

# Imaginary-time-dependent mean-field method for many-body tunneling

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# The problem

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$$i\frac{\partial}{\partial t}|\Psi\rangle = \hat{\mathcal{H}}|\Psi\rangle$$

$|\Psi\rangle$  is a complete many-fermion state, and the Hamiltonian takes into account all n-body interactions.

# TDHF

What we can solve is the time-dependent Hartree-Fock equation:

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Unfortunately it doesn't work for below-barrier dynamics.

# What we don't want

- A path of sub-barrier states constructed from above-barrier configurations
- A different framework for calculating evolution inside and outside the barrier
- A separate method for obtaining tunneling transmission probabilities
- A method that relies on knowledge of the tunneled state
- A method that can only be used for fusion/fission

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- If we add imaginary time paths to a semi-classical approximation i.e. TDHF, we may hope to recover TDHF that tunnels.
- Feynman path integrals further justify this more rigorously. See e.g. Levit et al. [1980], Negele [1989]

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We search for periodic solutions starting (and ending) at the initial state, where the tunneled state is partway through the evolution. This follows the same approach as e.g. *Nuclear fission with mean-field instantons* (Skalski [2008]), *Instanton - motivated study of spontaneous fission of odd-A nuclei* (Brodzinski and Skalski [2020])

# Transmission probability

We get out the transmission probability "for free" from the total reduced action of the path:

$$\Psi(\tau_f) = \exp\left(-\int_0^{\tau_f} \mathcal{H}(\tau) d\tau\right) \Psi(0)$$

It's a bit more complicated because we have to consider repeated paths. One half-cycle has integral  $W_1$ , and a full cycle has integrand  $W_2$  so the actual transmission amplitude is

$$T = \exp(-W_1) * \sum_{n=0}^{\infty} \exp(-nW_2) = \frac{\exp(-W_1)}{1 - \exp(-W_2)}$$

# Imaginary time extension to mean field

## Imaginary Time Mean-Field Method for Collective Tunneling

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(Dated: December 3, 2020)

**Background:** Quantum tunneling in many-body systems is the subject of many experimental and theoretical studies in fields ranging from cold atoms to nuclear physics. However, theoretical description of quantum tunneling with strongly interacting particles, such as nucleons in atomic nuclei, remains a major challenge in quantum physics.

**Purpose:** An initial-value approach to tunneling accounting for the degrees of freedom of each interacting particle is highly desirable.

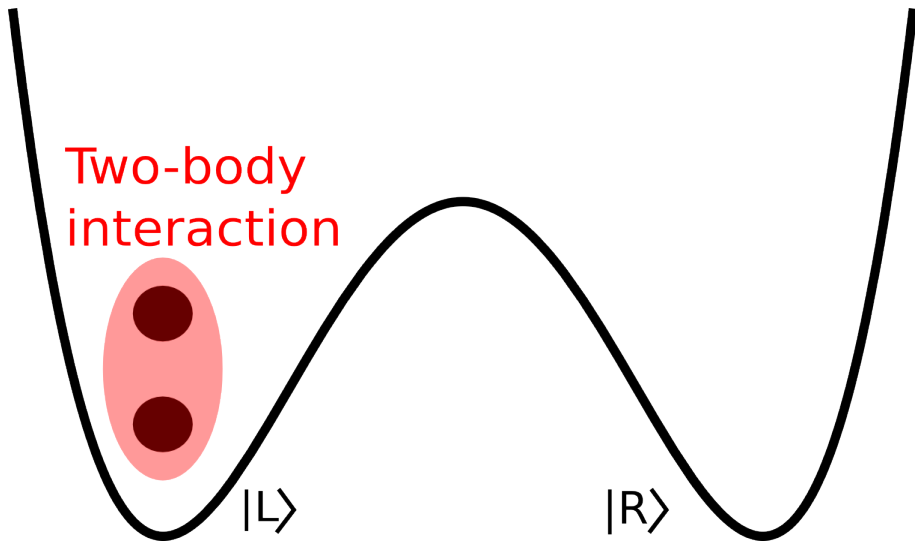
**Methods:** Inspired by existing methods to describe instantons with periodic solutions in imaginary time, we investigate the possibility to use an initial value approach to describe tunneling at the mean-field level. Real-time and imaginary-time Hartree dynamics are compared to the exact solution in the case of two particles in a two-well potential.

**Results:** Whereas real-time evolutions exhibit a spurious self-trapping effect preventing tunneling in strongly interacting systems, the imaginary-time-dependent mean-field method predicts tunneling rates in excellent agreement with the exact solution.

**Conclusions:** Being an initial-value method, it could be more suitable than approaches requiring periodic solutions to describe realistic systems such as heavy-ion fusion.

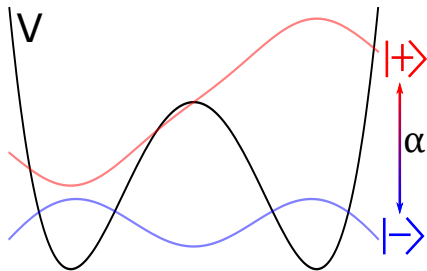
McGlynn and Simenel [2020]

# Simple model





# Two state model



With states defined by

$$|+\rangle = \frac{1}{\sqrt{2}}(|L\rangle - |R\rangle)$$

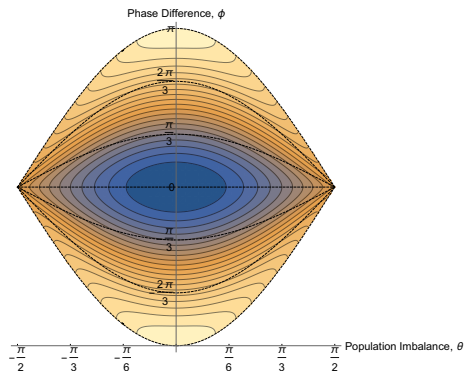
$$|-\rangle = \frac{1}{\sqrt{2}}(|L\rangle + |R\rangle)$$

Interaction is entirely local, i.e.

$$\hat{h}_{MF}[\{\psi_i\}] = \hat{h}_0 + \mu \sum_i (\langle \psi_i | L \rangle \langle L | \psi_i \rangle |L\rangle \langle L| + \langle \psi_i | R \rangle \langle R | \psi_i \rangle |R\rangle \langle R|)$$

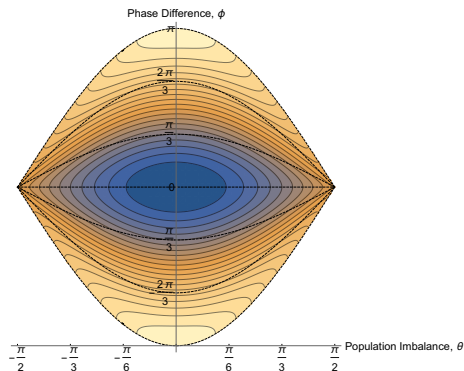
Sufficiently simple to solve exactly, which allows for comparison with imaginary time mean field technique.

# Contours in real time

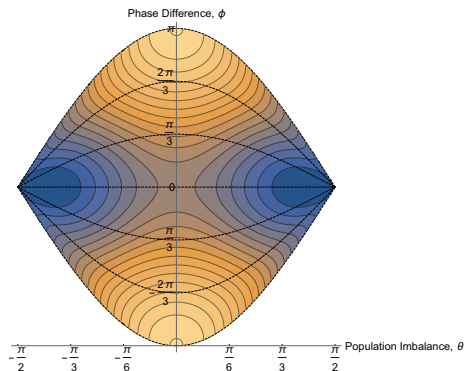


Contours for  $\mu = 0$

# Contours in real time

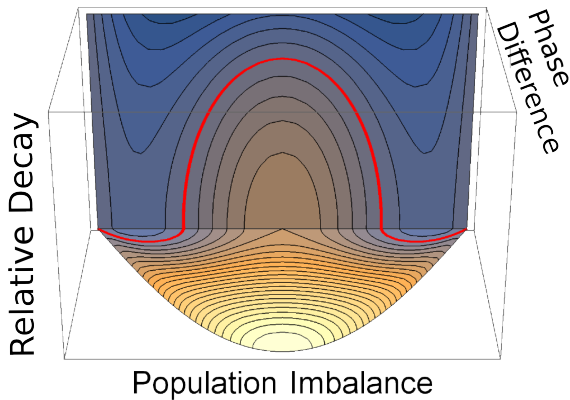


Contours for  $\mu = 0$



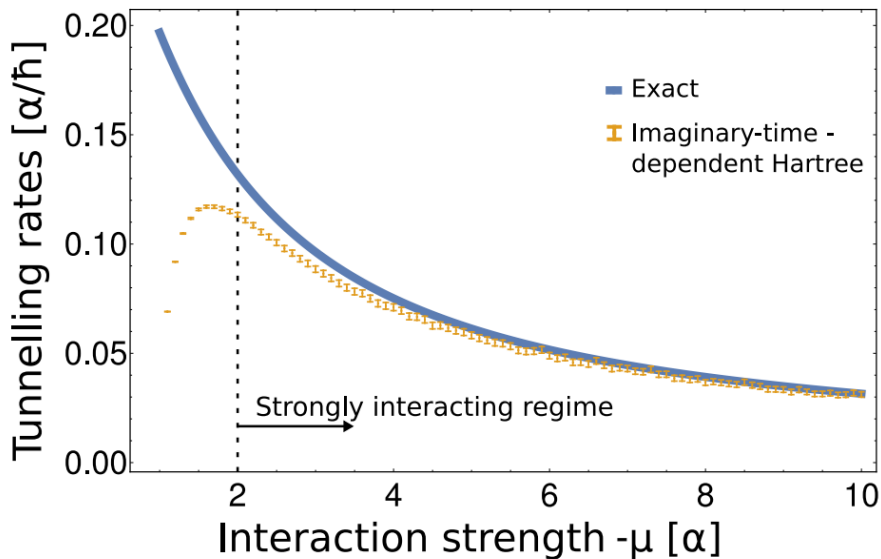
Contours for  $\mu = -4$

# Contours in imaginary time



Imaginary time contours for  $\mu = -4$

# Simple solution



# Extension

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## Approach

Take the continuous version of the toy problem and approximate it with many grid points, taking care to set parameters to match those in the two-state problem. Then we can identify what is different and why it breaks down.



# Equation of motion

$$\frac{\partial \Psi(x)}{\partial \tau} = \frac{1}{2} \frac{\partial^2}{\partial x^2} \Psi(x) - V(x) \Psi(x) - \mu U[\Psi(x)]$$

$$V(x) = \omega(x - d/2)^2(x + d/2)^2,$$

where  $\omega$  is chosen to fix the difference between the first and second energy eigenstates. Finding the eigenstates of that potential, we then define  $|L\rangle, |R\rangle$  as before.  $U[\Psi(x)]$  is calculated in the position vector basis, as the matrix representation of  $|L\rangle \langle L| \langle \Psi|L\rangle \langle L|\Psi\rangle + |R\rangle \langle R| \langle \Psi|R\rangle \langle R|\Psi\rangle$  to correlate with the local interaction in the two-state model.

# Conjugates and stiffness

As mentioned, the conjugate state  $\langle \Psi(\tau) | \neq |\Psi(\tau)\rangle^\dagger$  as it does in real time, instead  $\langle \Psi(\tau) | = |\Psi(-\tau)\rangle^\dagger$ . This is crucial for ensuring the norm remains constant, but it causes a huge problem.

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$$\partial_\tau \Psi = h[\rho] \Psi$$

$$\partial_\tau \tilde{\Psi} = -h[\rho] \tilde{\Psi}$$

## Stiffness

Stiffness is a poorly defined (Press et al. [1987]) attribute of some PDEs which makes them very resistant to numerical solutions. In this case, the equations appear to be stiff because the forward and backward evolving wavefunctions are exponentially growing and decaying respectively.

# Naïve attempts to resolve

- Improving discrete derivatives (time and space).
- Employing implicit PDE solving techniques.

All unsuccessful so far, numerical problems still arise as number of points in space grid increases (or number of energy eigenstates increases).

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- Identifying the form of the PDE and applying existing solution techniques.

# Floquet equations

If we have a linear differential equation of the form

$$x'(t) = Q(t)x(t)$$

where  $Q(t + T) = Q(t)$  for some period  $T$ , then the solution will take the form

$$x(t) = e^{gt} f(t)$$

where  $f(t + T) = f(t)$  and  $g$  is a constant. The easiest way to arrive at a solution is then to simply know the period  $T$  and thus easily calculate  $g = \frac{\ln(x(T)) - \ln(x(0))}{T}$ , and then solve the related linear equation

$$f'(t) = (Q(t) - g)f(t)$$

.

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The following two papers were published last year on similar topics, but not the same:

*Flow Equations for Disordered Floquet Systems* (Thomson et al. [2020]),  
*Chaos and subdiffusion in the infinite-range coupled quantum kicked rotors* (Russomanno et al. [2021])

## Specific example

We are looking for a solution to a self-consistent nonlinear Floquet equation of the form:

$$\begin{aligned}\frac{\partial}{\partial \tau} \begin{pmatrix} L \\ R \end{pmatrix} &= \begin{pmatrix} 1/2 & -1/2 + \mu L \tilde{L} \\ -1/2 + \mu R \tilde{R} & 1/2 \end{pmatrix} \begin{pmatrix} L \\ R \end{pmatrix} \\ \frac{\partial}{\partial \tau} \begin{pmatrix} \tilde{L} \\ \tilde{R} \end{pmatrix} &= - \begin{pmatrix} 1/2 & -1/2 + \mu L \tilde{L} \\ -1/2 + \mu R \tilde{R} & 1/2 \end{pmatrix} \begin{pmatrix} \tilde{L} \\ \tilde{R} \end{pmatrix}\end{aligned}$$

In principle solutions exist where  $L = \exp(\int g(\tau) d\tau) f(\tau)$  with  $g$  antisymmetric and  $f$  symmetric and periodic such that  $\tilde{L} = \exp(-\int g(\tau) d\tau) f(\tau)$ ,  $L\tilde{L} = f(\tau)^2$ . This ansatz gives rise to a natural decomposition of the equations of motion, but unfortunately does not yield an analytic form of the solution.

# Renormalising continuously

$$\psi_{n+1} = \psi_n + h[\psi_n, \tilde{\psi}_n] \cdot \psi_n \Delta t$$

Can also apply Runge-Kutta, Crank-Nicolson, etc. here.

$$\psi_{n+1} = \frac{\psi_{n+1}}{|\psi_{n+1}|}$$

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Act similarly on  $\tilde{\psi}$ . One-body observables are unchanged, so calculation of the mean-field is the same. This approach works, but it's very ad hoc, and it's not well suited to dealing with sudden jumps in one state, so it requires absurdly short time steps.

# Evolution of renormalised states

Define

$$\begin{aligned}
 |\phi\rangle &= \frac{|\psi\rangle}{\sqrt{\langle\psi|\psi\rangle}} = \frac{|\psi\rangle}{N} \\
 \partial_\tau \phi &= \frac{\partial_\tau \psi}{N} - \frac{|\psi\rangle}{N^2} \partial_\tau N \\
 &= h[\psi, \tilde{\psi}] |\phi\rangle - |\phi\rangle \partial_\tau \ln(N) \\
 &= \left( h[\phi, \tilde{\phi}] - \langle\phi| h[\phi, \tilde{\phi}] |\phi\rangle \right) |\phi\rangle
 \end{aligned}$$

And the same for  $\tilde{\phi}$ . This gives evolution of a norm-1 backwards and forwards state, without resorting to ad hoc renormalisation, and in fact captures the essential physics well.

# Results and continued issues

Much smoother than ad hoc division, but there are still numerical problems.

The problem arises from the highest energy eigenstates available in the problem. The forward evolving state quickly occupies these states, and machine precision is unable to maintain any occupancy in the lowest energy states (where the backwards evolving state is).

We need an approach which allows for enough precision in the numerics to stave off this runaway energy, but without simply diagonalising the Hamiltonian at each step.

# Conclusion and discussion

State of the work:

- The work is at the (possibly very long) stage of dealing with numerical issues.
- There may be room for a better mathematical foundation.
- There could also be choices of model problem which resolve this, but we may then lose the versatility of the approach.
- We still have the initial value problem and we get both probability and dynamics.

- S. Levit, J. W. Negele, and Z. Paltiel. Barrier penetration and spontaneous fission in the time-dependent mean-field approximation. *Physical Review C*, 22:1979–1995, 1980. ISSN 05562813. doi: 10.1103/PhysRevC.22.1979. Mostly just uses the previous two and a little bit more insight with imaginary time to get to some viable simulations.
- J. W. Negele. Microscopic theory of fission dynamics. *Nuclear Physics A*, 502:371–386, 10 1989. ISSN 03759474. doi: 10.1016/0375-9474(89)90676-3. URL [https://doi.org/10.1016/0375-9474\(89\)90676-3](https://doi.org/10.1016/0375-9474(89)90676-3)<http://linkinghub.elsevier.com/retrieve/pii/0375947489906763>.
- J. Skalski. Nuclear fission with mean-field instantons. *Physical Review C*, 77:64610, 2008. ISSN 1089490X. doi: 10.1103/PhysRevC.77.064610. URL <https://journals.aps.org/prc/pdf/10.1103/PhysRevC.77.064610>. uses the same ideas as Levit.
- W. Brodzinski and J. Skalski. Instanton - motivated study of spontaneous fission of odd-a nuclei. *arXiv*, 054603:1–25, 2020. ISSN 2469-9985. doi: 10.1103/physrevc.102.054603.
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- William H. Press, Brian P. Flannery, Saul A. Teukolsky, William T. Vetterling, and Harvey Gould. Numerical Recipes, The Art of Scientific Computing. *Am. J. Phys.*, 55(1):90–91, jan 1987. ISSN 0002-9505. doi: 10.1119/1.14981. URL <http://aapt.scitation.org/doi/10.1119/1.14981>.
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