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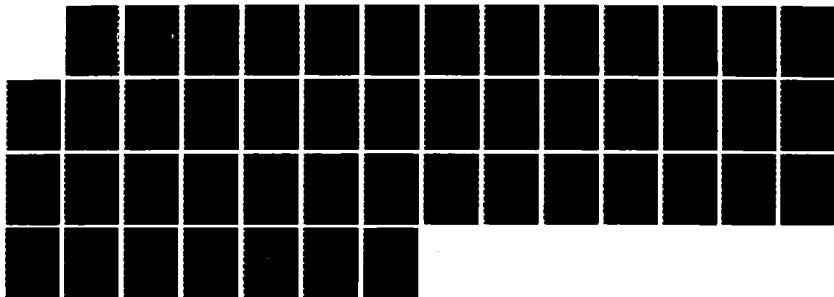
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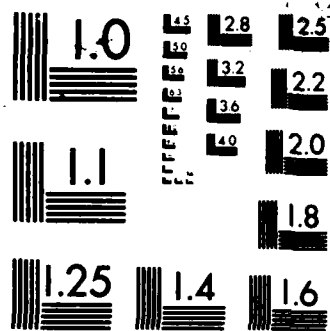
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by

LIT-DEH CHANG & WALTER KOHN

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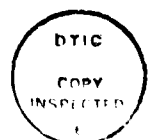
**Semiclassical Theory of Inelastic Scattering of a Particle
in the Near-Adiabatic Limit**

Lit-Deh Chang and Walter Kohn

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Santa Barbara CA 93106*

ABSTRACT: A semiclassical theory for inelastic scattering of a particle by a two-state system in the near-adiabatic limit is developed. The exponentially small transition amplitude is calculated. The theory is an extension of Pokrovskii and Khalatnikov's theory for above-barrier reflection. The analysis involves studies of the WKB solutions in the complex coordinate plane along certain contours. The region of validity of the theory is established. Our result has the same form as the Landau-Zener-Stückelberg formula; however, our theory is applicable to more general systems. Numerical comparisons with exact solutions are presented; the differences between our results and exact solutions become negligible as the adiabatic limit is approached.

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I. INTRODUCTION

The inelastic scattering problem of a particle by dynamical systems with internal degrees of freedom is an important problem in many fields of physics and chemistry. In various contexts the internal degrees of freedom could represent phonons in a solid, vibrational states of a molecule, atomic energy levels, ionization states, etc.. Consider the scattering of a particle by a harmonic oscillator for example. In the adiabatic limit in which a heavy particle is incident with low velocity, the oscillator wave function follows the interaction potential due to the particle adiabatically and returns to its initial state as the particle leaves the interaction region; even if inelastic scattering is energetically possible, the inelastic transition amplitude approaches zero in the adiabatic limit. For a small but finite incident velocity the transition amplitude is exponentially small as a function of a parameter which characterizes the deviation from the adiabatic limit. Near the adiabatic limit a WKB expansion in the appropriate small parameter is natural, such an expansion yields a vanishing transition amplitude in any finite order. Many approaches ¹ have been developed in the past to deal with the problem with various degrees of success. However, questions of the validity and generality of those approaches have remained unresolved. In this work we have developed a rigorous treatment of this problem to obtain exponentially small transition amplitudes for general interaction potentials between a particle and a system with two internal states.

Stückelberg ² was the first to applied a Zwaan type of analysis of the WKB solutions to the problem of the inelastic transition. His theory was based on the so-called Stokes constant method. Since the Stokes constant method has not been justified for general problems, the validity of his theory remains unclear ³. Our theory is an extension of Pokrovskii and Khalatnikov's theory ⁴ for above-barrier reflection. We obtain the same result as the Landau-Zener-Stückelberg formula in the near-adiabatic limit. Our theory

is however more general and we establish its region of validity. In Sec. II we review the work of Pokrovskii and Khalatnikov. In Sec. III we review the two-state model and the adiabatic basis. Our procedure for obtaining the transition amplitude is presented in Sec. IV. Numerical results are described in Sec. V. Mathematical proofs of the propositions used in Sec. IV are given in the appendix.

II. ABOVE-BARRIER REFLECTION

Consider a one-dimensional potential scattering problem with a localized repulsion potential $V(x)$. If $E > V(x)$ everywhere on the real axis, the Schrödinger equation

$$\frac{d^2\Psi(x)}{dx^2} + \alpha^2(E - V(x))\Psi(x) = 0 \quad , \quad (1)$$

$$\alpha \equiv \frac{\sqrt{2M}}{\hbar} \quad , \quad (2)$$

has a physical solution corresponding to incidence from the left, which satisfies the following asymptotic conditions:

$$\Psi(x) \rightarrow \frac{1}{\sqrt{q}} \left\{ e^{i\alpha\bar{q}x} + R e^{-i\alpha\bar{q}x} \right\} \quad , \quad x \rightarrow -\infty \quad , \quad (3)$$

$$\rightarrow \frac{T}{\sqrt{q}} e^{i\alpha\bar{q}x} \quad , \quad x \rightarrow +\infty \quad (4)$$

where

$$\bar{q} = \lim_{x \rightarrow \pm\infty} \sqrt{E - V(x)} \quad , \quad (5)$$

R is the reflection coefficient and T is the transmission coefficient. In the semiclassical limit $\alpha \rightarrow \infty$, T tends to one and R is exponentially small in α . On the real axis the WKB solutions of Eq.(1) are

$$\Psi^\pm(x, \tilde{z}) = \frac{1}{\sqrt{q(x)}} e^{\pm i\alpha \int_{\tilde{z}}^x q(x) dx} \quad , \quad (6)$$

where

$$q(x) = \sqrt{E - V(x)} \quad , \quad (7)$$

and $\tilde{z}$ is an arbitrary but fixed lower bound which may be real or complex. These solutions have an error of order α^{-1} . In the following we shall use the symbol $\approx$ to denote an approximate equality which becomes exact in the limit $\alpha \rightarrow \infty$. According to the boundary condition (3) , the physical solution can be expressed in terms of the WKB solution:

$$\Psi(x) \approx A^+ \Psi^+(x, \tilde{z}) \quad , \quad x \rightarrow \infty, \quad (8)$$

where A^+ is a constant. As we trace the solution along the real axis beginning at $+\infty$, Eq.(8) remains valid uniformly all the way to $-\infty$. But Ψ^+ does not include the exponentially small reflected wave. In fact R cannot be obtained even if we expand the solution to higher orders in powers of α^{-1} . Pokrovskii and Khalatnikov⁴ developed a method for obtaining the exponentially small R to leading order. We now review their work briefly.

Throughout this work we shall use z to denote a complex coordinate and use x to denote a real coordinate. We assume that all potentials can be analytically continued into those regions of the z plane which are relevant to our discussions. In order to obtain R we must construct a solution of the Schrödinger equation along a path in the z plane where, even as $\alpha \rightarrow \infty$, the ratio of reflected to incident wave functions (see Eq.(3)) remains finite and does not tend exponentially to zero. This path passes through a point z_c , defined by $q(z_c) = 0$ ⁵, where the WKB solution breaks down. However, similar to the familiar case of a classical turning point on the real axis, near z_c an exact solution of the Schrödinger equation can be obtained and joined to WKB solutions. If there are more than one z_c , the one closest to the real axis must be chosen.

Consider now the transition point z_c . The appropriate lines passing through z_c are given by the condition,

$$\text{Im} \int_{z_c}^z q(z') dz' = 0 \quad (9)$$

They are the so-called anti-Stokes lines, on which the functions $\Psi^+(z, z_c)$ and $\Psi^-(z, z_c)$ have the same magnitude, regardless of the value of α (see Eq.(6)). There are altogether three anti-Stokes lines, two of which are shown schematically in Fig. 1. L_1 and L_2 are useful to us because they form a contour connecting $+\infty$ and $-\infty$. Asymptotically they run parallel to the x -axis at a distance which we denote by y_1 . The procedure of Ref.(4) for obtaining R is as follows.

Starting with the right-going wave (4) at $+\infty$ on L_1 , we find the wave function in the

asymptotic region,

$$\Psi(z) = \frac{T}{\sqrt{q}} e^{i\alpha \bar{q} z} \quad , \quad (10)$$

where $z = x + iy_1$. Except in a small neighborhood of radius $O(\alpha^{-2/3})$ near z_c , $\Psi(z)$ can be represented on L_1 by

$$\Psi(z) \approx A^+ \Psi^+(z, z_c) \quad , \quad (11)$$

where

$$A^+ = T e^{-i\alpha \eta^+} \quad , \quad (12)$$

and

$$\eta^\pm = \pm \left\{ \int_{z_c}^{\pm\infty} (q(z') - q) dz' - q z_c \right\} \quad . \quad (13)$$

The solution is then matched to the exact solutions of the Schrödinger equation in the vicinity of z_c , which are the familiar Airy functions. The Airy solutions are valid in a neighborhood Ω_c of radius d_c around z_c (see Fig. 1), where d_c is the range in which the term $(E - V(z))$ can be approximated by the linear term of its Taylor expansion at z_c ; d_c is evidently independent of α . The matching region lies between $|z - z_c| = d_c$ and $|z - z_c| \sim \alpha^{-2/3}$. α must be large enough so that the matching region exists. Similarly, except for a small neighborhood of z_c , the physical solution on L_2 can be represented by a linear combination of the two WKB solutions, Eq.(6),

$$\Psi(z) \approx \{B^+ \Psi^+(z, z_c) + B^- \Psi^-(z, z_c)\} \quad , \quad (14)$$

where B^+ and B^- are determined by a similar matching procedure to the Airy solution in the vicinity of z_c . B^+ and B^- have the same magnitude. On L_2 , as $x \rightarrow -\infty$, $\Psi(z)$, Eq.(14) takes the form

$$\Psi(z) \approx \frac{1}{\sqrt{q}} \{B^+ e^{-i\alpha \eta^-} e^{i\alpha \bar{q} z} + B^- e^{i\alpha \eta^-} e^{-i\alpha \bar{q} z}\} \quad . \quad (15)$$

When the appropriate values of A^+ , B^+ and B^- are used and comparison with Eqs. (3) and (4) is made one finds

$$T \approx e^{i\alpha(\eta^+ + \eta^-)} \quad , \quad (16)$$

$$R \approx -ie^{2i\alpha\eta^-} \quad . \quad (17)$$

Notice that $|T| \approx 1$, while R is exponentially small.

Let us note in passing that R cannot be obtained by using a contour consisted of L_1^* and L_2^* , corresponding to L_1 and L_2 , but passing through z_c^* , the complex conjugate of z_c . The reason is that whereas on L_1 and L_2 , the asymptotic magnitudes of the incident, transmitted and reflected waves are all equal, on L_1^* and L_2^* , the magnitude of the reflected wave is exponentially smaller than those of the incident and transmitted waves by a factor of $e^{-4\alpha\eta^-}$. Such an exponentially small term is "missed" by our procedure.

III. ADIABATIC BASIS

We consider the one-dimensional scattering of a particle of mass M by a two-state system with energy splitting $\hbar\omega$. We denote the internal states by $|0\rangle$, the lower energy state, and $|1\rangle$, the higher energy one. They form the so-called diabatic basis for a two dimensional vector space. The Hamiltonian of the total system can be written as

$$H = H_p + H_s + H_{int} \quad , \quad (18)$$

$$H_p = -\frac{\hbar^2}{2M} \frac{d^2}{dx^2} + V_0(x) \quad , \quad (19)$$

$$H_s = -\frac{\hbar\omega}{2} \sigma_z \quad , \quad (20)$$

$$H_{int} = \tilde{V}_1(x) \sigma_x + V_2(x) \sigma_z \quad , \quad (21)$$

where H_p is the Hamiltonian of the particle, H_s is the Hamiltonian of the two-state system, H_{int} is the interaction Hamiltonian and σ_x , σ_z are Pauli matrices. The two-component Schrödinger equation in this basis is

$$H \begin{pmatrix} \Psi_0(z) \\ \Psi_1(z) \end{pmatrix} = E \begin{pmatrix} \Psi_0(z) \\ \Psi_1(z) \end{pmatrix} \quad . \quad (22)$$

We assume that $V_0(x)$, $\tilde{V}_1(x)$ and $V_2(x)$ all tend to zero as $x \rightarrow \infty$ and that the particle comes in from the right. For a fixed energy, the velocity of the incoming particle decreases as the mass is increased. In the limit of large α the particle acts on the two-state system as a slowly varying external field and the two-state system follows nearly adiabatically; in the infinite α limit there is no inelastic transition. In the extreme adiabatic limit ($\alpha = \infty$) the Hamiltonian is trivially diagonalized at each z by the transformation^{1,2}

$$U = \begin{pmatrix} \cos\theta(z) & \sin\theta(z) \\ -\sin\theta(z) & \cos\theta(z) \end{pmatrix} \quad , \quad (23)$$

where

$$\tan 2\theta(z) = \frac{V_2(z)}{V_1(z)} \quad , \quad (24)$$

with

$$V_1(z) \equiv \tilde{V}_1(z) - \frac{\hbar\omega}{2} \quad (25)$$

(25) does not determine $\theta(z)$ uniquely; we make the choice of $\theta(z)$ to tend to 0 as $x \rightarrow \infty$ so that

$$\cos\theta(z) = \frac{1}{\sqrt{2}} \left(1 - \frac{V_1(z)}{\sqrt{V_1^2(z) + V_2^2(z)}} \right)^{1/2}, \quad (26)$$

and

$$\sin\theta(z) = -\frac{1}{\sqrt{2}} \left(1 + \frac{V_1(z)}{\sqrt{V_1^2(z) + V_2^2(z)}} \right)^{1/2}. \quad (27)$$

We shall assume that there is a pair of points z_c and z_c^* where $V_1^2 + V_2^2$ vanishes. If there are more than one pair of z_c we choose the one which is closest to the real axis. $\sqrt{V_1^2 + V_2^2}$ is defined to be positive along the real axis with one cut going from z_c to $i\infty$ and the other from z_c^* to $-i\infty$. This choice of branch cuts insures that the mixing angle $\theta(z)$ is a continuous function of x on the real axis. For z real, U is unitary. The new basis vectors

$$\begin{pmatrix} |0, z\rangle \\ |1, z\rangle \end{pmatrix} = U \begin{pmatrix} |0\rangle \\ |1\rangle \end{pmatrix} \quad (28)$$

constitute the so-called adiabatic basis. In this basis the Hamiltonian takes the form

$$H_a = U H U^{-1} \quad (29)$$

$$= \begin{pmatrix} -\frac{\hbar^2}{2M} \frac{d^2}{dz^2} + \frac{\hbar^2}{2M} (\theta')^2 + U_0(z) & \frac{\hbar^2}{2M} \theta'' - \frac{\hbar^2}{M} \theta' \frac{1}{iz} \\ -\frac{\hbar^2}{2M} \theta'' - \frac{\hbar^2}{M} \theta' \frac{d}{dz} & -\frac{\hbar^2}{2M} \frac{d^2}{dz^2} - \frac{\hbar^2}{2M} \theta' - \dots \end{pmatrix}$$

where U_0, U_1 are the adiabatic potentials,

$$U_0(z) \equiv V_0(z) - \sqrt{V_1^2(z) + V_2^2(z)}$$

and

$$U_1(z) \equiv V_0(z) + \sqrt{V_1^2(z) + V_2^2(z)}$$

The Schrödinger equation becomes

$$H_a \begin{pmatrix} \Phi_0(z) \\ \Phi_1(z) \end{pmatrix} = E \begin{pmatrix} \Phi_0(z) \\ \Phi_1(z) \end{pmatrix}, \quad (33)$$

where

$$\begin{pmatrix} \Phi_0(z) \\ \Phi_1(z) \end{pmatrix} \equiv U \begin{pmatrix} \Psi_0(z) \\ \Psi_1(z) \end{pmatrix}. \quad (34)$$

It is easy to see that

$$\Psi_0(z)|0\rangle + \Psi_1(z)|1\rangle \equiv \Phi_0(z)|0, z\rangle + \Phi_1(z)|1, z\rangle. \quad (35)$$

If the off-diagonal terms of H_a are neglected, Φ_0 and Φ_1 are uncoupled. The WKB solutions ($\alpha \rightarrow \infty$) for these uncoupled equations have the usual form,

$$\Phi_0^\pm(z, z^{(0)}) = \frac{1}{\sqrt{q_0(z)}} e^{\pm i\alpha \int_{z^{(0)}}^z q_0(z) dz}, \quad (36)$$

and

$$\Phi_1^\pm(z, z^{(1)}) = \frac{1}{\sqrt{q_1(z)}} e^{\pm i\alpha \int_{z^{(1)}}^z q_1(z) dz}, \quad (37)$$

where

$$q_i(z) = \sqrt{E - U_i(z)}, \quad (38)$$

and $z^{(i)}$ is an arbitrary but fixed lower bound. The branch of $q_i(z)$ is defined so that $q_i(x) = \sqrt{|E - V_i(x)|}$ for $x > x_i$ and $q_i(x) = i\sqrt{|E - V_i(x)|}$ for $x < x_i$, where x_i is the classical turning point defined by

$$E - U_i(x_i) = 0, \quad i = 0, 1. \quad (39)$$

If we treat these solutions at the classical turning points x_i , we will obtain a reflection coefficient of magnitude 1 and a vanishing inelastic transition amplitude. This remains true in all higher order WKB approximations. We need to go into the complex z plane and follow the solutions along appropriate contours. We need to consider the singular

points : x_0 , x_1 and z_c (see Fig. 2). Note that at z_c the function $\theta(z)$ diverges and hence the off-diagonal terms of H_a also diverge, which signals the failure of the adiabatic solutions. In Fig. 2 we show the anti-Stokes lines defined as follows,

$$L_1, L_2 : \text{Im} \int_{z_c}^z (q_0(z) - q_1(z)) dz = 0 \quad , \quad (40)$$

$$L_3 : \text{Im} \int_{x_1}^z q_1(z) dz = 0 \quad , \quad (41)$$

and

$$L_4 : \text{Im} \int_{x_0}^z q_0(z) dz = 0 \quad . \quad (42)$$

L_3 and L_4 are just the anti-Stokes lines for ordinary potential scattering problems with classical turning points at x_1 and x_0 . L_1 and L_2 are the lines on which $\Phi_0^+(z, z_c)$ ($\Phi_0^-(z, z_c)$) have the same magnitude as $\Phi_1^+(z, z_c)$ ($\Phi_1^-(z, z_c)$). The topology of Fig. 2 depends on the potentials and the energy. Since $U_1 > U_0$, $x_1 > x_0$. Both x_0 and x_1 shift to the right as the energy is decreased, whereas z_c does not depend on the energy. In most previous discussions of Stückelberg's theory, only the cases where $\text{Re}(z_c) \gg x_0, x_1$ are discussed. We will see that this restriction is not necessary. The general features of L_1 and L_2 are:

1. L_1 extends to infinity and becomes parallel to the real axis at a distance y_1 for $x \rightarrow \infty$;
- and 2. L_2 intercepts the real axis at a point $\bar{x}$ which can easily be shown to be always less than x_1 . Both y_1 and $\bar{x}$ depend on the energy for given potentials.

IV INELASTIC TRANSITION AMPLITUDE

Consider the physical solution of the Schrödinger equation (23) along the real axis with the following asymptotic conditions:

$$\begin{aligned}\Psi_0(x) &\rightarrow \frac{1}{\sqrt{q_0}}(e^{-i\alpha\bar{q}_0x} + A_0^+ e^{i\alpha\bar{q}_0x}) & , x \rightarrow \infty & , \\ &\rightarrow 0 & , x \rightarrow -\infty & ,\end{aligned}\tag{43}$$

$$\begin{aligned}\Psi_1(x) &\rightarrow \frac{A_1^+}{\sqrt{q_1}} e^{i\alpha\bar{q}_1x} & , x \rightarrow \infty & , \\ &\rightarrow 0 & , x \rightarrow -\infty & ,\end{aligned}\tag{44}$$

where $\bar{q}_i = q_i(x \rightarrow \infty)$. In the adiabatic limit $A_1^+ = 0$ and $|A_0^+|$ is 1. In the near-adiabatic limit, A_1^+ cannot be determined from the usual treatment of the WKB solutions to all orders whereas A_0^+ can be determined to leading order, since its magnitude is ~ 1 . We have seen in Sec. III that at the complex transition point z_c the adiabatic solutions break down. We shall obtain the transition from one state to the other by a careful treatment of the Schrödinger equation near z_c : we need to obtain the exact solutions near z_c in order to connect the WKB solutions on L_1 and L_2 . One might hope to obtain the exponentially small amplitude following a procedure similar to that described in Sec. II; however, the geometry of L_1 and L_2 are very different for the two cases. In the case of above-barrier reflection L_2 extends to $-\infty$ where WKB solutions become the exact solutions and yield the exponentially small reflection amplitude. In the present case L_2 goes down to the real axis where the potentials do not vanish and hence the exact solutions are not known. A different strategy is needed in making use of the solutions on L_1 and L_2 .

It is helpful to think of the physical solution as a linear combination of two-component Jost functions (JF) ⁶. A JF is a (non-physical) solution of the Schrödinger equation which asymptotically has only one incoming or one outgoing wave in one channel. The exact physical solution corresponding to the asymptotic conditions (42) and (43) can be

written as,

$$\Psi_0(x) = \Psi_0^{(0-)}(x) + A_0^+ \Psi_0^{(0+)}(x) + A_1^+ \Psi_0^{(1+)}(x) \quad , \quad (45)$$

$$\Psi_1(x) = \Psi_1^{(0-)}(x) + A_0^+ \Psi_1^{(0+)}(x) + A_1^+ \Psi_1^{(1+)}(x) \quad , \quad (46)$$

where $\Psi_i^{(j\pm)}(x)$ is the component in channel i of the JF with unit incoming $(-)$ or outgoing $(+)$ amplitude in channel j . Our objective is to determine the coefficient A_1^+ which, by Eq.(44), is the transition amplitude. The procedure is as follows.

1. We first obtain A_0^+ , whose magnitude is ~ 1 , by ordinary WKB techniques, applied entirely within channel 0. (Ordinary reflection by a barrier.)
2. Next we note that, as $x \rightarrow -\infty$ each of the JF components in Eqs.(45) and (46) grows exponentially like Φ_1^+ , Eq.(37), which is the most rapidly growing exponential. We shall choose A_1^+ so that the total coefficient of Φ_1^+ vanishes.
3. To accomplish step 2, for Eq.(46), we need to know the coefficient of Φ_1^+ , for $x \rightarrow -\infty$, of each of the JF components $\Psi_1^{(0-)}(x)$, $\Psi_1^{(0+)}(x)$ and $\Psi_1^{(1+)}(x)$. The first two coefficients are exponentially small and need to be carefully calculated on appropriate contours (see below). The last coefficient is of order 1 and can be easily obtained by ordinary WKB techniques, applied entirely to channel 1.
4. Since this procedure determines A_1^+ uniquely, it is not surprising that, in fact, it also makes the leading exponentially growing term of Eq.(45) equal to zero.

We shall need a number of propositions which are proved in the appendix and which have been verified in our numerical calculations.

Proposition 1. Consider the Schrödinger equation (33) on the real axis. Under conditions detailed in the appendix, the physical solution, which vanishes at $-\infty$ and has an incoming wave in channel 0, has the following components,

$$\Phi_0(x) \approx \left(\frac{d\xi_0}{dx} \right)^{-\frac{1}{2}} A i(-\alpha^{\frac{2}{3}} \xi_0(x)) \quad , \text{ everywhere } \quad , \quad (47)$$

$$\begin{aligned}\frac{\Phi_1(x)}{\Phi_0(x)} &\approx 0, & x \leq x_0, \\ \alpha^{1/6} \Phi_1(x) &\approx 0, & x > x_0,\end{aligned}\tag{48}$$

where

$$\frac{2}{3} (\xi_i(x))^{3/2} = \int_{x_i}^x q_i dx, \tag{49}$$

and q_i is given by Eq.(38). The branch of ξ_i in Eq.(49) is defined so that $\xi_i(z) = [-U'(x_i)]^{1/3}(z - x_i)$ in the vicinity of x_i . Proposition 1 establishes the validity of the ordinary WKB solution.

Proposition 2 gives the exact solutions in the vicinity of z_c .

Proposition 2. Consider a circle Ω_c of radius d_c around z_c . We denote the intersection of Ω_c with L_1 and L_2 by $\tilde{z}_1$ and $\tilde{z}_2$ respectively (see Fig.2). Assume that $V_1'V_1 + V_2'V_2$ does not vanish at z_c . Then for sufficiently small d_c , the general solutions of the Schrödinger equation (23) in Ω_c are given by

$$\begin{aligned}\Psi_0(z) &\approx e^{i\alpha q_c \zeta} \left(a_+ Ai(-\alpha^{2/3} C^{2/3} \zeta) + b_+ Bi(-\alpha^{2/3} C^{2/3} \zeta) \right) \\ &\quad + e^{-i\alpha q_c \zeta} \left(a_- Ai(-\alpha^{2/3} C^{2/3} \zeta) + b_- Bi(-\alpha^{2/3} C^{2/3} \zeta) \right),\end{aligned}\tag{50}$$

to the leading order in ζ , where

$$\zeta = z - z_c, \tag{51}$$

$$q_c = \sqrt{E - V_0(z_c)}, \tag{52}$$

$$C = \frac{\sqrt{(V_1^2 + V_2^2)'}}{2q_c} \Big|_{z_c}, \tag{53}$$

and $a_{\pm}$ and $b_{\pm}$ are arbitrary constants.

Proposition 3 and 4 give the WKB solutions on L_1 and L_2 which are needed for finding $\Psi_0^{(0+)}(z)$.

Proposition 3. Consider the anti-Stokes line L_1 . Let z_1 denote a point on L_1 at a fixed distance from z_c and let L_1^- denote L_1 , excluding the segment from z_c to z_1 . Under

conditions detailed in the appendix, there is a solution of the following form,

$$\Phi_0(z) \approx \Phi_0^+(z, z_c) \quad , \quad (54)$$

$$\frac{\Phi_1(z)}{\Phi_0(z)} \approx 0 \quad , \quad (55)$$

for z on L_1^- .

Proposition 4. Consider the anti-Stokes line L_2 . Let z_2 denote a point on L_2 at a fixed distance from z_c and let L_2^- denote L_2 , excluding the segment from z_c to z_2 . Under conditions detailed in the appendix, there is a solution of the following form,

$$\Phi_0(z) \approx \Phi_0^+(z, z_c) \quad , \quad (56)$$

$$\Phi_1(z) \approx \Phi_1^+(z, z_c) \quad , \quad (57)$$

for z on L_2^- .

On L_2 , $\Phi_0^+(z, z_c)$ and $\Phi_1^+(z, z_c)$ have the same magnitude. Therefore their coefficients can be determined accurately. To the left of the point $\bar{x}$, $\Phi_1^+(z, z_c)$ becomes exponentially larger than $\Phi_0^+(z, z_c)$, since the real part of the exponent of the former is larger than that of the latter for $x < \bar{x}$.

We now proceed to find the leading exponentially growing parts (for $x \rightarrow -\infty$) of the JF components. Consider first the JF component $\Psi_0^{(0+)}(z)$ in Eq.(44). As $x \rightarrow +\infty$, $\Psi_0^{(0+)}(z)$ on L_1 is an outgoing wave in channel 0,

$$\Psi_0^{(0+)}(z) \rightarrow \frac{1}{\sqrt{q_0}} e^{i\alpha q_0 z} \quad , x \rightarrow +\infty \quad , \quad (58)$$

where $z = x + iy_1$. According to proposition 3, the continuation of this function on L_1 is given by

$$\Psi_0^{(0+)}(z) \approx A_{0,z_c}^{(0+)} \Phi_0^+(z, z_c) \cos\theta(z) \quad . \quad (59)$$

where $\Phi_0^+(z, z_c)$ is the WKB approximation, Eq.(37), of the component of the exact solution along the adiabatic basis vector $|0, z\rangle$;

$$A_{0,z_c}^{(0+)} \equiv e^{-i\alpha\eta_c} \quad , \quad (60)$$

$$\eta_c = \int_{z_c}^{\infty} (q_0 - \bar{q}_0) dz - \bar{q}_0 z_c \quad ; \quad (61)$$

and $\cos\theta(z)$ is given by Eq.(27). The approximation is valid on L_1 , from $+\infty$ up to a point a_1 , where $|a_1 - z_c| = O(\alpha^{-2/3})$.

We now match this WKB solution (59) to the appropriate linear combination of Airy functions, Eq.(50), at a point m_1 at which both the WKB solutions and the Airy solutions become exact in the limit $\alpha \rightarrow \infty$. By taking, for example $|m_1 - z_c| \sim \alpha^{-1/3}$, we see that $|m_1 - z_c|/|z_1 - z_c| \sim \alpha^{1/3}$, validating the WKB solutions, and $|m_1 - z_c|/|\tilde{z}_1 - z_c| \sim \alpha^{-1/3}$, validating the Airy solutions. At m_1 we can use the asymptotic form of the Airy functions, since the argument, $|\alpha^{2/3} C^{2/3} (m_1 - z_c)|$, is $O(\alpha^{1/3})$:

$$Ai(-w) \sim \frac{1}{\sqrt{\pi}} \frac{1}{w^{1/4}} \sin\left(\frac{2}{3} w^{3/2} + \frac{\pi}{4}\right) \quad , \quad (62)$$

$$Bi(-w) \sim \frac{1}{\sqrt{\pi}} \frac{1}{w^{1/4}} \cos\left(\frac{2}{3} w^{3/2} + \frac{\pi}{4}\right) \quad , \quad -\frac{2\pi}{3} < \arg(w) < \frac{2\pi}{3} \quad (63)$$

Accordingly, inside Ω_c , the JF component is given by

$$\Psi_0^{(0+)}(z) \approx e^{i\frac{\pi}{4}} \frac{\sqrt{\alpha^{1/3} C^{1/3} \pi}}{\sqrt{q_c}} \sqrt{-D} A_{0,z_c}^{(0+)} e^{i\alpha q_c \zeta} \times \{Ai(-\alpha^{2/3} C^{2/3} \zeta) - iBi(-\alpha^{2/3} C^{2/3} \zeta)\} \quad , \quad (64)$$

where C is given by Eq.(53) and

$$D \equiv \frac{V_1}{\sqrt{(V_1^2 + V_2^2)'}}|_{z_c} \quad (65)$$

In the same way we match the Airy-type solution (64) inside Ω_c , to the appropriate WKB solution on L_2 , where the asymptotic forms of Airy functions can be found using the following identities:

$$Ai(e^{-i2\pi/3} w) = e^{-i\pi/3} \left\{ \frac{1}{2} Ai(w) + \frac{i}{2} Bi(w) \right\} \quad , \quad (66)$$

$$Bi(e^{-i2\pi/3} w) = e^{-i\pi/3} \left\{ \frac{3}{2} i Ai(w) + \frac{1}{2} Bi(w) \right\} \quad . \quad (67)$$

This yields , on L_2 ,

$$\Psi_0^{(0+)}(z) \approx A_{0,z_c}^{(0+)} \Phi_0^+(z, z_c) \cos \theta(z) - A_{1,z_c}^{(0+)} \Phi_1^+(z, z_c) \sin \theta(z) \quad , \quad (68)$$

$$A_{1,z_c}^{(0+)} = \epsilon A_{0,z_c}^{(0+)} \quad , \quad (69)$$

where $\epsilon = \pm 1$, and for any specific potentials is given by

$$\epsilon = \lim_{z \rightarrow z_c} i \cot \theta(z) \quad . \quad (70)$$

To be definite we choose $\epsilon = +1$ for the following calculations. From Proposition 4, Eq.(68) is valid on the whole L_2^- down to the real axis. (See Fig. 2.) On the real axis, to the left of the point $\bar{x}$, the JF component is dominated by $\Phi_1^+(x, z_c)$.

Therefore, on the real axis, we have

$$\Psi_0^{(0+)}(x) \rightarrow \frac{1}{\sqrt{q_0}} e^{i\alpha \bar{q}_0 x} \quad , x \rightarrow +\infty, \quad (71)$$

$$\approx -\Phi_1^{(0+)}(x) \sin \theta(x) \quad , x < \bar{x} \quad , \quad (72)$$

where

$$\Phi_1^{(0+)}(x) = A_{1,x_1}^{(0+)} \Phi_1^+(x, x_1) \quad , \quad (73)$$

$$A_{1,x_1}^{(0+)} = e^{-\alpha \gamma} e^{i\alpha \eta - i\alpha \eta_0} \quad , \quad (74)$$

$$\eta_i = \int_{x_i}^{\infty} (q_i(x) - \bar{q}_i) dx - \bar{q}_i x_i \quad , \quad (75)$$

and

$$\eta + i\gamma = \int_{x_0}^{z_c} q_0(z) dz - \int_{x_1}^{z_c} q_1(z) dz \quad . \quad (76)$$

It is easy to see that γ is positive, hence, $A_{1,x_1}^{(0+)}$ is exponentially small. The 0-component of the JF, $\Psi_0^{(0-)}(x)$, needed in Eq.(44) can be obtained simply by taking the complex conjugate of $\Psi_0^{(0+)}(x)$:

$$\Psi_0^{(0-)}(x) \rightarrow \frac{1}{\sqrt{q_0}} e^{-i\alpha \bar{q}_0 x} \quad , x \rightarrow +\infty, \quad (77)$$

$$\approx -\Phi_1^{(0-)}(x) \sin \theta(x) \quad , x < \bar{x} \quad , \quad (78)$$

where

$$\Phi_1^{(0-)}(x) = A_{1,x_1}^{(0-)} \Phi_1^+(x, x_1) \quad , \quad (79)$$

$$A_{1,x_1}^{(0-)} = ie^{-\alpha\gamma} e^{-i\alpha\eta + i\alpha\eta_0} \quad . \quad (80)$$

Finally we require, for Eq.(44), $\Psi_0^{(1+)}$, the 0-component of the JF corresponding to channel 1 outgoing. In the adiabatic basis this JF is, for our purpose, obtainable everywhere on the real axis by ordinary WKB turning point methods:

$$\Phi_1^{(1+)}(x) \rightarrow \frac{1}{\sqrt{q_1}} e^{i\alpha q_1 x} \quad , x \rightarrow +\infty \quad , \quad (81)$$

$$\approx A_{1,x_1}^{(1+)} \Phi_1^+(x, x_1) \quad , x < x_1 \quad , \quad (82)$$

where

$$A_{1,x_1}^{(1+)} = e^{-i\alpha\eta_1} \quad . \quad (83)$$

and

$$\frac{\Phi_0^{(1+)}(x)}{\Phi_1^{(1+)}(x)} \approx 0 \quad , \text{ everywhere} \quad . \quad (84)$$

The reason is that for this JF a single component, $\Phi_1^{(1+)}(x)$, is dominant everywhere on the x -axis; this is not the case for the JF's $(0+)$ and $(0-)$, for which $\Phi_0^{(0\pm)}(x)$ is dominant for $x > x$, while $\Phi_1^{(0\pm)}(x)$ is dominant for $x < x$. The required component $\Psi_0^{(1+)}(x)$ in the diabatic basis is given by

$$\Psi_0^{(1+)}(x) \approx -\Phi_1^{(1+)}(x) \sin\theta(x) \quad , \text{ everywhere} \quad . \quad (85)$$

We are now ready to determine the required coefficient A_1^+ from the condition that the coefficient of the dominant exponential, for $x \rightarrow -\infty$, in Eq.(44) vanishes. Substituting Eqs.(72), (78) and (85) into Eq.(44) gives,

$$A_{1,x_1}^{(0-)} + A_0^+ A_{1,x_1}^{(0-)} + A_1^+ A_{1,x_1}^{(1+)} = 0 \quad . \quad (86)$$

For a wave incident in channel 0 with unit amplitude,

$$A_0^+ \approx -ie^{2i\eta_0} \quad . \quad (87)$$

Substituting in Eq.(86) for A_0^+ , $A_{1,x_1}^{(0-)}$, $A_{1,x_1}^{(0+)}$ and $A_{1,x_1}^{(1+)}$, we obtain, on solving for A_1^+ ,

$$A_1^+ \approx -2\sin(\alpha\eta)e^{-\alpha\gamma}e^{i\alpha(\eta_0+\eta_1)} \quad (88)$$

Incidentally, we can verify that the coefficient of $\Phi_1^+(x, x_1)$ in Eq.(45), for $x < x_1$, also vanishes as it should if A_1^+ is given by Eq.(88).

Following the standard definition of the S matrix,

$$\Psi_0(x) \rightarrow \frac{1}{\sqrt{q_0}} \left(e^{-i\alpha\bar{q}_0x} - S_{00}e^{i\alpha\bar{q}_0x} \right) \quad , x \rightarrow +\infty \quad , \quad (89)$$

$$\Psi_1(x) \rightarrow -\frac{S_{01}}{\sqrt{q_1}} e^{i\alpha\bar{q}_1x} \quad , x \rightarrow +\infty \quad , \quad (90)$$

we find that

$$S_{00} \approx ie^{2i\alpha\eta_0} \quad , \quad (91)$$

and

$$S_{01} \approx 2\sin(\alpha\eta)e^{-\alpha\gamma}e^{i\alpha(\eta_0+\eta_1)} \quad (92)$$

(If ϵ is chosen to be -1 , the right hand side of Eq.(92) would change sign.)

Eq.(92) has the same form as the Landau-Zener-Stückelberg formula in the near-adiabatic limit. However whereas the earlier derivation was limited to the case where z_c is near the real axis (almost crossing adiabats on the real axis) and well to the right of the classical turning points x_0 and x_1 , our derivation is not limited by these restrictions.

We shall now indicate the conditions under which our near-adiabatic approximation is valid. It requires the existence of admissible matching points m_1 , on L_1 and m_2 , on L_2 (see Fig.2). It is easy to see that if m_1 exists so does m_2 . The existence of m_1 requires that

$$|z_1 - z_c| \ll d_c \quad (93)$$

Here z_1 is given by the following condition

$$\left| \frac{1}{\alpha} \frac{d}{dz} \frac{1}{q_i(z) - q_c} \right|_{z_1} = 1 \quad , \quad (94)$$

which is the analog of of the condition signalling the breakdown of the standard WKB approximation ⁷,

$$\left| \frac{1}{\alpha} \frac{d}{dz} \frac{1}{q(z)} \right| = 1 \quad ; \quad (95)$$

and d_c is the distance from z_c over which the following expansion is valid

$$\begin{aligned} q_0(z) &\equiv \sqrt{E - V_0(z) + \sqrt{V_1(z)^2 + V_2(z)^2}} \\ &= q_c + C(z - z_c)^{1/2} \quad , \end{aligned} \quad (96)$$

where q_c and C are defined in Eqs.(52) and (53). Combining (93) and (94) gives

$$\alpha d_c^{3/2} |C| \gg 1 \quad . \quad (97)$$

Since $\alpha = \sqrt{M}/\hbar$ it is evident that for any given potentials and given incident energy, the condition (97) will always be satisfied for sufficiently large M .

The left hand side of Eq.(97) is the dimensionless large parameter which characterizes the deviation from the adiabatic limit. (Let us remark that condition (97) is not necessarily equivalent to the intuitively suggestive criterion that the exponent $\alpha\gamma$, in Eq.(92), be $\gg 1$.)

V COMPARISON WITH NUMERICAL RESULTS

We present comparisons between our results and exact numerical solutions. We choose exponential potentials,

$$V_0(z) = u_0 e^{-z} \quad , \quad (98)$$

$$V_1(z) = u_1 e^{-z} - \frac{\hbar\omega}{2} \quad , \quad (99)$$

$$V_2(z) = u_2 e^{-z} \quad , \quad (100)$$

where the u_i are the strengths of $V_i(z)$. Varying u_i 's we can study both curve crossing and curve noncrossing cases. We shall set $\hbar\omega = 1$.

1. Curve non-crossing. In this case we choose $u_0 = 1.02$, $u_1 = .02$, $u_2 = .2$. Two energies $E = 1, 10$ are studied for different values of α . The two cases have very different topology of z_c , x_0 , x_1 and anti-Stokes lines as shown in Figs. 2(a) and 2(b). Although the diabatic potentials $V_0(z) \pm \tilde{V}_1(z)$ cross at $z = -3.2$, this point is far to the left of the classical turning points. In the region where the transition takes place the adiabatic potentials are almost parallel to each other. In Fig. 3 the absolute values of $\Phi_0^{(0+)}(x)$ and $\Phi_1^{(0+)}(x)$ for $E = 10$ are plotted for different values of α . For large α , channel 1 is seen to dominate for $x < x$. Numerical results for the S matrix are listed in Table I. The differences between semiclassical and exact solutions diminish in the limit of large α for both energies.

2. Curve crossing. In this case we choose $u_0 = 1.2$, $u_1 = .5$, $u_2 = .2$. The diabatic potentials cross at $z = 0$. Two energies, $E = 0.7, 1.5$, are studied. For $E = 1.5$, the topology of z_c , x_0 , x_1 and anti-Stokes lines is similar to Fig. 2(a) and for $E = 0.7$, it is similar to Fig. (2b). Results of the S matrix are also included in Table I. The differences between semiclassical and exact solutions also diminish in the limit of large α for both energies.

VI CONCLUSION

We have presented a rigorous treatment of the semiclassical theory for obtaining exponentially small inelastic transition amplitudes. The region of validity of our theory is established. Our result, Eq.(92), has the same form as the Landau-Zener-Stückelberg formula in the near-adiabatic limit. However, our theory is more general and is applicable to a wide range of systems.

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APPENDIX

In the following propositions we make the same assumptions about the potentials as in the text. The proofs of propositions 1, 3 and 4 are analogous to Jeffreys' proof⁸ for the ordinary potential scattering problem. For convenience we shall use N to denote a bounded constant independent of α . The value and the dimensionality of N may be different at different places and are irrelevant to our discussions.

I. Proposition 1. Consider the Schrödinger equation (33) on the real axis. We assume that for the given energy E each adiabatic potential U_i , $i = 0, 1$, has only one classical turning point, x_i , and that $U'_i(x_i) < 0$, which will normally be the case. If the following functions are bounded,

$$F_0(x) = \int_{-\infty}^x \left(|f_{00}(x')| + |f_{01}(x')| \sqrt{\frac{\xi_0(x')}{\xi_1(x')}} \right) \left| \frac{q_0(x')}{\xi_0(x')} \right| dx' \quad , \quad (101)$$

$$F_1(x) = \int_{-\infty}^x \left(|f_{11}(x')| + |f_{10}(x')| \sqrt{\frac{\xi_1(x')}{\xi_0(x')}} \right) \left| \frac{q_1(x')}{\xi_1(x')} \right| dx' \quad , \quad (102)$$

and if the following quantities can be bounded by $\alpha^{1/6}N$,

$$F_2^{\pm} = \int_{-\infty}^{x_i^-} + \int_{x_i^+}^{\infty} \left| \frac{d}{dx'} \left(\frac{q_j(x')h(x')}{\sqrt{\xi_0(x')\xi_1(x')(q_0(x') \pm q_1(x'))}} \right) \right| dx' ,$$

$$(i, j) = (0, 1), (1, 0), \quad (103)$$

where $x_i^{\pm} = x_i \pm N\alpha^{-2/3}$, ξ_i is given by Eq.(49), f_{ij} , and h are given by Eqs.(109)–(112), then the physical solution, which vanishes at $-\infty$ and has an incoming wave in channel 0, has the following form,

$$\Phi_0(x) \approx \left(\frac{d\xi_0}{dx} \right)^{-\frac{1}{2}} Ai(-\alpha^{\frac{2}{3}}\xi_0(x)) \quad , \text{everywhere} . \quad (104)$$

$$\begin{aligned} \frac{\Phi_1(x)}{\Phi_0(x)} &\approx 0 & , x \leq x_0, \\ \alpha^{1/6}\Phi_1(x) &\approx 0 & , x > x_0, \end{aligned} \quad (105)$$

Proof. Defining a new set of variables

$$\chi_i(\xi_i(x)) = \left(\frac{d\xi_i}{dx} \right)^{\frac{1}{2}} \Phi_i(x) \quad , i = 0, 1 \quad , \quad (106)$$

the Schrödinger equation (33) can be written as

$$\frac{d^2}{d\xi_0^2} \chi_0 + \alpha^2 \xi_0 \chi_0 = f_{00}(\xi_0) \chi_0 + f_{01}(\xi_0) \chi_1 + h(\xi_0) \frac{d}{d\xi_0} \chi_1 \quad , \quad (107)$$

$$\frac{d^2}{d\xi_1^2} \chi_1 + \alpha^2 \xi_1 \chi_1 = f_{11}(\xi_1) \chi_1 + f_{10}(\xi_1) \chi_0 - h(\xi_1) \frac{d}{d\xi_1} \chi_0 \quad , \quad (108)$$

where

$$h(\xi_i) = \frac{2\theta'}{(\xi_0' \xi_1')^{1/2}} \quad , \quad (109)$$

$$f_{ii}(\xi_i) = \frac{1}{2} \frac{\xi_i'''}{(\xi_i')^3} - \frac{3}{4} \frac{(\xi_i'')^2}{(\xi_i')^4} + \frac{(\theta')^2}{(\xi_i')^2} \quad , i = 0, 1 \quad , \quad (110)$$

$$f_{01}(\xi_0) = \frac{1}{(\xi_0' \xi_1')^{3/2}} (\theta'' \xi_1' - \theta' \xi_1'') \quad , \quad (111)$$

$$f_{10}(\xi_1) = \frac{1}{(\xi_0' \xi_1')^{3/2}} (-\theta'' \xi_0' + \theta' \xi_0'') \quad . \quad (112)$$

In Eqs.(107) and (108) χ_i are functions of ξ_i . The correspondence between ξ_0 and ξ_1 is one-to-one. If χ_1 is negligible, Eq.(107) involves only channel 0. The solution of χ_0 is given by Eq.(104). To show that χ_1 is indeed negligible we transform Eq.(108) into an integral equation⁸. We need to construct the Green's function. The general solutions of the homogeneous equation,

$$\frac{d^2}{d\xi_1^2} \chi_1^{(0)} + \alpha^2 \xi_1 \chi_1^{(0)} = 0 \quad , \quad (113)$$

are Airy functions:

$$\chi_1^{(0)}(\xi_1) = a_1 Ai(-\alpha^{2/3} \xi_1) + b_1 Bi(-\alpha^{2/3} \xi_1) \quad , \quad (114)$$

where a_1 and b_1 are arbitrary constants. The required Green's function which satisfies the differential equation,

$$\frac{d^2}{d\xi_1^2} G_1(\xi_1, \tilde{\xi}_1) + \alpha^2 \xi_1 G_1(\xi_1, \tilde{\xi}_1) = \delta(\xi_1 - \tilde{\xi}_1) \quad , \quad (115)$$

has the following form:

$$\begin{aligned} G_1(\xi_1, \tilde{\xi}_1) &= Ai(-\alpha^{2/3}\xi_1)P_1(\tilde{\xi}_1) & , \xi_1 < \tilde{\xi}_1, \\ &= \{+iAi(-\alpha^{2/3}\xi_1) + Bi(-\alpha^{2/3}\xi_1)\}\tilde{P}_1(\tilde{\xi}_1) & , \xi_1 > \tilde{\xi}_1, \end{aligned} \quad (116)$$

where $G_1 \rightarrow 0$ as $\xi_1 \rightarrow -\infty$ and, as $\xi_1 \rightarrow +\infty$, G_1 is an outgoing wave in channel 1 for fixed $\tilde{\xi}_1$. Solving for G_1 , we obtain,

$$\begin{aligned} G_1(\xi_1, \tilde{\xi}_1) &= -\frac{\pi}{\alpha^{2/3}}Ai(-\alpha^{2/3}\xi_1)\{iAi(-\alpha^{2/3}\tilde{\xi}_1) + Bi(-\alpha^{2/3}\tilde{\xi}_1)\} & , \xi_1 < \tilde{\xi}_1, \\ &= -\frac{\pi}{\alpha^{2/3}}Ai(-\alpha^{2/3}\tilde{\xi}_1)\{iAi(-\alpha^{2/3}\xi_1) + Bi(-\alpha^{2/3}\xi_1)\} & , \xi_1 > \tilde{\xi}_1. \end{aligned} \quad (117)$$

The integral equation for the required solutions is,

$$\chi_1(\xi_1) = \int_{-\infty}^{+\infty} d\tilde{\xi}_1 G_1(\xi_1, \tilde{\xi}_1) \left\{ f_{11}\chi_1 + f_{10}\chi_0 - h\frac{d}{d\tilde{\xi}_1}\chi_0 \right\} , \quad (118)$$

where the homogeneous term is chosen to be 0. (We have omitted some arguments of the functions to shorten the notation.) The first iteration of Eq.(118) is obtained by substituting χ_1 with 0 and χ_0 with $Ai(-\alpha^{2/3}\xi_0)$:

$$\chi_1(\xi_1) = \int_{-\infty}^{+\infty} d\tilde{\xi}_1 G_1(\xi_1, \tilde{\xi}_1) \left\{ f_{10} - h\frac{d}{d\tilde{\xi}_1} \right\} Ai(-\alpha^{2/3}\xi_0) . \quad (119)$$

The right hand side of Eq.(119) can be written as a sum of three terms,

$$\chi_1^{(1)}(\xi_1) = i\frac{\pi}{\alpha^{2/3}}Ai(-\alpha^{2/3}\xi_1) \int_{-\infty}^{+\infty} d\tilde{\xi}_1 Ai(-\alpha^{2/3}\tilde{\xi}_1) \left\{ f_{10} - h\frac{d}{d\tilde{\xi}_1} \right\} Ai(-\alpha^{2/3}\xi_0) , \quad (120)$$

$$\chi_1^{(2)}(\xi_1) = -\frac{\pi}{\alpha^{2/3}} \int_{-\infty}^{\xi_1} d\tilde{\xi}_1 K_{\alpha}^{+}(\xi_1, \tilde{\xi}_1) \left\{ f_{10} - h\frac{d}{d\tilde{\xi}_1} \right\} Ai(-\alpha^{2/3}\xi_0) , \quad (121)$$

$$\chi_1^{(3)}(\xi_1) = \frac{\pi}{\alpha^{2/3}} \int_{+\infty}^{\xi_1} d\tilde{\xi}_1 K_{\alpha}^{-}(\xi_1, \tilde{\xi}_1) \left\{ f_{10} - h\frac{d}{d\tilde{\xi}_1} \right\} Ai(-\alpha^{2/3}\xi_0) , \quad (122)$$

where

$$K_{\alpha}^{+}(\xi_i, \tilde{\xi}_i) = Bi(-\alpha^{2/3} \xi_i) Ai(-\alpha^{2/3} \tilde{\xi}_i) \quad , \quad (123)$$

$$K_{\alpha}^{-}(\xi_i, \tilde{\xi}_i) = Ai(-\alpha^{2/3} \xi_i) Bi(-\alpha^{2/3} \tilde{\xi}_i) \quad . \quad (124)$$

Since $Ai(-\alpha^{2/3} \xi_1)$ is bounded everywhere and $Ai(-\alpha^{2/3} \xi_1)$ is exponentially smaller than $Ai(-\alpha^{2/3} \xi_0)$ for $x < x_0$, we have

$$\frac{\chi_1^{(1)}(x)}{Ai(-\alpha^{2/3} \xi_0(x))} \approx 0 \quad , x \leq x_0 \quad , \quad (125)$$

$$\alpha^{1/6} \chi_1^{(1)}(x) \approx 0 \quad , x > x_0 \quad . \quad (126)$$

Both $\chi_1^{(2)}$ and $\chi_1^{(3)}$ satisfy equations similar to (125) and (126). We shall give the bound for the second term of $\chi_1^{(2)}$:

$$\tilde{\chi}_1^{(2)}(\xi_1) \equiv -\frac{\pi}{\alpha^{2/3}} \int_{-\infty}^{\xi_1} d\tilde{\xi}_1 K_{\alpha}^{+} h \frac{d}{d\tilde{\xi}_1} Ai(-\alpha^{2/3} \tilde{\xi}_0) \quad ; \quad (127)$$

the bound for other terms in $\chi_1^{(2)}$ and $\chi_1^{(3)}$ can be obtained similarly. Consider first the region $x \leq x_0$. In order to utilize the asymptotic form of $Ai(-\alpha^{2/3} \tilde{\xi}_0)$ we discuss two cases, $x < x_0^-$ and $x_0^- \leq x \leq x_0$, separately.

For $x < x_0^-$, using the asymptotic forms of Airy functions, we have,

$$\tilde{\chi}_1^{(2)} \approx \frac{i}{4\alpha^{1/6} \sqrt{-\xi_1}} e^{\alpha \int_{x_0}^{x_1} |q_1| dx''} \int_{-\infty}^x dx' q_0(x') \bar{h}(x') e^{-\alpha (\int_{x'}^{x_1} |q_1| dx'' + \int_{x'}^{x_0} |q_0| dx'')} \quad , \quad (128)$$

where

$$\bar{h}(x) = \frac{h(x)}{\sqrt[4]{\tilde{\xi}_1(x) \tilde{\xi}_0(x)}} \quad . \quad (129)$$

The integral in Eq.(134) can be written as

$$\int_{-\infty}^x dx' \frac{q_0(x') \bar{h}(x')}{-i\alpha(q_0(x') + q_1(x'))} \frac{d}{dx'} \left\{ e^{-\alpha (\int_{x'}^{x_1} |q_1| dx'' + \int_{x'}^{x_0} |q_0| dx'')} \right\}$$

Performing an integration by part in this form, we obtain,

$$|\tilde{\chi}_1^{(2)}| \leq \left| \frac{1}{\alpha^{7/6} \sqrt[4]{\xi_1(x)}} \frac{q_0 \bar{h}(x)}{(q_0(x) + q_1(x))} e^{-\alpha \int_x^{x_0} |q_0| dx'} \right| + \left| \frac{1}{\alpha^{7/6} \sqrt[4]{\xi_1(x)}} \int_{-\infty}^x dx' \left(\frac{d}{dx'} \frac{q_0 \bar{h}}{q_0 + q_1} \right) e^{-\alpha \left(\int_x^{x_1} |q_1| dx'' + \int_{x'}^{x_0} |q_0| dx'' - \int_x^{x_1} |q_1| dx'' \right)} \right| \quad (130)$$

Since we have assumed that there is only one classical turning point for each adiabatic potential, the function $\int_x^{x_1} |q_1| dx'' + \int_x^{x_0} |q_0| dx''$ is monotonically increasing as x moves from x_0 to $-\infty$. Hence the exponential term in the integral of Eq.(130) is bounded by $\exp(-\alpha \int_x^{x_0} |q_0| dx'')$. From this and the assumption about F_2^{0+} , it is not difficult to see that

$$|\tilde{\chi}_1^{(2)}| \leq \frac{N}{\alpha} \text{Ai}(-\alpha^{2/3} \xi_0(x)) \quad , x < x_0^- \quad (131)$$

For $x_0^- \leq x \leq x_0$ the asymptotic forms of Airy functions are not valid. However, both Ai and Bi are bounded, we can estimate the magnitude of the integral easily. In this region the integrand can be bounded as follows:

$$\frac{1}{\alpha^{2/3}} |K_\alpha^+| \leq \frac{N}{\alpha} \quad , \quad (132)$$

and

$$\left| \frac{d}{d\xi_1} \text{Ai}(-\alpha^{2/3} \tilde{\xi}_0) \right| \leq \alpha^{2/3} N \quad (133)$$

Since the integration region is only of $O(\alpha^{-2/3})$, the integral is only $O(\alpha^{-1})$. Therefore we conclude that

$$\frac{\tilde{\chi}_1^{(2)}(x)}{\Phi_0(x)} \approx 0 \quad , x \leq x_0 \quad (134)$$

For $x > x_0$, $\tilde{\chi}_1^{(2)}$ can be analyzed for regions $x_0 < x < x_1^-$, $x_1^- \leq x \leq x_1^+$ and $x > x_1^+$ by a similar treatment. We obtain $\alpha^{1/6} \tilde{\chi}_1^{(2)}(x) \approx 0$.

II. Proposition 2. Consider a circle Ω_c of radius d_c around z_c . Assume that $V_1' V_1 + V_2' V_2$ does not vanish at z_c then for sufficiently small d_c and sufficiently large α , the general

solutions of the Schrödinger equation (23) in Ω_c is

$$\begin{aligned}\Psi_0(z) \approx e^{i\alpha q_c \zeta} & \left(a_+ A i(\alpha^{2/3} C^{2/3} \zeta) + b_+ B i(\alpha^{2/3} C^{2/3} \zeta) \right) \\ & + e^{-i\alpha q_c \zeta} \left(a_- A i(\alpha^{2/3} C^{2/3} \zeta) + b_- B i(\alpha^{2/3} C^{2/3} \zeta) \right),\end{aligned}\quad (135)$$

to the leading order in ζ , where ζ , q_c and C are given by Eqs.(51), (52) and (53); and $a_{\pm}$ and $b_{\pm}$ are arbitrary constants.

Proof. Eliminating $\Psi_1(z)$ from the Schrödinger equation we obtain the fourth order differential equation for $\Psi_0(z)$,

$$\begin{aligned}D\Psi_0(z) \equiv & \left\{ \frac{d^4}{dz^4} + f_3(z) \frac{d^3}{dz^3} + f_2(z) \frac{d^2}{dz^2} + f_1(z) \frac{d}{dz} + f_0(z) \right\} \Psi_0(z) \\ & = 0,\end{aligned}\quad (136)$$

where

$$f_3 = -2 \frac{V_2'}{V_2}, \quad (137)$$

$$f_2 = 2(E - V_0) + \alpha^2 \left(-\frac{V_2''}{V_2} + 2 \left(\frac{V_2'}{V_2} \right)^2 \right), \quad (138)$$

$$f_1 = -2\alpha^2 \left[V_0' + V_1' + \frac{V_2'}{V_2} (E - V_0 - V_1) \right], \quad (139)$$

$$\begin{aligned}f_0 = & \alpha^4 ((E - V_0)^2 V_1^2 - V_2^2) \\ & + \alpha^2 \left[-(V_0'' + V_1'') + \frac{2(V_2')^2 - V_2 V_2''}{V_2^2} (E - V_0 - V_1) + 2 \frac{V_2'}{V_2} (V_0' + V_1') \right].\end{aligned}\quad (140)$$

Pulling out a fast oscillating part of Ψ_0 ,

$$\Psi_0(z) = e^{i\alpha q_c \zeta} \chi(\zeta), \quad (141)$$

the solutions of $\chi(\zeta)$ include two slowly varying solutions (for sufficiently small $|\zeta|$) and two fast oscillating solutions; we will find the former. The equation for χ reads

$$\left\{ \frac{d^4}{dz^4} + g_3(z) \frac{d^3}{dz^3} + g_2(z) \frac{d^2}{dz^2} + g_1(z) \frac{d}{dz} + g_0(z) \right\} \chi(z) = 0, \quad (142)$$

where

$$g_3(z) \approx -4i\alpha q_c \quad (143)$$

$$g_2(z) \approx 2\alpha^2(E - V_0 - 3q_c^2) \quad (144)$$

$$g_1(z) \approx 4\alpha^3 i q_c (E - V_0 - q_c^2) + 2\alpha^2 [V_0' - V_1' - (V_0 - V_1 + 3q_c^2) \frac{V_2'}{V_2}] \quad (145)$$

$$g_0(z) \approx \alpha^4 [(q_c^4 - 2q_c^2(E - V_0) + (E - V_0)^2) - (V_1^2 + V_2^2)] + 2\alpha^3 i q_c [V_1' - V_0' + (E - V_0 - V_1 - q_c^2) \frac{V_2'}{V_2}] \quad (146)$$

Linearizing the potentials at z_c and changing variable from z to ζ we obtain

$$\left\{ \frac{d^4}{d\zeta^4} + \alpha S_3 \frac{d^3}{d\zeta^3} + (\alpha^2 S_2 + \alpha^3 T_2 \zeta) \frac{d^2}{d\zeta^2} + \alpha^2 S_1 \frac{d}{d\zeta} + (\alpha^3 S_0 + \alpha^4 T_0 \zeta) \right\} \chi(\zeta) = 0 \quad (147)$$

where

$$S_3 = -2 \frac{a_2}{b_2} \quad (148)$$

$$S_2 = -4q_c^2 \quad (149)$$

$$S_1 = -2a_1 - 2a_0 + 2 \frac{b_1 a_2}{b_2} + 4q_c^2 \frac{a_2}{b_2} \quad (150)$$

$$T_2 = 4i q_c a_0 \quad (151)$$

$$S_0 = -i \frac{2q_c i}{b_2} (b_1 a_2 - a_1 b_2) \quad (152)$$

$$T_0 = 2(a_2 b_2 + a_1 b_1) \quad (153)$$

with

$$a_i = V_i'(z_c) \quad (154)$$

$$b_{1,2} = V_{1,2}(z_c) \quad (155)$$

Making a scale transformatin

$$\eta = \alpha^{2/3} \zeta \quad (156)$$

and assuming that $|\frac{d^m \chi}{d\eta^m}|$ are of the same order as $|\chi|$, Eq.(153) can be reduced to the leading order in α :

$$\frac{d^2 \chi}{d\eta^2} + C^2 \eta \chi + \frac{1}{S_2 \alpha^{1/3}} [S_3 \frac{d^3 \chi}{d\eta^3} + T_1 \frac{d\chi}{d\eta} - S_0 \chi] = 0 \quad (157)$$

For $\eta > O(\alpha^{-1/3})$ the last term is negligible, the solutions are the Airy functions. For $\eta < O(\alpha^{-1/3})$ the last term is not smaller than the second term, however, all terms are small; the correction to the Airy functions vanishes in the large α limit. Hence the slowly varying solutions are

$$\chi(\zeta) \approx a_+ Ai(\alpha^{2/3} C^{2/3} \zeta) + b_+ Bi(\alpha^{2/3} C^{2/3} \zeta) \quad (158)$$

where a_+ and b_+ are arbitrary constants. This shows that the scaling, Eq.(156), is indeed a correct one. Eqs.(141) and (158) give one set of solutions. Pulling out another fast oscillating factor $e^{-i\alpha\eta\zeta}$ (cf. Eq.(141)) we can obtain the other set of solutions in Eq.(135).

III. Proposition 3. Consider the anti-Stokes line L_1 . Let z_1 denote a point at a fixed distance from z_c and let L_1^- denote L_1 , excluding the segment from z_c to z_1 . We assume the following conditions to be true: 1. L_1 does not pass through singularities of the potentials. 2. the mappings $\xi_i(z) = \int_{z_*}^z q_i(z) dz$, $i = 0, 1$, are one to one⁹; 3. $\text{Im}(\xi_i)$ increases monotonically as z moves to the right on L_1 ¹⁰. If the following functions can be bounded by N ,

$$F_0(z) = \int_z^\infty (|f_{00}(z)| + |f_{01}(z)|) |q_0(z) dz| \quad (159)$$

$$F_1(z) = \int_z^\infty (|f_{11}(z)| + |f_{10}(z)|) |q_1(z) dz| \quad (160)$$

$$F_2^{i\pm}(z) = \int_z^\infty \left| \frac{d}{dz} \left(\frac{q_i(z) h(z)}{q_0(z) \pm q_1(z)} \right) \right| |dz| \quad , i = 0, 1 \quad (161)$$

where f_{ij} and h are given by Eqs.(167)-(170), then, for z on L_1^- , there is a solution of the following form,

$$\Phi_0(z) \approx \Phi_0^+(z, z_c) \quad (162)$$

$$\frac{\Phi_1(x)}{\Phi_0(x)} \approx 0, \quad (163)$$

where $\Phi_0^+(x, z_c)$ is defined in Eq.(36).

Proof. Defining a new set of variables

$$\chi_i(\xi_i(x)) = \left(\frac{d\xi_i}{dx} \right)^{\frac{1}{2}} \Phi_i(x), \quad i = 0, 1, \quad (164)$$

the Schrödinger equation (33) can be written as

$$\frac{d^2}{d\xi_0^2} \chi_0 + \alpha^2 \chi_0 = f_{00}(\xi_0) \chi_0 + f_{01}(\xi_0) \chi_1 + h(\xi_0) \frac{d}{d\xi_0} \chi_1, \quad (165)$$

$$\frac{d^2}{d\xi_1^2} \chi_1 + \alpha^2 \chi_1 = f_{11}(\xi_1) \chi_1 + f_{10}(\xi_1) \chi_0 - h(\xi_1) \frac{d}{d\xi_1} \chi_0, \quad (166)$$

where

$$h(\xi_i) = \frac{2\theta'}{(\xi_0' \xi_1')^{1/2}}, \quad (167)$$

$$f_{ii}(\xi_i) = \frac{1}{2} \frac{\xi_i'''}{(\xi_i')^3} - \frac{3}{4} \frac{(\xi_i'')^2}{(\xi_i')^4} + \frac{(\theta')^2}{(\xi_i')^2}, \quad i = 0, 1, \quad (168)$$

$$f_{01}(\xi_0) = \frac{1}{(\xi_0' \xi_1')^{3/2}} (\theta'' \xi_1' - \theta' \xi_1''), \quad (169)$$

$$f_{10}(\xi_1) = \frac{1}{(\xi_0' \xi_1')^{3/2}} (-\theta'' \xi_0' + \theta' \xi_0''), \quad (170)$$

The correspondence between variables ξ_0 and ξ_1 is one-to-one. Similar to the proof of proposition 1, we transform (165) and (166) into coupled integral equations ⁶:

$$\chi_0(\xi_0) = \chi_0^{(0)}(\xi_0) + \int_{\xi_0}^{\xi_1} d\tilde{\xi}_0 K_\alpha(\xi_0, \tilde{\xi}_0) \times \left\{ f_{00}(\tilde{\xi}_0) \chi_0(\tilde{\xi}_0) + f_{01}(\tilde{\xi}_0) \chi_1(\tilde{\xi}_1) + h(\tilde{\xi}_0) \frac{d}{d\tilde{\xi}_0} \chi_1(\tilde{\xi}_1) \right\}, \quad (171)$$

$$\chi_1(\xi_1) = \chi_1^{(0)}(\xi_1) + \int_{\xi_1}^{\xi_0} d\tilde{\xi}_1 K_\alpha(\xi_1, \tilde{\xi}_1) \times \left\{ f_{11}(\tilde{\xi}_1) \chi_1(\tilde{\xi}_1) + f_{10}(\tilde{\xi}_1) \chi_0(\tilde{\xi}_0) - h(\tilde{\xi}_1) \frac{d}{d\tilde{\xi}_1} \chi_1(\tilde{\xi}_1) \right\}, \quad (172)$$

where $\chi_0^{(0)}$ and $\chi_1^{(0)}$ are solutions of the homogeneous equations:

$$\chi_0^{(0)}(\xi_0) = a_0 e^{i\alpha\xi_0} + b_0 e^{-i\alpha\xi_0} , \quad (173)$$

$$\chi_1^{(0)}(\xi_1) = a_1 e^{i\alpha\xi_1} + b_1 e^{-i\alpha\xi_1} , \quad (174)$$

and K_α is the kernel,

$$K_\alpha(\xi_i, \tilde{\xi}_i) = -\frac{\pi}{\alpha} \left(e^{i\alpha(\xi_i - \tilde{\xi}_i)} - e^{-i\alpha(\xi_i - \tilde{\xi}_i)} \right) . \quad (175)$$

Choosing the lower bounds of the integrals to be ξ_i^∞ , where $z(\xi_i^\infty) = \infty + iy_1$, and choosing

$$\chi_0^{(0)} = e^{i\alpha\xi_0} , \quad (176)$$

$$\chi_1^{(0)} = 0 , \quad (177)$$

the integral equations become,

$$\chi_0(\xi_0) = e^{i\alpha\xi_0} + \int_{\xi_0^\infty}^{\xi_0} d\tilde{\xi}_0 K_\alpha \left\{ f_{00}\chi_0 + f_{01}\chi_1 + h \frac{d}{d\tilde{\xi}_0} \chi_1 \right\} , \quad (178)$$

$$\chi_1(\xi_1) = \int_{\xi_1^\infty}^{\xi_1} d\tilde{\xi}_1 K_\alpha \left\{ f_{11}\chi_1 + f_{10}\chi_0 - h \frac{d}{d\tilde{\xi}_1} \chi_0 \right\} . \quad (179)$$

The first iteration of Eqs.(178) and (179) gives

$$\chi_0(\xi_0) = e^{i\alpha\xi_0} + \int_{\xi_0^\infty}^{\xi_0} d\tilde{\xi}_0 K_\alpha f_{00} e^{i\alpha\tilde{\xi}_0} , \quad (180)$$

$$\chi_1(\xi_1) = \int_{\xi_1^\infty}^{\xi_1} d\tilde{\xi}_1 K_\alpha \left(f_{10} - h \frac{d}{d\tilde{\xi}_1} \right) e^{i\alpha\tilde{\xi}_0} . \quad (181)$$

Eq.(180) includes only one channel, which is similar to the ordinary potential scattering problem; the integral is negligible. We will only show the bound for the second term of (181):

$$\chi_1^{(1)}(\xi_1) \equiv - \int_{\xi_1^\infty}^{\xi_1} d\tilde{\xi}_1 K_\alpha h \frac{d}{d\tilde{\xi}_1} e^{i\alpha\tilde{\xi}_0} . \quad (182)$$

Performing an integration by part (which is similar to the step from Eq.(128) to Eq.(130)), we obtain

$$\chi_1^{(1)} = \frac{1}{\alpha} e^{i\alpha\xi_0} (B_1 + B_2 + B_3 + B_4) \quad , \quad (183)$$

where

$$B_1 = -\frac{h(z)q_0(z)}{q_0(z) - q_1(z)} \quad , \quad (184)$$

$$B_2 = \frac{h(z)q_0(z)}{q_0(z) + q_1(z)} \quad , \quad (185)$$

$$B_3 = \int_{\infty}^z dz' \left(\frac{d}{dz'} \frac{h_1(z')q_0(z')}{q_0(z') - q_1(z')} \right) e^{i\alpha(\xi_1(z') - \xi_0(z'))} \quad , \quad (186)$$

$$B_4 = \int_{\infty}^z dz' \left(\frac{d}{dz'} \frac{h_1(z')q_0(z')}{q_0(z') + q_1(z')} \right) e^{2i\alpha[(\xi_1(z') + \xi_0(z')) - (\xi_0(z) + \xi_1(z))]} \quad . \quad (187)$$

From the definition of L_1 , $|e^{i\alpha(\xi_0 - \xi_1)}|$ is 1. Therefore B_1 , B_2 and B_3 are bounded for z on L_1^- . From condition 3 about L_1 we see that the real part of the exponent of B_4 is always less than 0. Thus B_4 is also bounded. Therefore we have

$$\frac{\chi_1^{(1)}(z)}{\Phi_0(z)} \approx 0 \quad . \quad (188)$$

The proof of proposition 4 is similar to what we have just shown. We only give the statement.

Proposition 4. Consider the anti-Stokes lines L_2 . Let z_2 denote a point at a fixed distance from z_c and let L_2^- denote L_2 , excluding the segment from z_c to z_2 . We assume the following conditions to be true: 1. L_2 does not pass through singularities of the potentials. 2. the mappings $\xi_i(z) = \int_{z_c}^z q_i(z) dz$, $i = 0, 1$, are one to one; 3. $\text{Im}(\xi_i)$ increases monotonically as z moves down to $\bar{z}$ on L_2 ¹¹. If the following functions can be bounded by N ,

$$F_0(z) = \int_{z_2}^z (|f_{00}(z)| + |f_{01}(z)|) |q_0(z) dz| \quad , \quad (189)$$

$$F_1(z) = \int_{z_2}^z (|f_{11}(z)| + |f_{10}(z)|) |q_1(z) dz| \quad , \quad (190)$$

$$F_2^{i\pm}(z) = \int_{z_2}^z \left| \frac{d}{dz'} \left(\frac{q_i(z')h(z')}{q_0(z') \pm q_1(z')} \right) \right| |dz'| \quad , i = 0, 1 \quad , \quad (191)$$

where f_{ij} , and h are given by Eqs.(167)-(170), then, for z on L_2^- , there is a solution of the following form,

$$\Phi_0(z) \approx \Phi_0^+(z, z_c) \quad , \quad (192)$$

$$\Phi_1(z) \approx \Phi_1^+(z, z_c) \quad , \quad (193)$$

where $\Phi_0(z, z_c)$ and $\Phi_1(z, z_c)$ are defined in Eqs.(36) and (37) respectively.

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5. If z_c satisfies this condition so does z_c^* .
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9. The ξ_i defined here are different from those used in proposition 1.
10. This condition is not restrictive at all; it is satisfied for all numerical examples presented in Sec. V. A weaker condition is sufficient: there exists a path from z to ∞ along which $\text{Im}(\xi_i)$ increases monotonically. (Such a path need not be L_1 .)
11. This is also true for our numerical examples. A weaker condition is sufficient: there exists a path from z_c to z along which $\text{Im}(\xi_i)$ increases monotonically.

FIGURE CAPTIONS

Fig. 1. The typical topology of the complex transition point z_c and anti-Stokes lines L_1 and L_2 are shown for above barrier reflection problem. L_1 extends to $+\infty$ and becomes parallel to the real axis at a distance y_1 asymptotically. L_2 behaves similarly as it extends to $-\infty$.

Fig. 2. The transition points x_0 , x_1 , $\bar{x}$, z_c and anti-Stokes lines L_1 , L_2 , L_3 , L_4 are shown for the curve noncrossing case in Sec. V: 2(a) for $E = 10$ and 2(b) for $E = 1$.

Fig. 3. The absolute values of $\Phi_0^{(0+)}(x)$ and $\Phi_1^{(0+)}(x)$ for the case of Fig. 2(a) are shown for several values of α : 3(a) for $\alpha = 1$, 3(b) for $\alpha = 5$ and 3(c) for $\alpha = 10$. $|\Phi_0^{(0+)}(x)|$ is represented by the solid line and $|\Phi_1^{(0+)}(x)|$ by the dash line. The vertical dot-dash line marks the position of $\bar{x}$. Note that for large α , $\Phi_1^{(0+)}(x)$ becomes greater than $\Phi_0^{(0+)}(x)$ as x moves to the left of $\bar{x}$.

TABLE CAPTION

Table I. The numerical results of exact and semiclassical solutions for the S matrix are shown. The semiclassical results are calculated from Eqs.(91) and (92). Note that the differences between them decrease as α is increased.

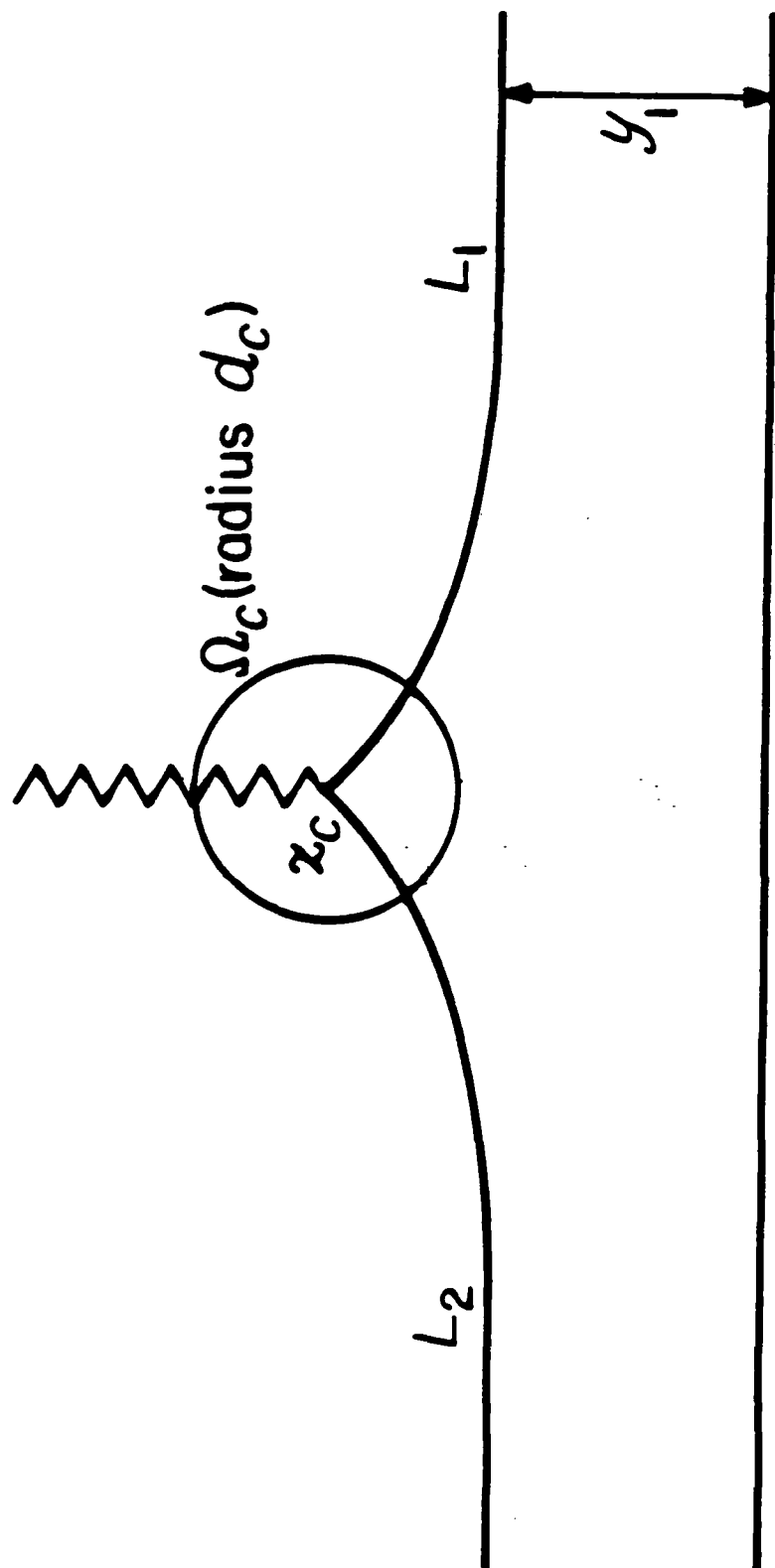


Fig.1

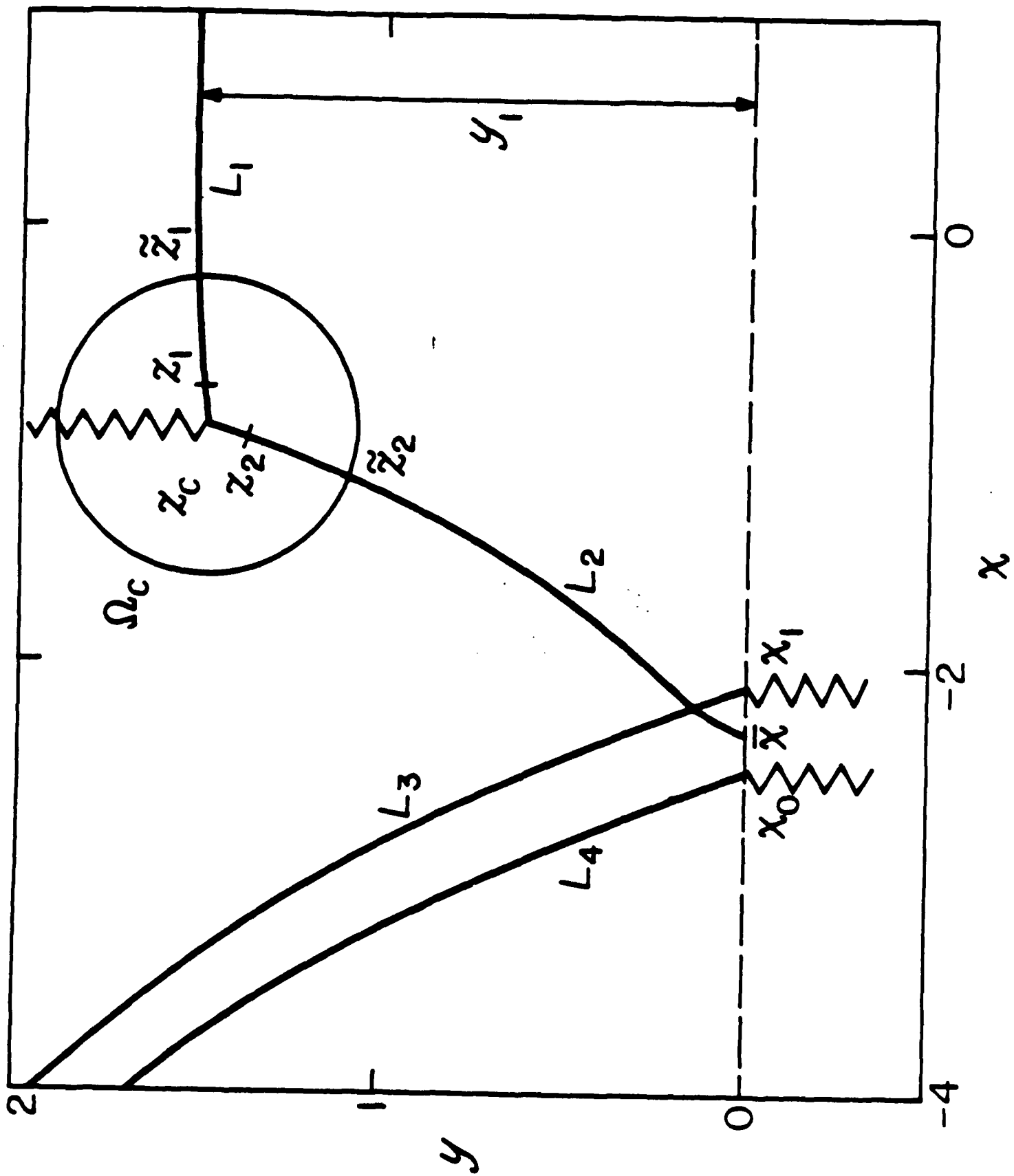


Fig. 2(a)

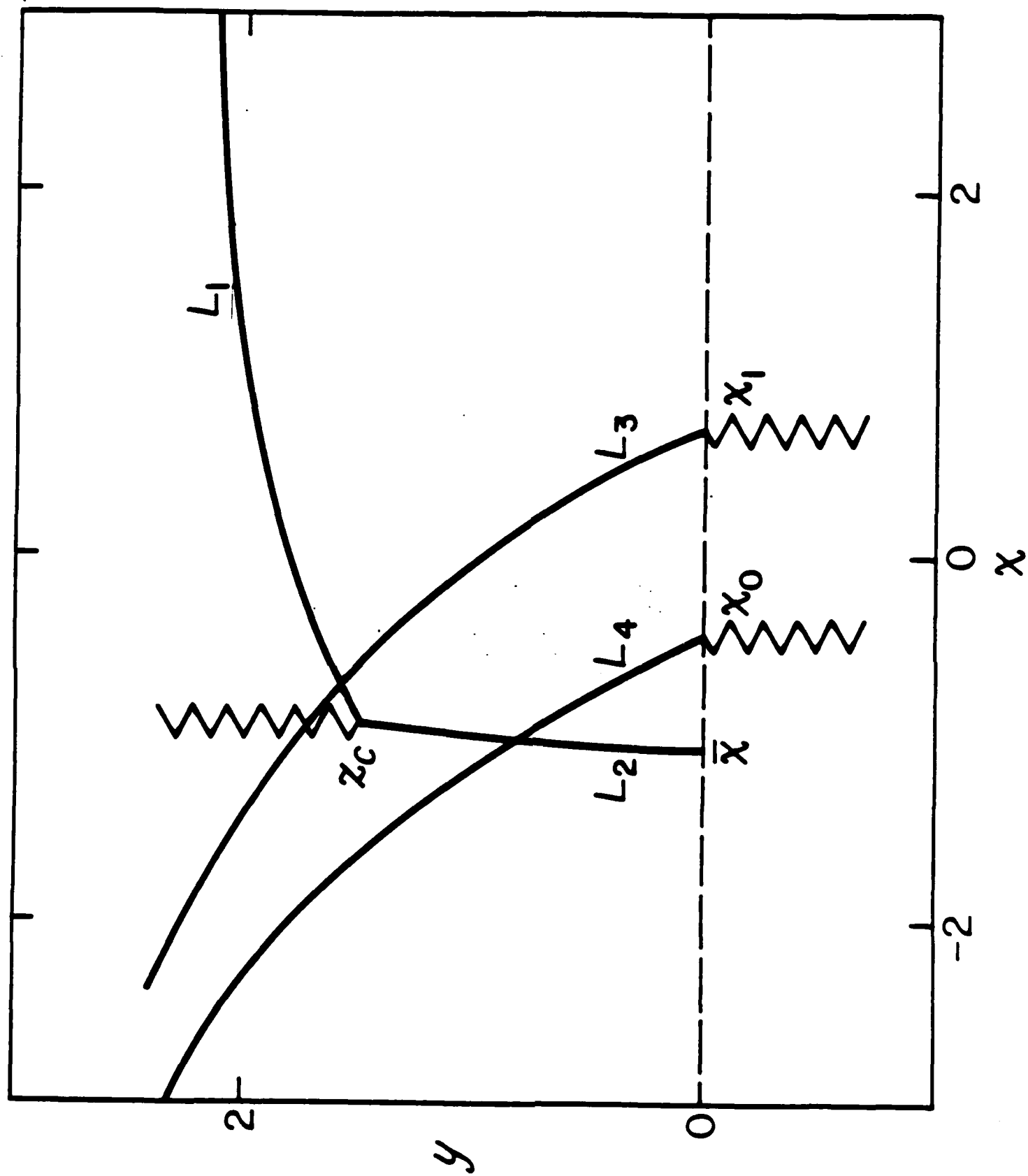


Fig 2(b)

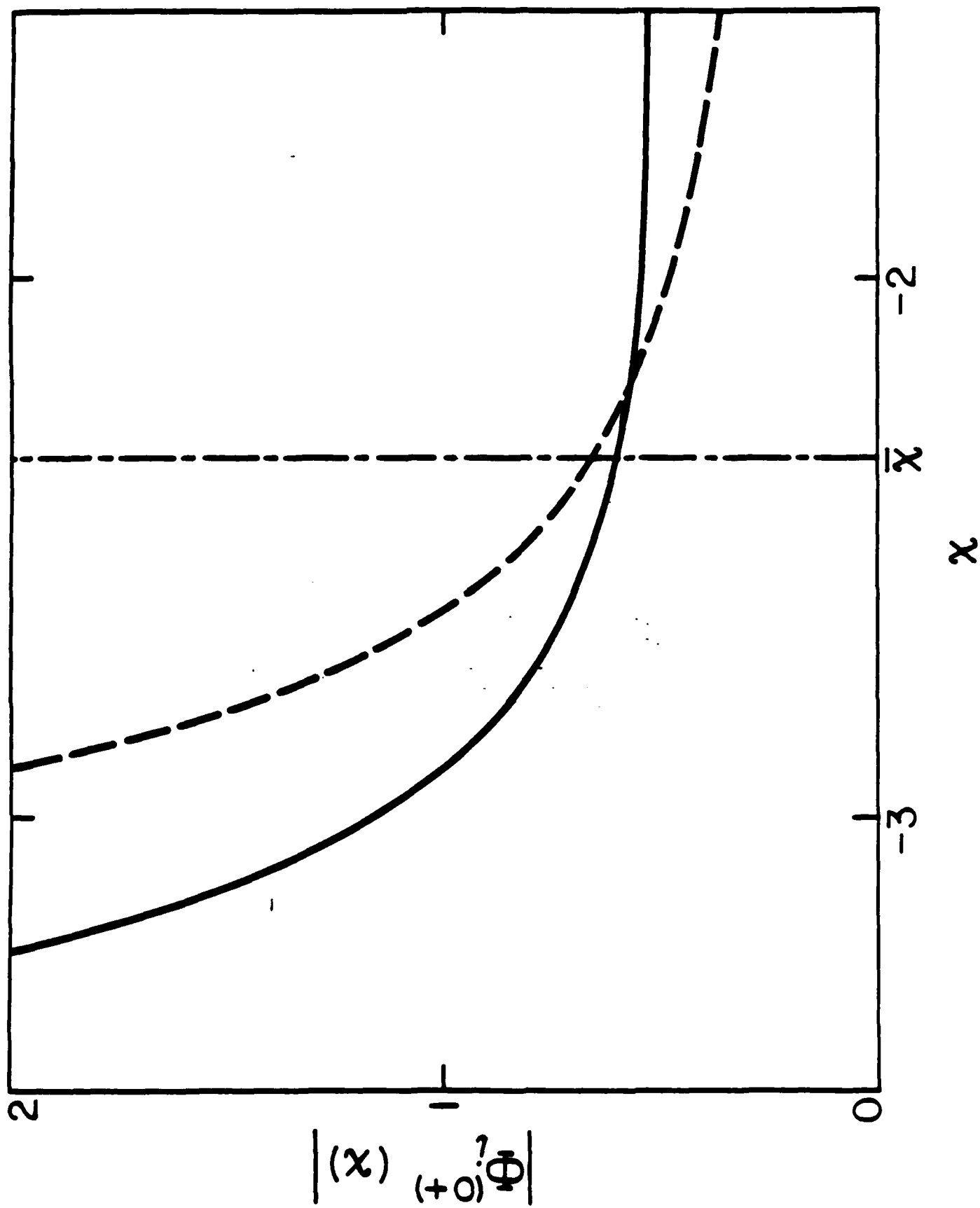


Fig. 3(a)

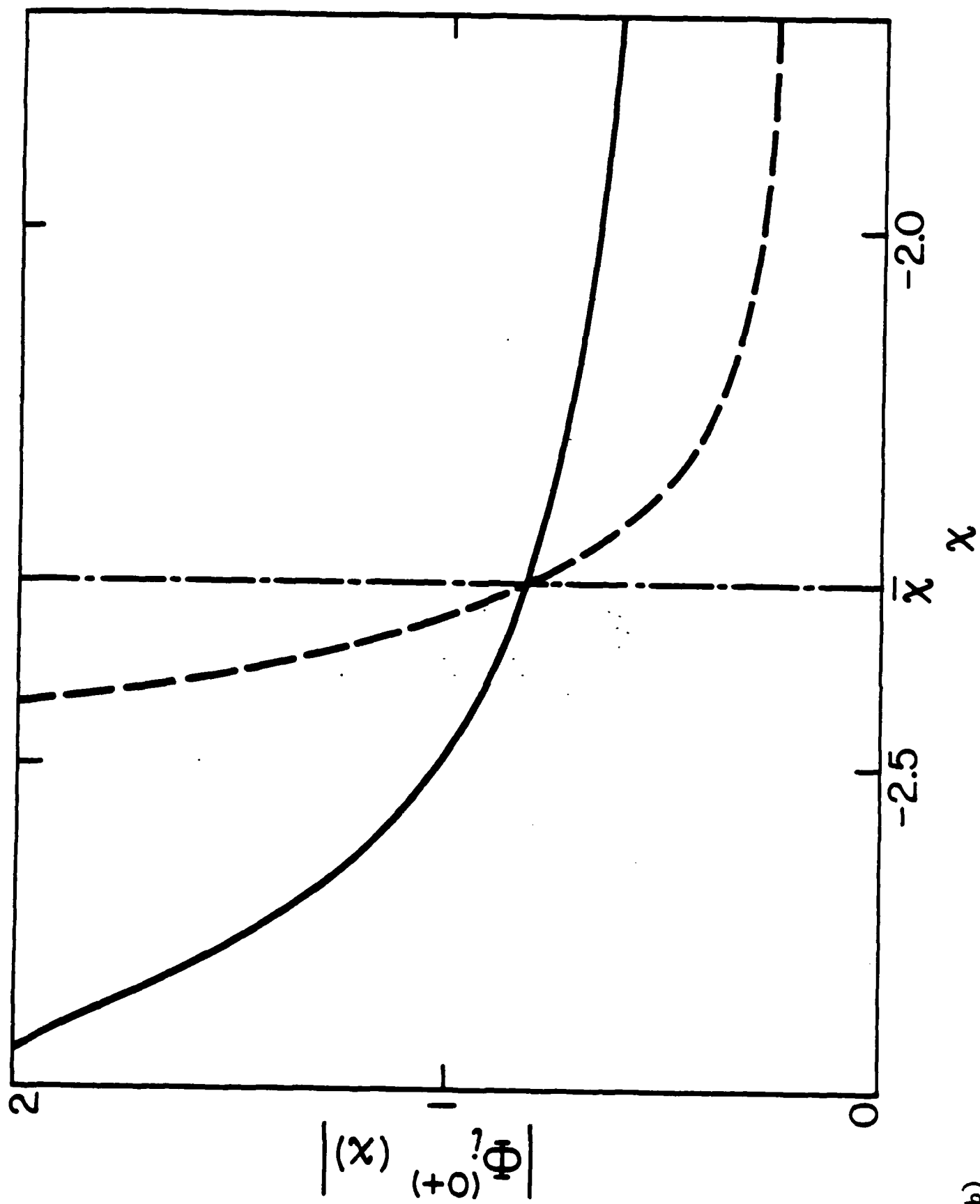


Fig. 3(b)

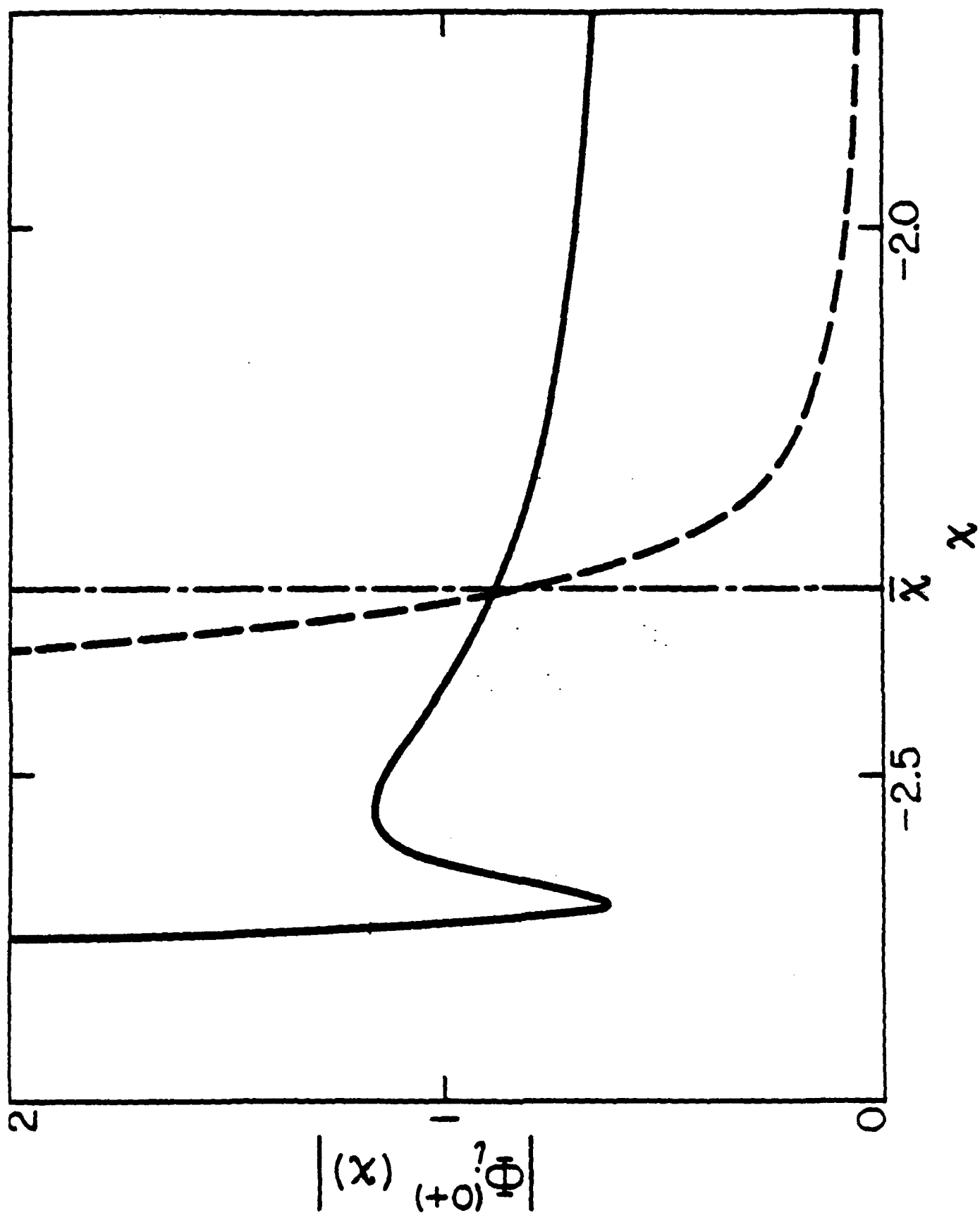


Fig. 3(c)

TABLE I

Case I.		S_{00}		S_{01}	
E	α	Exact	Semiclassical	Exact	Semiclassical
1	1	(.532, .808)	(.488, .873)	(.072, -.243)	(.130, -.323)
	5	(.552, -.834)	(.557, -.831)	(.308, .103) $\cdot 10^{-2}$	(.260, .092) $\cdot 10^{-2}$
	10	(-.924, .383)	(-.925, .380)	(-.166, -.132) $\cdot 10^{-4}$	(-.157, -.127) $\cdot 10^{-4}$
10	5	(.564, -.825)	(.343, -.939)	(.454, -.017) $\cdot 10^{-1}$	(.574, -.019) $\cdot 10^{-1}$
	10	(-.734, .678)	(-.644, .765)	(-.328, .022) $\cdot 10^{-1}$	(-.345, .022) $\cdot 10^{-1}$
	20	(-.993, .115)	(-.985, .171)	(-.608, .080) $\cdot 10^{-2}$	(-.613, .080) $\cdot 10^{-2}$

Case II.		S_{00}		S_{01}	
E	α	Exact	Semiclassical	Exact	Semiclassical
0.7	10	(.999, -.038)	(.999, -.038)	(.207, .042) $\cdot 10^{-1}$	(.165, .035) $\cdot 10^{-1}$
	20	(-.079, -.997)	(-.079, -.997)	(.258, .114) $\cdot 10^{-3}$	(.227, .102) $\cdot 10^{-3}$
	30	(-.993, .119)	(-.993, .118)	(.143, .104) $\cdot 10^{-5}$	(.126, .093) $\cdot 10^{-5}$
1.5	10	(.979, -.126)	(.739, -.674)	(-.103, -.120)	(-.258, -.305)
	20	(-.874, -.402)	(-.996, -.091)	(.045, -.269)	(.053, -.311)
	30	(.430, .887)	(.604, .797)	(.144, -.085)	(.147, -.087)

END

3-87

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