1d ITDHF Example

Eric Flynn

July 2022

1 What is this?

This is a document that will detail all examples we try to solve in the imaginary time mean field theory approach. This includes the mathematical framework and the numerical methods/algorithms we use for each problem.

2 1d Slab Example

Setup:
This example is taken from the last sections of [1] and here we re-derive their results. We now detail the setup. In this paper, we use units

$$E_0 = \frac{\hbar^2}{2ml_0^2}, \quad t_0 = \frac{\hbar}{E_0} \tag{1}$$

such that xx_0 and tt_0 define a length and time respectively. Here, m is the mass of the fermion (will probably take it to be mass of proton). We define

$$l_0 = \frac{1}{\rho_0} \tag{2}$$

where $\rho_0 = 0.16 \text{ fm}^{-3} = 1/l_0^3$ is nuclear saturation density. So $l_0 = 1.85$ fm. This makes $E_0 = 6.03$ MeV and $t_0 = 1.09 \times 10^{-22}$ seconds. Since we are in complex time, the conjugate wavefunction denoted a $\bar{\phi}_\alpha(x,t)$ has the form

$$\bar{\phi}_\alpha(x,t) = \begin{cases} \phi^*(x,t) & t \in \mathbb{R} \\ \phi^*(x,-\tau) & t \in \mathbb{C}, \tau = Im(t) \end{cases} \tag{3}$$

where * denotes the usual complex conjugate. The Hamiltonian density for this model is going to be of BKN-type.

$$\mathcal{H} = -s \sum_\alpha \bar{\phi}_\alpha(x,t) \frac{\partial^2}{\partial x^2} \phi_\alpha(x,t) + \frac{1}{2} \int \rho(x,t) V(x-x') \rho(x',t) dx' + \frac{1}{2} V_3 \rho^3 \tag{4}$$

γ_1	2
γ_2	10
V_1	-1.489
V_2	0.4
V_3	0.5

Table 1: Constants used in Eq. 4.

where $s = 4$ for the spin and isotopic spin dengeneracy and the sum over α is over all occupied states. The fields are defined as

$$\rho(x,t) = s\sum_{\alpha} \bar{\phi}_\alpha(x,t)\phi_\alpha(x,t) \tag{5}$$

$$V(x-x') = \sum_{j=1}^{2} \frac{V_j}{\sqrt{\pi}\gamma_i} e^{-(x-x')^2/\gamma_i^2} \tag{6}$$

Values for the interactions constants in Eq. 4 are given in Table 1

Static Solutions:

Static bound states are given by the HF equations

$$\Big(\frac{d^2}{dx^2} + \int V(x-x')\rho(x')dx' + V_3\rho^2(x) + V_\lambda(x)\Big)u_\alpha(x) = \varepsilon_\alpha u_\alpha(x) \tag{7}$$

where we take $u_\alpha(x) = \phi_\alpha(x, t = 0)$. If Ω is the domain, boundary conditions will be taken to be $u(\partial\Omega) = 0$, i.e we enforce Dirichlet boundary conditions on the spatial domain. $V_\lambda(x)$ is a constraining potential added to make the saddle points resulting from the SPA. This potential makes converging to the saddle point more stable; the solutions with the constraining potential are stable against small perturbations. The form of the constraint used in [1] is

$$V_\lambda(x) = \lambda\Big[\int_{-1/2}^{1/2} d\eta \int dx' x'^2 \rho(x',\eta) - x_0^2\Big]x^2 \tag{8}$$

where λ is some constant? The bounce solutions correspond to where

$$\int_{-1/2}^{1/2} d\eta \int dx' x'^2 \rho(x',\eta) = x_0^2 \tag{9}$$

[1] focus on solving this for $A = 4, 8, 16$. With computers these days, we can easily include $A = 40, 48$.

Dynamic Solutions:

Let $T \in \mathbb{C}$ be a complex time period and let $\eta = t/T$. There are two forms of the ITDHF equations

$$\Big[\frac{\partial}{\partial\eta} + T\Big(-\frac{\partial^2}{\partial x^2} + \int V(x-x')\rho(x',\eta)dx' + V_3\rho^2(x,\eta) + V_\lambda(x)\Big)\Big]u_\beta(x,\eta) = \lambda_\beta u_\beta(x,\eta) \tag{10}$$

with boundary conditons

$$u_\beta(x, \frac{1}{2}) = u_\beta(x, -\frac{1}{2}) \tag{11}$$

Alternatively, we can cast the ITDHF equations as

$$-\frac{\partial \phi_\beta(x,\eta)}{\partial \eta} = T\Big(-\frac{\partial^2}{\partial x^2} + \int V(x-x')\rho(x',\eta)dx' + V_3\rho^2(x,\eta) + V_\lambda(x)\Big)\phi_\beta(x,\eta) = h[\rho]\phi_\beta(x,\eta) \tag{12}$$

with boundary conditions

$$\phi_\beta(x, \frac{1}{2}) = e^{-\lambda_\beta}\phi(x, -\frac{1}{2}) \tag{13}$$

Here,

$$u_\beta(x,\eta) = e^{\lambda_\beta(\eta+\frac{1}{2})}\phi_\beta(x,\eta) \tag{14}$$

<u>Calculation of the Bounce Action</u>

Once we have solutions of the ITDHF equations, we can calculate the action of the "bounce trajectory", that is, the phase contribution to the probability amplitude $\langle f|U|i\rangle$.

$$\langle f|U(t_f,t_i)|i\rangle = \int D\sigma e^{iS[\sigma]} \tag{15}$$

In the SPA approximation to zeroth order, $\sigma = \rho$ as defined earlier.

$$\langle f|U(t_f,t_i|i\rangle = e^{iS[\sigma]} \tag{16}$$

So the probability for the tunneling to occur is

$$|\,\langle f|U(t_f,t_i|i\rangle\,|^2 = |e^{iS[\sigma]}|^2 \tag{17}$$

Since S is now in general complex, this can be ≤ 1. The action is then given by

$$W_2^{(a)} = \sum_\alpha \int_{-1/2}^{1/2} d\eta \int dx u_\alpha(x,-\eta)\frac{\partial}{\partial \eta}u_\alpha(x,\eta) \tag{18}$$

where (a) is labeling all periodic solutions corresponding to a a particular stationary point of the action S. Evolving from the static HF solution evolving to the a-th distinct fragment configuration, the sum of all periodic trajectories is given by

$$\sum_{k=1}^{\infty}\Big[e^{iW_1}\Big(\sum_{n=0}^{\infty}e^{-nW_2^{(a)}}\Big)\Big]^k = \frac{e^{iW_1}}{1-e^{iW_1}-e^{-W_2^{(a)}}} \tag{19}$$

where W_1 is the action in the classically allow region. The total width/ decay rate is then given by

$$\Gamma = \sum_a \Gamma^{(a)} \tag{20}$$

$$\Gamma^{(a)} = 2\Big(\frac{\partial W_1}{\partial E}\Big)^{-1} e^{-W_2^{(a)}(E)} = 2\omega e^{-W_2^{(a)}(E)} \tag{21}$$

where ω is the "frequency of assaults" on the barrier. Thus, each bounce solution corresponds to a partial width. This is great since we can study the competition between different modes of fission for example.

3 Double Well Example

This example is taken from [2] and we try to re-derive their results.

References

[1] S Levit, JW Negele, and Z Paltiel. Barrier penetration and spontaneous fission in the time-dependent mean-field approximation. *Physical Review C*, 22(5):1979, 1980.

[2] Patrick McGlynn and Cédric Simenel. Imaginary-time mean-field method for collective tunneling. *Physical Review C*, 102(6):064614, 2020.