{A12}$$

Thus any vector χ in the old system of axis corresponds to $S\chi$ in the new one and the Hamiltonian becomes SHS^{-1}

$$SHS^{-1} = \begin{pmatrix} B_1 & B_2 - iB_3 \\ B_2 + iB_3 & -B_1 \end{pmatrix}$$

$$\text{in the basis } \left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\} \ . \tag{A13}$$

In particular, if ψ satisfies the Schrödinger equation for H, $S\psi$ satisfies it for SHS^{-1} and if $\varphi_k(z) = U(z)\varphi_k(0)$ is such that $H(z)\varphi_k(z) = e_k(z)\varphi_k(z)$, $S\varphi_k(z) = [SU(z)S^{-1}]S\varphi_k(0)$ satisfies $SH(z)S^{-1}[S\varphi_k(z)] = e_k(z)[S\varphi_k(z)]$. Thus we can write with the *same* coefficients c_j as before,

$$S\psi_T = \sum_{j=1}^{2} c_j e^{-iT\lambda_j}(S\varphi_j) \ . \tag{A14}$$

Then we proceed as we did in the old set of axes to compute the eigenvectors $S\varphi_k$ and coefficients a_{kj}, but this time with B_1 in place of B_3, B_2 in place of B_1, and B_3 in place of B_2 in formulas (A11) and (3.1).

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