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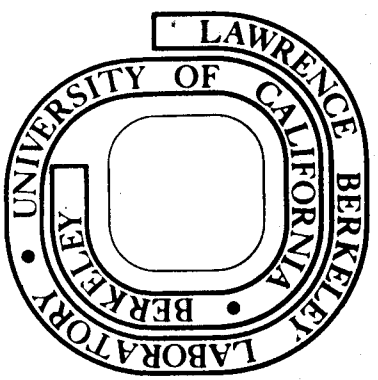

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QUANTUM MECHANICAL AND SEMICLASSICAL DESCRIPTION OF A TWO - DIMENSIONAL FISSION MODEL *

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Abstract

The penetration through a two dimensional fission barrier is investigated by a fully quantum mechanical coupled channel calculation and by a new semiclassical method. One finds a quantitative agreement.

In recent years much progress has been made in the determination of collective Hamiltonian describing the fission process[1,2]. One finds that in order to understand better the physics behind the fission process, one has to take into account more than one degree of freedom, and the inertial tensor seems to depend strongly on the coordinates. A fully quantum mechanical solution of this multidimensional barrier penetration problem is possible by the method of coupled channels. We discuss in the first part of this letter how to carry out such a calculation and apply it to a simple two dimensional model. However, for computational reasons such an approach may break down for realistic surfaces with several minima and saddles. Therefore one usually looks for approximations. The common approach is to make a one dimensional problem by introducing a suitable fission path[3]. The traditional choice of the path is along the bottom of the valley in the potential surface. The potential energy along the valley is taken as the potential energy of the one-dimensional problem; some suitable expression for the mass parameter, from the hydrodynamic or the cranking model, is taken, and the one dimensional WKB formula is applied. Starting with one dimensional wavefunctions of this type one can take into account the other degrees of freedom in a fully quantum mechanical way by some kind of DWBA approach if the coupling is not too strong[4]. For realistic cases with winding valleys and variable inertial tensor the Strutinsky-Pauli group[1] applied the one dimensional WKB formula for many paths, looking for the minimum action integral. In this two dimensional approach however, one still ignores the kinetic energy tied up in the motion orthogonal to the fission path.

Based on the formulation of quantum mechanics by path integrals given by Feynman [5] together with the correspondence principle, a unified semiclassical theory has been developed in the field of molecular reactions [6-9]. In the second part of this letter we will describe briefly this method and apply it to the same model for which the quantum mechanical calculation was done.

In the following we use a model for a collective Hamiltonian which depends on the fission coordinate x and a coordinate y perpendicular to that, which describes collective excitations along the fission path:

$$H = p_x^2/2m_x + p_y^2/2m_y + V_o \exp(-x^2/a^2) + \frac{1}{2} C (1 + \alpha \exp(-x^2/a^2)) y^2 \qquad (1)$$

The barrier in the x-direction has a simple Gaussian shape, and the potential in the y-direction is harmonic but with an x-dependent spring constant. This allows a coupling between the two degrees of freedom. The parameters are chosen so as to reproduce roughly a typical fission barrier: m_x=500 MeV^{-1}, m_y= 4.7 MeV^{-1}, V_o=7 MeV, a=0.185, C=5.1 MeV and α is variable. The coordinates x, y are dimensionless corresponding for instance to the deformation parameters ε_2 and ε_4; C and m_y are chosen in such a way, that the corresponding frequency is around 1 MeV.

The quantum mechanical description of the barrier penetration is given by the solution of the stationary Schrödinger equation:

$$H \Psi = E \Psi \tag{2}$$

with certain boundary conditions. This equation can be solved by a decomposition:

$$\psi^{(\mu)} = \sum_{\nu} u_{\mu\nu}(x)\ \phi_\nu(y) \tag{3}$$

where $\{\phi_\nu\}$ is the orthonormal set of eigenfunctions of the y dependent oscillator for $|x| \to \infty$. The index μ indicates the boundary condition; in the channel μ one has for $x \to -\infty$ an incoming wave, but in the other channels only outgoing waves. Multiplying eq.(2) from the left hand side with $\phi_\mu^*(y)$ and integrating over y yields a set of coupled channel equations for the functions $u_{\mu\nu}(x)$, which is solved numerically within the appropiate boundary conditions. From the amplitude of the outgoing waves for $|x| \to \infty$ one can deduce in the usual way the trasmission probabilities $P_{\mu\nu}$ for a transition from the incoming channel μ to the outgoing channel ν and corresponding reflection coefficients $R_{\mu\nu}$.

A first approximation for the diagonal transitions is the so-called adiabatic approximation. One assumes that during the fission process the system always stays in the same oscillator state μ. Then one carries out a one dimensional calculation, taking into account only the change of the oscillator energy. This gives a change of the available translational energy along the fission path.

Fig. 1 shows in its upper part the shape of the barrier together with the adiabatic translational energies for the channels n = 0,2,4 and their change along the fission path for a coupling constant $\alpha = 0.1$. This corresponds to a narrowing of the fission valley at the top of the barrier. The oscillator energy therefore increases and the coupling reduces the transition probabilities. Table I shows the diagonal transition probabilities for no coupling ($\alpha = 0$) and for a coupling $\alpha = 0.1$ for the exact quantum mechanical (QM) solution and for the adiabatic approximation (QM_{ad}). It turns out that in this case the adiabatic approximation is good.

For the ground state this diagonal transition is the most important one. However, for excited states this is no longer true. In this case the transition probabilities to the ground state are always higher by some orders of magnitude than the ones to excited states. The reason is that the system can penetrate more easily within the groundstate. The lower part of Fig. 1 shows the quantum mechanical probabilities $|u_{2\nu}(x)|^2$ for a barrier penetration starting from channel $\mu=2$. Within the inner region ($x<0$) we have, because of the high reflection probability in the $\mu=2$ channel, nearly a standing wave and in all the other channels outgoing waves. For $x>0$ we have only outgoing waves. the amplitude for $\nu=0$ however is larger than the one for $\nu=2$. That means it is much more probable for the system after the penetration to be found in the ground state than in the excited state. This feature does not depend very much on the value of the coupling constant α. As is shown in Fig.2 the diagonal transitions do not change very much. The same is true more or less also for transitions between different oscillator states. Only for very small values of α the transitions are reduced. For $\alpha=0$ they vanish obviously.

The coupled-channel code described above can take into account only a finite number of channels. It therefore is useful only for problems where one can get convergence after inclusion of a reasonable number of channels. Actually in the calculations described here we included the three open channels. A further closed channel changed the results only in the fourth significant figure. For realistic surfaces, in order to expand the wavefunction eq.(3), many more channels have to be included. This does not only involve more computer time, but also closed channels with higher energy require a special

handling. Therefore we carried out these calculationsonly for not too strong coupling in order to test the validity of the uniform semiclassical approximation (USCA), as discussed in the following section.

The underlying idea of this approach is that one uses an analytical continuation of the classical equations of motion for the description of the dynamics of the system together with quantized boundary conditions and the quantum mechanical superposition principle in adding amplitudes for different trajectories. The foundations of the USCA and many applications to molecular scattering and reaction problems have been given by Miller in great detail; (see refs. 6,7,8). Here we will therefore only give the results of the USCA as applied to our model.

We introduce in the asymptotic region, that is for $|x| \to \infty$, the action-angle variables (J,q) for the transverse collective degree of freedom. The action variable J is related by the correspondence principle to the "quantum number" n of the harmonic oscillator through $J = 2\pi\hbar(n+1/2)$ and the angle variable q to the phase ϕ of the oscillator through $q = \phi/2\pi$.

The semiclassical S-matrix describing a transition between two quantum states $n_\mu \to n_\nu$ is given by [6]:

$$S_{\nu\leftarrow\mu} = \sum \left(-2\pi i \, (\partial n_f(q_i)/\partial q_i)_{n_\mu} \right)^{-1/2} \exp(i\Phi(n_\nu, n_\mu)) \qquad (4)$$

where the phase Φ is the classical action integral:

$$\Phi(n_\nu, n_\mu) = -\frac{1}{\hbar}\int_{t_i}^{t_f} (x\dot{p}_x + y\dot{p}_y)\, dt \; - (Jq - \frac{1}{2} yp_y)\Big|_{t_i}^{t_f} \qquad (5)$$

The sum in eq.(4) goes over all possible classical paths which satisfy the appropriate boundary conditions, that is, correspond to trajectories which tunnel through the barrier and are such that $n(t_i \to -\infty) = n_\mu$ and $n(t_f \to \infty) = n_\nu$.

There are several differences between this USCA method and the two-dimensional method used by Pauli et. al.[1]. The main difference lies in the different boundary conditions used in the two methods. The way in which the boundary conditions are handled in the USCA method, allows one to calculate

penetrabilities from particular initial states (i.e. not only from the ground state but also from excited states) to particular final states. In the USCA one also takes the full dynamics of the problem along, that is the energy tied up in the motion perpendicular to the fission path is included.

One way to proceed in order to find the paths with the correct boundary conditions is the following: integrate the coupled classical Hamilton equations of motion starting from the left side at some distance $x=x_i$ (<0) outside of the interaction region, with the collective oscillation in the quantum state n_μ and with some arbitrary angle variable q_i. The integration is directed so that tunneling is achieved and continued until $x=x_f$ (>0) outside of the interaction region. The final "quantum number" n_f (usually not an integer) in which the transverse oscillatory degree of freedom is found is then a function of q_i . This way one finds the final quantum number function $n_f(q_i)$. The classical paths which satisfy the correct boundary conditions are then those satisfying the equation:

$$n_f(q_i) = n_\nu \tag{6}$$

The way to obtain a trajectory that tunnels is to follow a time path in the complex time plane around the appropiate branch points of the solution of the equations of motion.[7]. How one has to proceed is most easily seen on a simple one-dimensional example: the barrier penetration through a symmetrical Eckard potential barrier [9]. This problem can be solved analytically [9] and the main results are summarized in Fig.3. In the complex time plane the solution to this problem has pairs of branch points joined by cuts. If the time increments are kept real then the particle is reflected at the barrier; if a purely imaginary time increment is chosen when the particle has reached the barrier then the particle penetrates into the barrier. If one switches to real time increments when the particle has reached the other side of the barrier, then the particle continues moving to the right and tunneling has been achieved. In essentially the same way one has to proceed in our two-dimensional example.

It is noted, that in applying this semiclassical method one needs the analytical continuation of the equations of motion into the complex plane.

For this to be possible one has to have an analytical expression for the potential energy in the Hamiltonian.A potential consisting of piecewise analytical functions can not be continued analytically in a unique way into the complex plane and therefore the USCA can not be applied in this case. This however doesn't pose a major restriction to the method since any potential energy surface can be approximated,in the region of interest, in some way by an analytical function.

For our model problem we find that eq.(6) has always two solutions: that is, there are two values of q_i (usually complex) that satisfy $n_f(q_i)=n_\nu$. That one has complex initial and final phases should cause no problems, since these phases are not observable quantities. The quantities that are observables (for example, the initial and final quantum numbers n_μ and n_ν) are real in the asymptotic regions. In our calculations we have used for the coupling constant $\alpha=0.1$ and $\alpha=0.01$ which correspond to a weak coupling and therefore , as in the case of Coulomb excitation [10] and other cases studied [9] one has that for the off-diagonal transitions, only one of the two solutions of eq.(6) contributes to the S-matrix, (this may not necessarily be true for larger coupling constants). For the diagonal transition however both roots contribute. Since the quantum number function is very flat (due to the weak coupling) a uniform semiclassical expression for the S-matrix, based on Bessel functions is the appropiate one for this case [9,11]. We used here an expression slightly modified and generalized from the one given by Stine and Marcus[11].

Once the S-matrix is known, the transition probabilities $P_{\nu\leftarrow\mu}=|S_{\nu\leftarrow\mu}|^2$ follow directly. It is found (see Fig.2 and Table II) that there is a very good agreement between the USCA calculations and the exact quantum mechanical coupled channel calculations, even though the model here considered is highly nonclassical.

This very good agreement makes us confident that the semiclassical method may also be applied to more realistic cases with stronger coupling, where the numerical effort does not change very much and where a quantum mechanical calculation would be unfeasible.

Since to handle coordinate-dependent inertial parameters introduces

no additional difficulty, we hope that it will be a useful tool to investigate the full dynamics of the coupling between the fission coordinate and the other degrees of freedom such as hexadecupole deformations, mass asymmetries and change in pairing correlation [12].

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Table I. Comparison between the quantum mechanical (QM), adiabatic (QM_{ad}) and semiclassical (USCA) calculations of the diagonal penetrability $P_{\mu\mu}$. For $\alpha=0$ QM corresponds to QM_{ad} and USCA is the usual WKB formula.

	$\alpha = 0$		$\alpha = 0.1$		
	QM	USCA	QM	QM_{ad}	USCA
$0 \leftrightarrow 0$	$1.67\ 10^{-5}$	$1.60\ 10^{-5}$	$1.40\ 10^{-5}$	$1.40\ 10^{-5}$	$1.44\ 10^{-5}$
$2 \leftrightarrow 2$	$5.48\ 10^{-13}$	$5.21\ 10^{-13}$	$2.67\ 10^{-13}$	$2.42\ 10^{-13}$	$2.52\ 10^{-13}$
$4 \leftrightarrow 4$	$1.44\ 10^{-22}$	$1.34\ 10^{-22}$	$4.66\ 10^{-23}$	$3.62\ 10^{-23}$	

Table II. Comparison between the QM and USCA penetrabilties $P_{\mu\nu}$

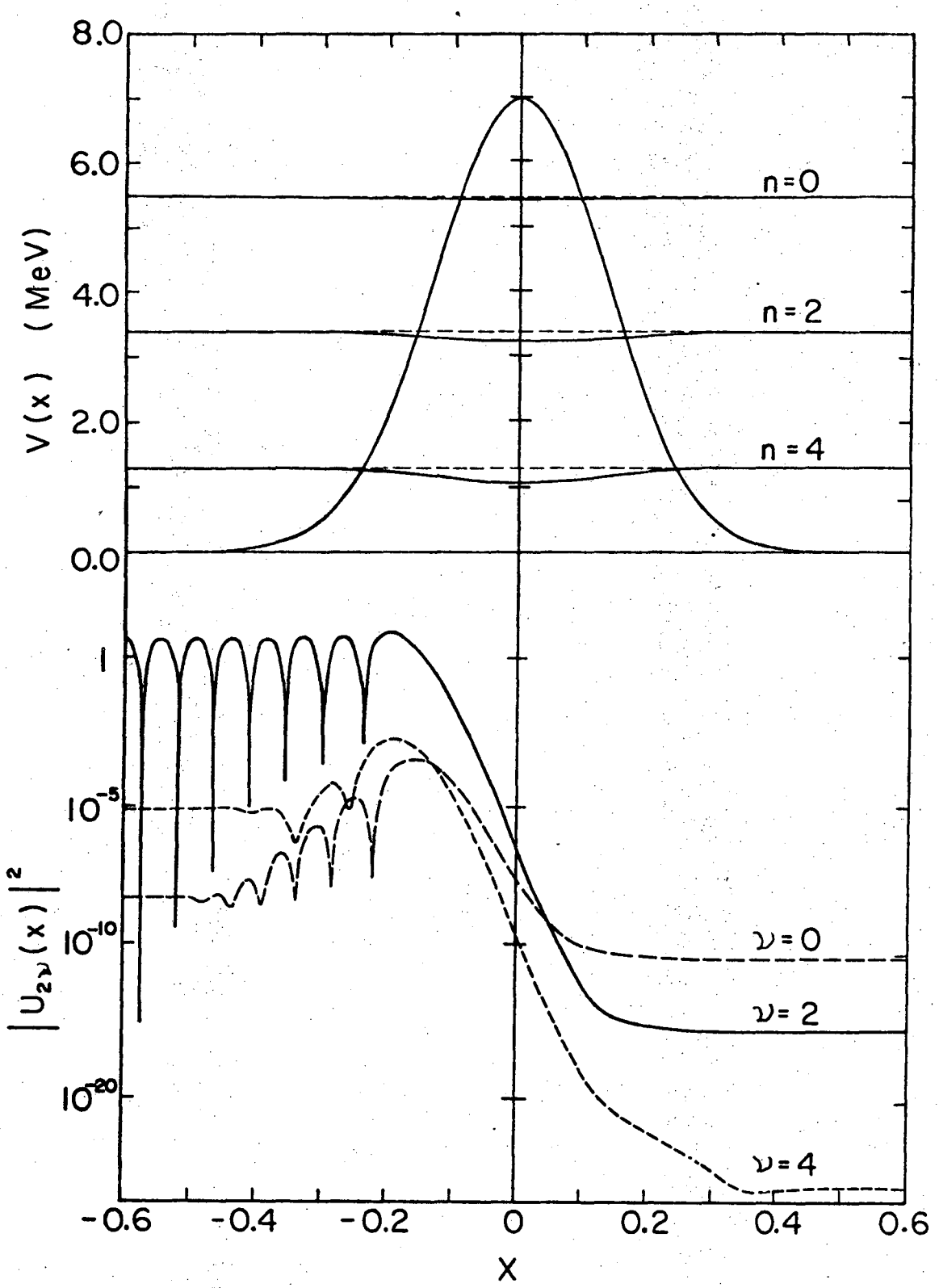
	$\alpha = 0.1$					$\alpha = 0.01$		
	$0 \leftrightarrow 0$	$0 \leftrightarrow 2$	$0 \leftrightarrow 4$	$2 \leftrightarrow 2$	$2 \leftrightarrow 4$	$0 \leftrightarrow 0$	$0 \leftrightarrow 2$	$0 \leftrightarrow 4$
QM	$1.40\ 10^{-5}$	$9.30\ 10^{-11}$	$1.03\ 10^{-16}$	$2.67\ 10^{-13}$	$9.86\ 10^{-19}$	$1.64\ 10^{-5}$	$1.22\ 10^{-12}$	$1.49\ 10^{-20}$
USCA	$1.44\ 10^{-5}$	$9.49\ 10^{-11}$	$0.97\ 10^{-16}$	$2.52\ 10^{-13}$	$9.15\ 10^{-19}$	$1.56\ 10^{-5}$	$1.30\ 10^{-12}$	$1.42\ 10^{-20}$

Figure Captions

Fig.1 Fission barrier and the square of the quantum mechanical channel functions $u_{2\nu}(x)$ for an incoming wave in the channel $\mu=2$.

Fig.2 Penetrabilities $P_{\mu\nu}$ for different values of the coupling constant α. The lines correspond to the QM coupled channel calculations (solid line for the diagonal and broken lines for the off-diagonal penetrabilities) and the dots correspond to the USCA calculations.

Fig.3 Diagram showing on the right hand side the different time paths one has to follow in order to obtain the trajectories shown on the left hand side. The crosses represent the branch points and the wiggly line corresponds to the cuts joining them.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6.0
4.0
2.0
0.0
V(x) (MeV)
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n=2
n=4
1
10^{-5}
10^{-10}
10^{-20}
$|U_{2\nu}(x)|^2$
$\nu=0$
$\nu=2$
$\nu=4$
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-0.4
-0.2
0
0.2
0.4
0.6
X
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Fig. 1

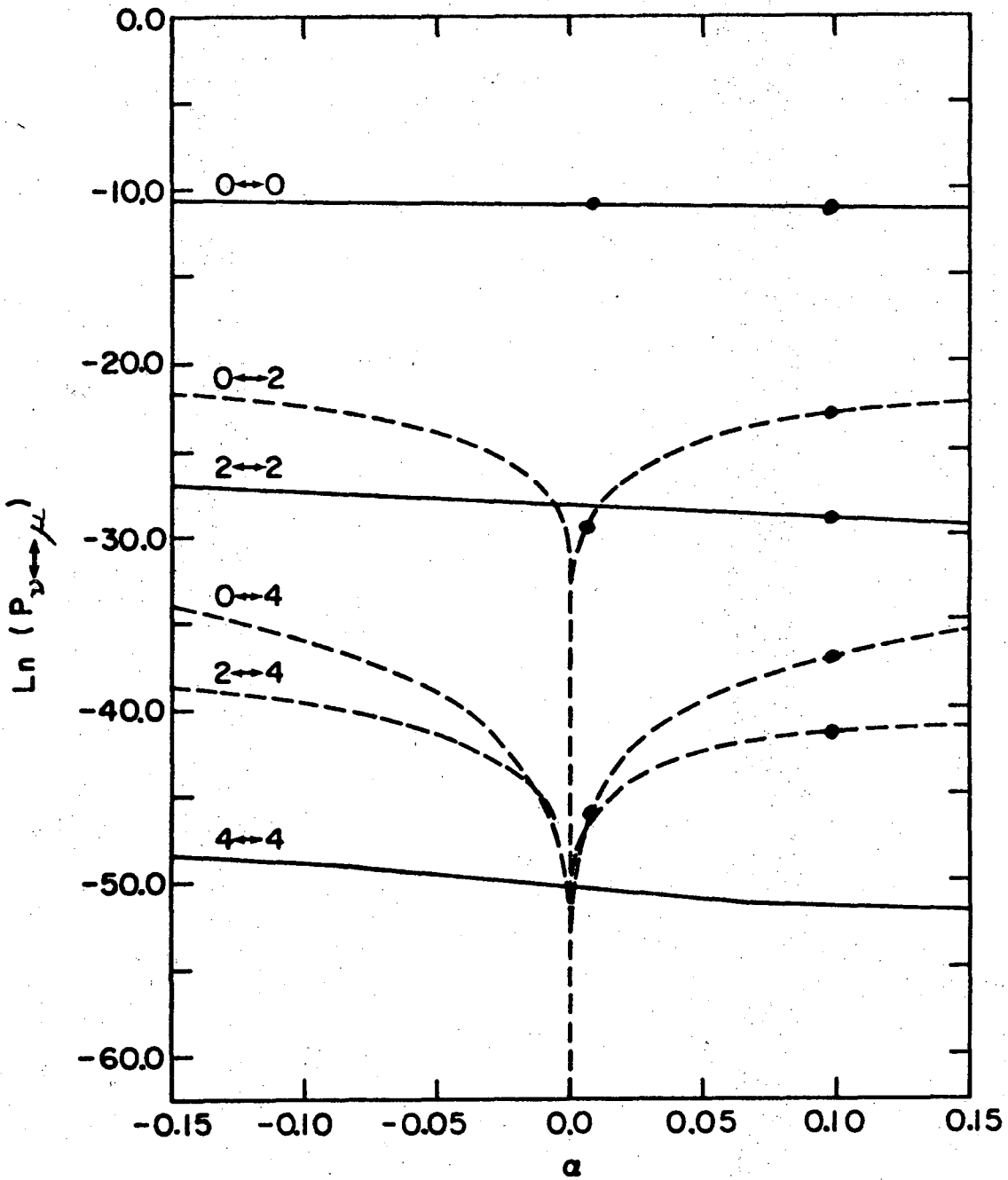

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Fig. 2

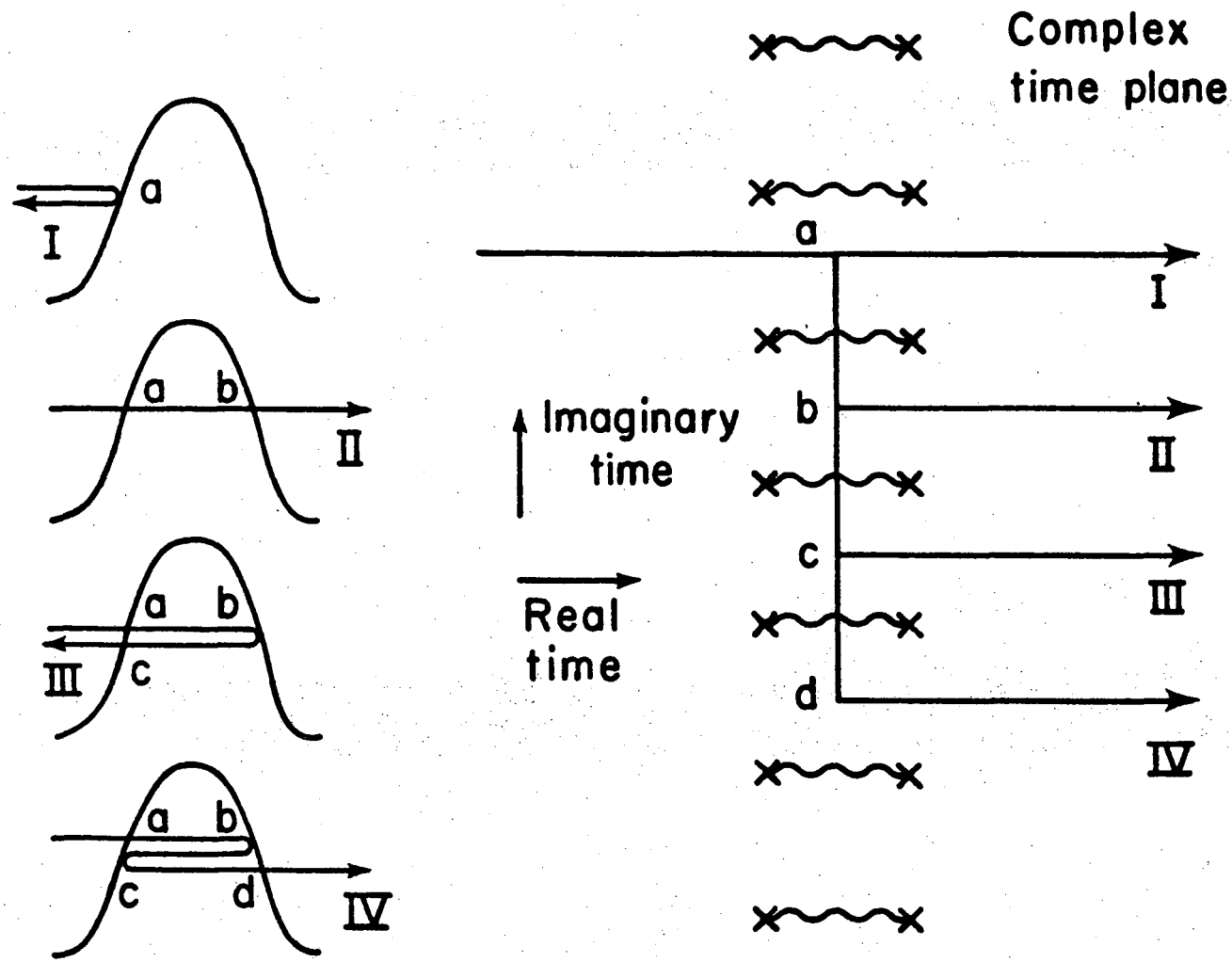

Fig. 3

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