

## Polychronic Tunneling

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N. Oshita, YS, M. Yamaguchi, PRD 107 (2023) 4

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## Mixed tunneling

## Mixed tunneling phenomena

This has been discussed from 1970's

the journal of chemical physics $\qquad$
Classical $S$ Matrix: Numerical Application to Inelastic Collisions

## Wiluam H. Miller*

norganic Materials Research Divisions, Lawrence Radiation Laboratory and The Department of Chemistry, University of Califormia Berkeley, California 94720 (Received 26 June 1970)

A previously developed semiclassical theory of molecular collisions based on exact classical mechanic is applied to the linear atom-diatom collision (vibrational excitation). Classical, semiclassical, and unifor emiclassical results for individual vibrational transition probabilities corresponding to the $\mathrm{H}_{2}+$ He syste are presented and compared to the exact quantum mechanical results of Secrest and Johnson. hee purely
classical results (the classical limit of the exact quantum mechanical transition probability) are seen to be accurate only in an average sense; ste semiclassical and uniform semiclassical results, which contain inter-
ference effects omitted by the classical treatent, are in excellent arrement (within a few percent ) ference effects omitted by the classical treatment, are in excellent agreement (within a few percent) wit
the exact quantum transition probabilities. An integral representation for the $S$-matrix elements is als developed which, although it involves only classical quantitities, appears to have a region of validity beyon that of the semiclassical or uniform semiclassical expressions themselves. The general conclusion seems
to be that the dynamics of these inelastic collisions is basically classical, with all quantum mechanical to be that the dynamich of these inelastic coilisions
structure being of a rather simple interference nature.

## There are a few known techniques

Complex trajectories
No first principle derivation
Adiabatic approximation
Only for adiabatic, diabatic or weak-coupling cases
Tunneling time itself has been a controversial issue of QM
Huygens principle
Construction of wave fronts, computationally very hard

## Separable problem



## Hamiltonian

There are $(2 N+1)$ independent particles

$$
H=\sum_{a=-N}^{N} \frac{p_{a}^{2}}{2 m}+\delta_{a 0} V\left(x^{a}\right), \quad V(x)= \begin{cases}V_{0} & 0<x<1 \\ 0 & \text { otherwise }\end{cases}
$$

Initial kinetic energy
All particles have the same energy

$$
\mathcal{E}<V_{0}
$$

What is expected?
Only a=0 particle tunnels with probability

$$
P=\frac{\left|\psi\left(s_{f}\right)\right|^{2}}{\left|\psi\left(s_{i}\right)\right|^{2}} \simeq \exp \left[-\frac{2}{\hbar} \int_{0}^{1} \mathrm{~d} x \sqrt{2 m\left(V_{0}-\mathcal{E}\right)}\right]
$$

## The wrong calculation

## Standard way of solving the Hamilton-Jacobi equation


$a=-1$


Shroedinger equation

$$
\hat{H} \psi=E \psi . \quad E=(2 N+1) \mathcal{E}
$$

WKB approximation
§ Semi-classical expansion

$$
\psi=\exp \left[\frac{i}{\hbar} \Theta^{(0)}+\Theta^{(1)}+\ldots\right]
$$

2 Oth-order WKB equation

$$
\frac{1}{2 m} \sum_{a}\left(\frac{\partial \Theta^{(0)}}{\partial x^{a}}\right)^{2}=E-V\left(x^{0}\right) .
$$

3 Solution of the Hamilton-Jacobi equation (method of characteristics)

$$
\Theta^{(0)}\left(\left\{x^{a}\left(s_{f}\right)\right\}\right)-\Theta^{(0)}\left(\left\{x^{a}\left(s_{i}\right)\right\}\right)=\int_{s_{i}}^{s_{f}} \mathrm{~d} s \sqrt{2 m\left(E-V\left(x^{0}\right)\right)} \sqrt{\sum_{a}\left(\frac{\mathrm{~d} x^{a}}{\mathrm{~d} s}\right)^{2}}
$$

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$$

No tunneling if $V_{0}<E$ ???

## What was wrong?

## Shroedinger equation for each particle

$$
\hat{\mathcal{H}}_{a} \psi=0, \quad \mathcal{H}_{a}=\frac{p_{a}^{2}}{2 m}+\delta_{a 0} V\left(x^{a}\right)-\mathcal{E}
$$

## WKB approximation

Execute the WKB approximation for each particle

$$
\begin{gathered}
\Theta^{(0)}\left(\left\{x^{a}\left(s_{f}\right)\right\}\right)-\Theta^{(0)}\left(\left\{x^{a}\left(s_{i}\right)\right\}\right)=\sum_{a=-N}^{N} \int_{s_{i}}^{s_{f}} \mathrm{~d} s \sqrt{2 m\left(\mathcal{E}-\delta_{a 0} V\left(x^{a}\right)\right)} \sqrt{\left(\frac{\mathrm{d} x^{a}}{\mathrm{~d} s}\right)^{2}} \\
\text { Correct result! } \\
P=\frac{\left|\psi\left(s_{f}\right)\right|^{2}}{\left|\psi\left(s_{i}\right)\right|^{2}} \simeq \exp \left[-\frac{2}{\hbar} \int_{0}^{1} \mathrm{~d} x \sqrt{2 m\left(V_{0}-\mathcal{E}\right)}\right]
\end{gathered}
$$

## What was wrong?

2 Oth-order WKB equation

$$
\frac{1}{2 m} \sum_{a}\left(\frac{\partial \Theta^{(0)}}{\partial x^{a}}\right)^{2}=E-V\left(x^{0}\right)
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$$

Coupled Anharmonic Oscillators. I. Equal-Mass Case

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$$
\text { Tai Tsun } \mathrm{Wu}^{\ddagger}
$$

Gordon McKay Laboratory, Harvard University, Cambridge, Massachusetts 02138 (Received 7 May 1973)
equation for the phase $S$ of a wave function with energy $E$ is ${ }^{15}$

$$
\begin{equation*}
(\vec{\nabla} S)^{2}=V-E . \tag{3.1}
\end{equation*}
$$

This is just the Hamilton-Jacobi equation for a classical system with Hamiltonian $\overrightarrow{\mathrm{p}}^{2}+V$. In one dimension it reduces to $(d S / d x)^{2}=V-E$, whose solution is $S= \pm \int(V-E)^{1 / 2}$. For the general multidimensional case it is a nonlinear partial differential equation. Of course, if the Hamiltonian has a continuous symmetry, Eq. (3.1) will be separable. However, Eq. (3.1) is nontrivial in general. The new multidimensional techniques which we have discovered simplify the problem of solving Eq. (3.1) because now we need to solve it only in a small, approximately one-dimensional region. Our technique is expressly designed to deal with problems which do not have continuous symmetries, and is thus complementary to the separation of variables idea.

## What was wrong?

## Shroedinger equation for each particle

$$
\hat{\mathcal{H}}_{a} \psi=0, \quad \mathcal{H}_{a}=\frac{p_{a}^{2}}{2 m}+\delta_{a 0} V\left(x^{a}\right)-\mathcal{E}
$$

## WKB approximation

Execute the WKB approximation for each particle



Mixed tunneling

What was wrong?
2 Oth-order WKB equation

$$
\frac{1}{2 m} \sum_{a}\left(\frac{\partial \Theta^{(0)}}{\partial x^{a}}\right)^{2}=E-V\left(x^{0}\right) .
$$

3 Solution of the Hamilton-Jacobi equation (method of characteristics)

$$
\left.\Theta^{(0)}\left(\left\{x^{a}(s)\right\}\right)\right\}-\Theta^{(0)}\left(\left\{x^{a}\left(s_{s}\right)\right\}\right)=\int_{s i s}^{s i s} d \sqrt{2 m\left(E-V\left(x^{0}\right)\right)} \sqrt{\sum_{a}\left(\frac{d d^{a}}{d s}\right)^{2}} .
$$

## What was wrong?

## Shroedinger equation for each particle

$$
\hat{\mathcal{H}}_{a} \psi=0, \quad \mathcal{H}_{a}=\frac{p_{a}^{2}}{2 m}+\delta_{a 0} V\left(x^{a}\right)-\mathcal{E} . \quad \text { Local energy conservation law }
$$

## WKB approximation

Execute the WKB approximation for each particle



What was wrong?
2 Oth-order WKB equation

$$
\frac{1}{2 m} \sum_{a}\left(\frac{\partial \Theta^{(0)}}{\partial x^{a}}\right)^{2}=E-V\left(x^{0}\right) .
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$$

## Path integral

## Constructed from the local energy conservation law

$$
\begin{aligned}
& \text { Path integral formula } \\
& \int \mathcal{D} X \delta_{\eta} \exp \left[\frac{i}{\hbar} \sum_{a=-N}^{N} \int_{s_{1}}^{s_{n}} \mathrm{~d} s 2 \sqrt{\mathcal{K}^{a}(s)} \sqrt{-\mathcal{V}^{a}(s)}\right] \\
& \text { Here, 22] } \\
& \qquad \mathcal{K}^{a}=\frac{m}{2}\left(\frac{\mathrm{~d} x^{a}}{\mathrm{~d} s}\right)^{2}, \\
& \qquad \mathcal{V}^{a}=\delta_{a 0} V\left(x^{a}\right)+\frac{w}{2} \frac{\left(x^{a}-x^{a+1}\right)^{2}+\left(x^{a}-x^{a-1}\right)^{2}}{2}-\eta^{a}+\eta^{a-1} . \\
& \text { With eta satisfying } \\
& \qquad \frac{\mathrm{d} \eta^{a}(s)}{\mathrm{d} s}=\frac{w}{2}\left(x^{a+1}(s)-x^{a}(s)\right)\left(\frac{\mathrm{d} x^{a+1}(s)}{\mathrm{d} s}+\frac{\mathrm{d} x^{a}(s)}{\mathrm{d} s}\right)
\end{aligned}
$$

## Path integral

## Constructed from the local energy conservation law

Path integral formula [YS; 22]
$\int \mathcal{D} X \delta_{\eta} \exp \left[\frac{i}{\hbar} \sum_{a=-N}^{N} \int_{s_{1}}^{s_{n}} \mathrm{~d} s 2 \sqrt{\mathcal{K}^{a}(s)} \sqrt{-\mathcal{V}^{a}(s)}\right]$
Here,

$$
\begin{aligned}
\mathcal{K}^{a} & =\frac{m}{2}\left(\frac{\mathrm{~d} x^{a}}{\mathrm{~d} s}\right)^{2} \\
\mathcal{V}^{a} & =\delta_{a 0} V\left(x^{a}\right)+\frac{w}{2} \frac{\left(x^{a}-x^{a+1}\right)^{2}+\left(x^{a}-x^{a-1}\right)^{2}}{2}-\eta^{a}+\eta^{a-1}
\end{aligned}
$$

With eta satisfying

$$
\frac{\mathrm{d} \eta^{a}(s)}{\mathrm{d} s}=\frac{w}{2}\left(x^{a+1}(s)-x^{a}(s)\right)\left(\frac{\mathrm{d} x^{a+1}(s)}{\mathrm{d} s}+\frac{\mathrm{d} x^{a}(s)}{\mathrm{d} s}\right)
$$

## Lorentzian path integral



$$
=\int \mathcal{D} X \exp \left[i \int_{s_{1}}^{s_{n}} \mathrm{~d} s L\left(\left\{x^{a}\right\},\left\{\dot{x}^{a}\right\}\right)\right]
$$

Euclidean path integral

$$
=\int \mathcal{D} X \exp \left[-\int_{s_{1}}^{s_{n}} \mathrm{~d} s L_{E}\left(\left\{x^{a}\right\},\left\{\dot{x}^{a}\right\}\right)\right]
$$

## Separable example

$$
\sum_{a=-N}^{N} \int_{s_{i}}^{s_{f}} \mathrm{~d} s \sqrt{2 m\left(\mathcal{E}-\delta_{a 0} V\left(x^{a}\right)\right)} \sqrt{\left(\frac{\mathrm{d} x^{a}}{\mathrm{~d} s}\right)^{2}}
$$

## Polychronic tunneling ~ new tunneling process in QFT ~

## One-dimensional chain explanation CDL tunneling



## One-dimensional chain explanation

## Polychronic tunneling

Potential is higher due to springs


Euclidean evolution

Potential is lower due to springs


Lorentzian evolution


Repetition in infinitesimal time

Complex exponent

## Numerical analysis

## Setup

## Potential

$$
V(\phi)=\frac{\phi^{4}}{4}-\frac{k+1}{3} \phi^{3}+\frac{k}{2} \phi^{2}+V_{0}
$$

SO(3) x R Ansatz


$$
\begin{aligned}
\phi & =\phi(s, r) \\
h_{i j} \mathrm{~d} x^{i} \mathrm{~d} x^{j} & =e^{\eta(s, r)} \mathrm{d} r^{2}+r^{2}\left(\mathrm{~d} \theta^{2}+\sin ^{2} \theta \mathrm{~d} \phi^{2}\right),
\end{aligned}
$$

## False vacuum

$$
\begin{aligned}
& \phi(0, r)=\phi_{\mathrm{F}}, \\
& \eta(0, r)=-\ln \left(1-\frac{\kappa r^{2}}{3} V\left(\phi_{\mathrm{F}}\right)\right) .
\end{aligned}
$$

=> Search for a complex saddle point

## Numerical analysis

## CDL vs PT

[N. Oshita, YS, M. Yamaguchi, '23]
$\left(\kappa, k, V_{0}\right)=(0.5,0.3,0)$


## Numerical analysis <br> CDL vs PT

[N. Oshita, YS, M. Yamaguchi, '23]



## Numerical analysis <br> CDL vs PT

[N. Oshita, YS, M. Yamaguchi, '23]


## Summary

- Quantum tunneling in a many-body system is much more non-trivial than that in a one-body system and the conventional technique sometimes fails to give the correct results
- Mixed tunneling is a tunneling process that has a complex exponent, and has been discussed and observed in quantum many-body systems
- We have formulated path integral that can be used for the mixed/polychronic tunneling
- Extending it to QFT, we have found faster tunneling processes than the CDL one

