Lattice EFT note 1

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Chapter 1

Introduction

1.1 Euclidean Time

Analytic continuation to Eucliean time ,$it \to t_E$, enables the numerical calculation of path integral.

1.1.1 Euclidean action for Boson

Consider a Quantum mechanical path integral,

$$\begin{aligned}
&\langle x_f|U(t_f,t_i)|x_i\rangle = \int \mathcal{D}x(t)e^{iS[x]}, \quad S[x] = \int_{t_i}^{t_f} dtL(x,\dot{x}),\\
&L(x,\dot{x}) = \frac{m}{2}\dot{x}(t)^2 - V(x(t)) = \dot{x}p - \left(\frac{p^2}{2m} + V(x)\right), \quad p = m\dot{x}
\end{aligned} \tag{1.1}$$

Let us transform into a Euclidean time by $it \to t_E$, then (Note overall $-$ sign comes from the Lagrangian itself.)

$$\begin{aligned}
&e^{i\int dt(\frac{m}{2}\dot{x}(t)^2 - V(x(t)))} \to e^{\int dt_E(-\frac{m}{2}\dot{x}(t_E)^2 - V(x(t_E)))} = e^{-S_E[x]},\\
&S_E[x] = \int dt_E L_E = \int dt_E \left[\frac{m}{2}\dot{x}(t_E)^2 + V(x(t_E))\right].
\end{aligned} \tag{1.2}$$

Then, the following path integral gives the complete information for the quantum theory,(in Euclidean time)

$$\langle x_f|e^{-\tilde{H}(t_f-t_i)}|x_i\rangle = \int_{x_i}^{x_f} \mathcal{D}x(t)e^{-S[x]}. \tag{1.3}$$

Be careful for the sign. In other words, it goes like $e^{-S_E} = e^{-H_E t}$

Let us consider for a pion action for example. (interaction with nucleon will be considered later and also the time derivative of pion will not be considered because we will not treat dynamic pion. π_I where I is an iso-spin index.)

$$\begin{aligned}
& iS[\pi_I] = i\int dt \int d^3x \left[\frac{1}{2}\partial_\mu\pi_I\partial^\mu\pi_I - \frac{1}{2}m_\pi^2\pi_I^2 - V(\pi_I)\right]\\
\to\ & \int d\tau \int d^3x \left[-\frac{1}{2}(\partial_\tau\pi_I)^2 - \frac{1}{2}(\nabla\pi_I)^2 - \frac{1}{2}m_\pi^2\pi_I^2 - V(\pi_I)\right]\\
=\ & -\int d\tau \int d^3x \left[\frac{1}{2}(\partial_\tau\pi_I)^2 + \frac{1}{2}(\nabla\pi_I)^2 + \frac{1}{2}m_\pi^2\pi_I^2 + V(\pi_I)\right]
\end{aligned} \tag{1.4}$$

1.1.2 Euclidean action for Fermion

Let us consider a non-relativistic Fermion action,

$$\begin{aligned} i\int dtd^3x\psi^\dagger(i\partial_t+\frac{\hbar^2\nabla^2}{2m})\psi-V &\rightarrow \int d\tau d^3x\psi^\dagger(-\partial_\tau+\frac{\hbar^2\nabla^2}{2m})\psi-V \\ &= -\int d\tau d^3x\psi^\dagger(\partial_\tau-\frac{\hbar^2\nabla^2}{2m})\psi+V \end{aligned} \tag{1.5}$$

1.1.3 Path integral in Euclidean time

In a similar way, let us consider action for the QFT. Once Wick rotate to Euclidean time, the partition function can be written as

$$Z_T=\mathrm{Tr}(e^{-TH})=\sum_n\langle n|e^{-TH}|n\rangle=\sum_n e^{-TE_n}. \tag{1.6}$$

Here, it is important to remind that $|n\rangle$ is a multi particle states.

Euclidean correlator is defined

$$\langle O_1(t)O_2(0)\rangle_T=\frac{1}{Z_T}\mathrm{Tr}\left[e^{-(T-t)H}\hat{O}_2e^{-tH}\hat{O}_1\right] \tag{1.7}$$

Inserting complete states between operators, we have the first important relation,

$$\lim_{T\to\infty}\frac{1}{Z_T}\mathrm{Tr}\left[e^{-(T-t)H}\hat{O}_2e^{-tH}\hat{O}_1\right]=\sum_n\langle 0|\hat{O}_2|n\rangle\langle n|\hat{O}_1|0\rangle e^{-t(E_n-E_0)} \tag{1.8}$$

This means, if we can compute the left hand-side by path integral, we can extract the information on excited states, energy E_n and wave function or observables $\langle 0|\hat{O}_2|n\rangle\langle n|\hat{O}_1|0\rangle$.

We can obtain information on quantum system by computing average of operators. Now the second key equation is

$$\frac{1}{Z_T}\mathrm{Tr}\left[e^{-(T-t)\hat{H}}\hat{O}_2e^{-t\hat{H}}\hat{O}_1\right]=\frac{1}{Z_T}\int\mathcal{D}[\Phi]e^{-S_E[\Phi]}O_2[\Phi(.,t)]O_1[\Phi(.,0)]. \tag{1.9}$$

This means that if we compute the path integral numerically, we can extract physical information we want from the first relation.

From now on, let us represent any physical quantity as power of lattice size a, so that all quantoty can be written as dimensionless.

1.2 Example: Numerical Path Integral for scalar field

In this example, some details on how to construct the path integral for a scalar field is shown.

In Minkowski space, Lagrangian of scalar field is

$$L(\Phi,\partial_\mu\Phi)=\frac{1}{2}\dot{\Phi}^2-\frac{1}{2}(\nabla\Phi)^2-\frac{m^2}{2}\Phi^2-V(\Phi). \tag{1.10}$$

The Hamiltonian of scalar field becomes

$$\hat{H} = \int d^3x \left(\frac{1}{2}\hat{\Pi}(\boldsymbol{x})^2 + \frac{1}{2}(\nabla\hat{\Phi}(\boldsymbol{x}))^2 + \frac{m^2}{2}\hat{\Phi}(\boldsymbol{x})^2 + V(\hat{\Phi}(\boldsymbol{x})) \right), \tag{1.11}$$

with equal time commutation relation,

$$\left[\hat{\Phi}(\boldsymbol{x}), \hat{\Pi}(\boldsymbol{y})\right] = i\delta(\boldsymbol{x}-\boldsymbol{y}), \quad \left[\hat{\Phi}(\boldsymbol{x}), \hat{\Phi}(\boldsymbol{y})\right] = \left[\hat{\Pi}(\boldsymbol{x}), \hat{\Pi}(\boldsymbol{y})\right] = 0, \tag{1.12}$$

where,

$$\hat{\Pi}(t, \boldsymbol{x}) = \frac{\partial}{\partial\dot{\Phi}(t, \boldsymbol{x})} L(\Phi, \partial_\mu\Phi) = \dot{\Phi}(t, \boldsymbol{x}), \tag{1.13}$$

or equivalently, from the commutation relation, we can considering $\hat{\Pi}$ as an operator in Φ representation,

$$\hat{\Pi}(\boldsymbol{x}) = i\frac{\partial}{\partial\Phi(\boldsymbol{x})}. \tag{1.14}$$

By introducing 3-D lattice Λ_3,

$$\boldsymbol{x} \to a\boldsymbol{n}, \quad n_i = 0, 1, \ldots, N-1 \quad i = 1, 2, 3. \tag{1.15}$$

We change Hamiltonian into lattice form,

$$\hat{H} = a^3 \sum_{\boldsymbol{n}\in\Lambda_3} \left(\frac{1}{2}\hat{\Pi}(\boldsymbol{n})^2 + \frac{1}{2}\sum_{j=1}^{3} \left(\frac{\hat{\Phi}(\boldsymbol{n}+j) - \hat{\Phi}(\boldsymbol{n}-j)}{2a} \right)^2 + \frac{m^2}{2}\hat{\Phi}(\boldsymbol{n})^2 + V(\hat{\Phi}(\boldsymbol{n})) \right) \tag{1.16}$$

With,

$$\left[\hat{\Phi}(\boldsymbol{n}), \hat{\Pi}(\boldsymbol{m})\right] = ia^{-3}\delta_{\boldsymbol{n},\boldsymbol{m}}, \quad \left[\hat{\Phi}(\boldsymbol{n}), \hat{\Phi}(\boldsymbol{m})\right] = \left[\hat{\Pi}(\boldsymbol{n}), \hat{\Pi}(\boldsymbol{m})\right] = 0, \tag{1.17}$$

And, $\hat{\Pi}(\boldsymbol{n})$ can be considered as a derivative operator according to the commutation relation,

$$\hat{\Pi}(\boldsymbol{n}) = -\frac{i}{a^3}\frac{\partial}{\partial\Phi(\boldsymbol{n})}. \tag{1.18}$$

Then considering action of operators,

$$\begin{aligned} &\hat{\Phi}(\boldsymbol{n})|\Phi\rangle = \Phi(\boldsymbol{n})|\Phi\rangle, \\ &\langle\Phi'|\Phi\rangle = \delta(\Phi'-\Phi) \equiv \prod_{\boldsymbol{n}\in\Lambda_3} \delta(\Phi'(\boldsymbol{n}) - \Phi(\boldsymbol{n})), \\ &1 = \int D\Phi|\Phi\rangle\langle\Phi|, \quad D\Phi = \prod_{\boldsymbol{n}\in\Lambda_3} d\Phi(\boldsymbol{n}). \end{aligned} \tag{1.19}$$

One can write the eigen state of $\hat{\Pi}(\boldsymbol{n})$ operator as $\langle\Phi|\Pi\rangle$,

$$\langle\Phi|\Pi\rangle = \prod_{\boldsymbol{n}\in\Lambda_3} \sqrt{\frac{a^3}{2\pi}} e^{ia^3\Pi(\boldsymbol{n})\Phi(\boldsymbol{n})}, \quad \hat{\Pi}(\boldsymbol{n})\langle\Phi|\Pi\rangle = \Pi(\boldsymbol{n})\langle\Phi|\Pi\rangle. \tag{1.20}$$

Then, free Hamiltonian evolves as

$$\begin{aligned}
\langle\Phi|\hat{H}_0|\Pi\rangle &= -\frac{1}{2a^3}\sum_{\boldsymbol{n}\in\Lambda_3}\frac{\partial^2}{\partial\Phi(\boldsymbol{n})^2}\langle\Phi|\Pi\rangle = \frac{a^3}{2}\sum_{\boldsymbol{n}\in\Lambda_3}\Pi(\boldsymbol{n})^2\langle\Phi|\Pi\rangle, \\
\langle\Phi'|e^{-t\hat{H}_0}|\Phi\rangle &= \int D\Pi\langle\Phi'|e^{-t\hat{H}_0}|\Pi\rangle\langle\Pi|\Phi\rangle = \int D\Pi\langle\Phi'|\Pi\rangle\langle\Pi|\Phi\rangle e^{-t\frac{a^3}{2}\sum_n\Pi(\boldsymbol{n})^2} \\
&= \prod_{\boldsymbol{n}\in\Lambda_3}\frac{a^3}{2\pi}\int d\Pi(\boldsymbol{n})e^{ia^3\Pi(\boldsymbol{n})(\Phi'(\boldsymbol{n})-\Phi(\boldsymbol{n}))}e^{-ta^3\Pi(\boldsymbol{n})^2/2} \\
&= \prod_{\boldsymbol{n}\in\Lambda_3}\sqrt{\frac{a^3}{2\pi t}}e^{-a^3/(2t)(\Phi'(\boldsymbol{n})-\Phi(\boldsymbol{n}))^2} = \left(\frac{a^3}{2\pi t}\right)^{\frac{N^3}{2}}e^{-\frac{a^3}{2t}\sum_n(\Phi'(\boldsymbol{n})-\Phi(\boldsymbol{n}))^2} \qquad (1.21)
\end{aligned}$$

With interaction,

$$\begin{aligned}
\hat{W}_\epsilon &= e^{-\epsilon\hat{U}/2}e^{-\epsilon\hat{H}_0}e^{-\epsilon\hat{U}/2}, \\
\langle\Phi'|e^{-t\hat{H}}|\Phi\rangle &= \lim_{n_t\to\infty}\langle\Phi'|\hat{W}_\epsilon^{n_t}|\Phi\rangle = \lim_{n_t\to\infty}\int D\Phi_1\dots D\Phi_{n_t-1}\langle\Phi'|\hat{W}_\epsilon|\Phi_{n_t-1}\rangle\dots\langle\Phi_1|\hat{W}_\epsilon|\Phi\rangle \qquad (1.22)
\end{aligned}$$

And the transfer matrix elements

$$\begin{aligned}
\langle\Phi_{i+1}|\hat{W}_\epsilon|\Phi_i\rangle &= \langle\Phi_{i+1}|e^{-\epsilon\hat{U}/2}e^{-\epsilon\hat{H}_0}e^{-\epsilon\hat{U}/2}|\Phi_i\rangle = e^{-\epsilon U[\Phi_{i+1}]/2}\langle\Phi_{i+1}|e^{-\epsilon\hat{H}_0}|\Phi_i\rangle e^{-\epsilon U[\Phi_i]/2} \\
&= C^{N^3}e^{-\epsilon U[\Phi_i]/2-a^3/(2\epsilon)\sum_n(\Phi(\boldsymbol{n})_i-\Phi(\boldsymbol{n})_{i+1})^2-\epsilon U[\Phi_{i+1}]/2} \qquad (1.23)
\end{aligned}$$

Finally, the partition function can be written as a path integral,

$$\begin{aligned}
Z_T^\epsilon &= \int D\Phi_0\langle\Phi_0|\widehat{W}_\epsilon^{N_T}|\Phi_0\rangle = C^{N^3N_T}\int D\Phi_0\dots D\Phi_{N_T-1}e^{-S_E[\Phi]} \\
&= C^{N^3N_T}\int\mathcal{D}[\Phi]e^{-S_E[\Phi]}, \quad \mathcal{D}[\Phi] = \prod_{(\boldsymbol{n},n_4)\in\Lambda}d\Phi(\boldsymbol{n},n_4), \qquad (1.24)
\end{aligned}$$

where

$$\begin{aligned}
S_E[\Phi] &= \epsilon a^3\sum_{(\boldsymbol{n}n_4)\in\Lambda_4}\left[\frac{1}{2}\left(\frac{\Phi(\boldsymbol{n},n_4+1)-\Phi(\boldsymbol{n},n_4)}{\epsilon}\right)^2\right. \\
&\left.+\frac{1}{2}\sum_{j=1}^{3}\left(\frac{\Phi(\boldsymbol{n}+\hat{j},n_4)-\Phi(\boldsymbol{n}-\hat{j},n_4)}{2a}\right)^2+\frac{m^2}{2}\Phi(\boldsymbol{n},n_4)^2+V(\Phi(\boldsymbol{n},n_4))\right] \qquad (1.25)
\end{aligned}$$

1.3 Example: non-relativistic quantum mechanics of 1-body in a potential.

This example shows how to construct path integral and how to compute it numerically. Also how to extract the information for ground state or excited state.

As an example of numerical calculation, let us evaluate

$$\langle x|e^{-H(t_f-t_i)}|x\rangle. \qquad (1.26)$$

for a particle in an external potential in quantum mechanics.

Discretize the time as

$$t_j = t_i + ja, \quad \text{for } j = 0,1,\dots N, \quad a_t = \frac{t_f-t_i}{N} \qquad (1.27)$$

A path(or a configuration) is described by a vector

$$x = \{x(t_0), x(t_1), \dots, x(t_N)\}. \qquad (1.28)$$

Then, in a notation $x_j = x(t_j)$ and b.c. $x_0 = x_N = x$,

$$\int \mathcal{D}x(t) \to A \int_{-\infty}^{+\infty} dx_1 dx_2 \dots dx_{N-1}, \tag{1.29}$$

where endpoints(x_0 and x_N) are fixed (not integrated).[1] And, in a simple approximation

$$\int_{t_j}^{t_{j+1}} dt L \simeq a \left[\frac{m}{2} \left(\frac{x_{j+1} - x_j}{a} \right)^2 + \frac{1}{2}(V(x_{j+1}) + V(x_j)) \right] \tag{1.30}$$

Thus,

$$\begin{aligned} \langle x | e^{-\tilde{H}T} | x \rangle &\simeq A \int_{-\infty}^{\infty} dx_1 \dots dx_{N-1} e^{-S_{lat}[x]}, \\ S_{lat}[x] &\equiv \sum_{j=0}^{N-1} \left[\frac{m}{2a}(x_{j+1} - x_j)^2 + aV(x_j) \right], \end{aligned} \tag{1.31}$$

we can evaluate the path integral numerically.

One way to do this integration is using Monte Carlo integration for all (N-1) variables by choosing random numbers.

Let us consider now excited states by sum over end points. To analyze excited states using path integral, interrupt the propagation of the ground state by new operators.

$$G(t) \equiv \sum_x \langle x | x(t_2) x(t_1) | x \rangle = \langle\langle x(t_2) x(t_1) \rangle\rangle \equiv \frac{\int \mathcal{D}x(t) x(t_2) x(t_1) e^{-S[x]}}{\int \mathcal{D}x(t) e^{-S[x]}} \tag{1.32}$$

where now we integrate over all $x_i = x_f = x$ as well as the intermediate $x(t)$'s. In a very large time limit $T = t_f - t_i$, the ground state contribution will be dominant, and large $t = t_2 - t_1$ limit,

$$\begin{aligned} \int \mathcal{D}x(t) x(t_2) x(t_1) e^{-S[x]} &= \int dx \langle x | e^{-\tilde{H}(t_f - t_2)} \tilde{x} e^{-\tilde{H}(t_2 - t_1)} \tilde{x} e^{-\tilde{H}(t_1 - t_i)} | x \rangle, \\ \langle\langle x(t_2) x(t_1) \rangle\rangle &= \frac{\sum e^{-E_n T} \langle E_n | \tilde{x} e^{-(\tilde{H} - E_n)t} \tilde{x} | E_n \rangle}{\sum e^{-E_n T}} \\ &\to \langle E_0 | \tilde{x} e^{-(\tilde{H} - E_0)t} \tilde{x} | E_0 \rangle \to |\langle E_0 | \tilde{x} | E_1 \rangle|^2 e^{-(E_1 - E_0)t} \end{aligned} \tag{1.33}$$

Thus, one can extract the excited state by

$$\log(G(t)/G(t+a)) \to (E_1 - E_0)a \tag{1.34}$$

and also matrix element $|\langle E_0 | \tilde{x} | E_1 \rangle|^2$.

For example, we may analyze the time dependence

$$G(t) = \frac{1}{N} \sum_j \langle\langle x(t_j + t) x(t_j) \rangle\rangle \to G_n = \frac{1}{N} \sum_j \langle\langle x_{(j+n) mod N} x_j \rangle\rangle \tag{1.35}$$

for all $t = 0, a_t, 2a_t, \dots (N-1)a_t$. And get energy difference,

$$\Delta E_n \equiv \log(G_n / G_{n+1}) \to_{large\ n} (E_1 - E_0)a \tag{1.36}$$

One can extract any information on quantum mechanical system by using some operator,

$$\langle\langle \Gamma[x] \rangle\rangle = \frac{\int \mathcal{D}x(t) \Gamma[x] e^{-S[x]}}{\int \mathcal{D}x(t) e^{-S[x]}}, \tag{1.37}$$

[1] Normalization factor $A = (\frac{m}{2\pi a})^{N/2}$.

where it is a weighted average with weight $e^{-S[x]}$, over large N_{cf} configurations. If we choose particular paths(configuration (α)) with probability

$$P[x^{(\alpha)}] \propto e^{-S[x^{(\alpha)}]}, \tag{1.38}$$

we get

$$\langle\langle\Gamma[x]\rangle\rangle \simeq \bar{\Gamma} \equiv \frac{1}{N_{cf}} \sum_{\alpha=1}^{N_{cf}} \Gamma[x^{(\alpha)}]. \tag{1.39}$$

Monte Carlo uncertainty in this approximation is estimated as

$$\sigma_{\bar{\Gamma}}^2 \simeq \frac{\langle\langle\Gamma^2\rangle\rangle - \langle\langle\Gamma\rangle\rangle^2}{N_{cf}} \tag{1.40}$$

One way to update $x^{(\alpha)}$ to $x^{(\alpha+1)}$ configuration is Metropolis algorithm.

More details on the algorithm is given in later chapter. But one have to take into account (1) avoid correlation between updates. (This can be done by keeping only N_{cor}-th path) (2) when starting the procedure requires "thermalizing the lattice"(This can be done by discarding some initial configurations).

1.4 Example: 1D QFT of scalar particle

This is a continuation from previous example for the case of scalar particle.

For QFT, we change $x(t) \to \phi(t) \to \phi(t, x)$.

$$\langle\langle\Gamma[\phi]\rangle\rangle \equiv \frac{1}{\mathcal{Z}} \int \prod_{x_j \in grid} d\phi(x_j) e^{-S[\phi]} \Gamma[\phi], \tag{1.41}$$

$$\mathcal{Z} \equiv \int \prod_{x_j \in grid} d\phi(x_j) e^{-S[\phi]} \tag{1.42}$$

For example, one may use operators like

$$\Gamma(t) \equiv \frac{1}{\sqrt{N}} \sum_{x_j} \phi(x_j, t), \tag{1.43}$$

which corresponds to zero momentum state $\phi(p = 0, t)$. Then, in large time limit, only the lowest energy excitation state ,which is one particle state, will contribute to the average

$$\langle\langle\Gamma(t)\Gamma(0)\rangle\rangle \to |\langle 0|\Gamma(0)|\phi : p = 0\rangle|^2 e^{-m_\phi t} \tag{1.44}$$

1.5 Example: Non-relativistic free particle action in lattice

This example shows how to write the approximate discretized lattice action for free particle.

Relativistic single particle energy spectrum in lattice have a doubling problem because of the relation $E = \pm\sqrt{p^2 + m^2}$. But, non-relativistic case does not have doubling problem.

After discretization,

$$\int_0^L dx \to a \sum_{n=0}^{N-1}, \quad a(x) \to a(n) \tag{1.45}$$

We may approximate the free Hamiltonian as(note that this is just one possibility.)

$$\begin{aligned} H_{free} &= -\frac{1}{2m}\int_0^L dx a^\dagger(x)\frac{\partial^2}{\partial x^2}a(x) = \frac{1}{2m}\int_0^L dx(\frac{\partial}{\partial x}a^\dagger(x))(\frac{\partial}{\partial x}a(x)) \\ &\to -\frac{a}{a^2}\frac{1}{2m}\sum_{n=0}^{N-1}[a^\dagger(n+1)a(n)+a^\dagger(n)a(n+1)-2a^\dagger(n)a(n)] \\ &= -\frac{a}{a^2}\frac{1}{2m}\sum_{n=0}^{N-1}[a^\dagger(n+1)a(n)+a^\dagger(n-1)a(n)-2a^\dagger(n)a(n)] \end{aligned} \tag{1.46}$$

where, $a(N) = a(0)$ with periodic boundary condition. We expect the energy of one particle momentum eigenstate $|\boldsymbol{p}\rangle$ to be $\frac{\boldsymbol{p}^2}{2m}$ in continuum limit. However, as shown below, the energy eigen value for this approximation does not give the exact continuum limit value.

A momentum eigen state on 1-D lattice can be defined(as a translation operator eigen state) as

$$|p\rangle = \frac{1}{\sqrt{N}}\sum_{n=0}^{N-1}e^{ipn}a^\dagger(n)|0\rangle, \quad p = \frac{2\pi k}{N} \text{ with k integer} \tag{1.47}$$

Then the energy of this state for approximate H^{free} is

$$\begin{aligned} H^{free}|p\rangle &= -\frac{1}{2m}\sum_{n'=0}^{N-1}[a^\dagger(n'+1)a(n')+a^\dagger(n')a(n'+1)-2a^\dagger(n')a(n')]\left(\frac{1}{\sqrt{N}}\sum_{n=0}^{N-1}e^{ipn}a^\dagger(n)|0\rangle\right) \\ &= -\frac{1}{2m}\frac{1}{\sqrt{N}}\sum_{n=0}^{N-1}e^{ipn}[a^\dagger(n+1)+a^\dagger(n-1)-2a^\dagger(n)]|0\rangle \\ &= -\frac{1}{2m}\frac{1}{\sqrt{N}}\sum_{n=0}^{N-1}[e^{-ip}+e^{ip}-2]e^{ipn}a^\dagger(n)|0\rangle \\ &= -\frac{1}{2m}(e^{-ip}+e^{ip}-2)|p\rangle = \frac{1}{m}(1-\cos p)|p\rangle \end{aligned} \tag{1.48}$$

Thus, the dispersion relation for this approximate Hamiltonian is

$$E(p) = \frac{1}{m}(1-\cos p) = \frac{p^2}{2m}+\mathcal{O}(p^4) \tag{1.49}$$

and only approximately the same with continuum limit.

1.5.1 Improved action

We may "improve" the Hamiltonian so that it gives better agreement in continuum limit. Suppose we discretize the Hamiltonian by

$$\boxed{H_{free} = \frac{1}{2m}\sum_{n=0}^{N-1}\sum_{\Delta=0}^{\Delta_{max}}(-1)^\Delta\omega_\Delta[a^\dagger(n+\Delta)a(n)+a^\dagger(n)a(n+\Delta)].} \tag{1.50}$$

Then the spectrum of single particle state is

$$\begin{aligned} H_{free}|p\rangle &= \left(\frac{1}{2m}\sum_{\Delta=0}^{\Delta_{max}}(-1)^\Delta\omega_\Delta(e^{i\Delta p}+e^{-i\Delta p})\right)|p\rangle = Q(p)|p\rangle \\ Q(p) &= \frac{1}{m}\sum_{\Delta=0}^{\Delta_{max}}(-1)^\Delta\omega_\Delta\cos(\Delta\cdot p) \\ &= \frac{1}{m}(\omega_0-\omega_1\cos(p)+\omega_2\cos(2p)+\dots) \end{aligned} \tag{1.51}$$

Then by expanding in power of p,

$$Q(p) = \frac{1}{m}\sum_{\Delta=0}^{\Delta_{max}}\sum_{\nu=0}^{\infty}\frac{(-1)^\nu}{(2\nu)!}\omega_\Delta \Delta^{2\nu}p^{2\nu} \tag{1.52}$$

By choosing appropriate ω_Δ, one can set $Q(p) = \frac{p^2}{2m} + \mathcal{O}(p^n)$, and approximate Hamiltonian which eliminates lattice artifact.

In 3-d lattice dispersion relation of free particle, $Q^{(n)}(p) = \frac{1}{2m}\sum_{l=1,2,3} p_l^2[1 + O(a^{2n+2})]$,

$$\boxed{H_{free} = \frac{1}{2m}\sum_{l=1,2,3}\sum_{n=0}^{N-1}\sum_{\Delta=0}^{\Delta_{max}}(-1)^\Delta\omega_\Delta[a^\dagger(n+\Delta\hat{l})a(n) + a^\dagger(n)a(n+\Delta\hat{l})].} \tag{1.53}$$

lowest order approximation is

$$\omega_0 = 1, \quad \omega_1 = 1. \tag{1.54}$$

At $\mathcal{O}(a^2)$ improved,

$$\omega_0 = \frac{5}{4}, \quad \omega_1 = \frac{4}{3}, \quad \omega_2 = \frac{1}{12}. \tag{1.55}$$

At $\mathcal{O}(a^4)$ improved,

$$\omega_0 = \frac{49}{36}, \quad \omega_1 = \frac{3}{2}, \quad \omega_2 = \frac{3}{20}, \quad \omega_3 = \frac{1}{90}. \tag{1.56}$$

and for $Q(p) = \frac{p^2}{2m} + \mathcal{O}(p^{10})$, we get(sign error?)

$$\omega_0 = \frac{205}{144}, \quad \omega_1 = -\frac{8}{5}, \quad \omega_2 = \frac{1}{5}, \quad \omega_3 = -\frac{8}{315}, \quad \omega_4 = \frac{1}{560}. \tag{1.57}$$

Sometimes, "well-tempered(wt) action" can be used. They are defined implicitly in terms of their dispersion relation,

$$\omega^{(wtn)}(\boldsymbol{p}) = \omega^{(n-1)}(\boldsymbol{p}) + c[\omega^{(n)}(\boldsymbol{p}) - \omega^{(n-1)}(\boldsymbol{p})], \tag{1.58}$$

where the unknown constant c was determined by the integral constraint,

$$\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} dp_1 dp_2 dp_3 \left[\omega^{(wtn)}(\boldsymbol{p}) - \frac{1}{2m}\sum_{l=1,2,3} p_l^2\right] = 0. \tag{1.59}$$

Note that this does not mean that dispersion relation is exact for $|\boldsymbol{p}\rangle$.

1.6 Example: lattice QCD action

This section discuss about the QCD lattice action. One may skip this section.

In case of QCD, before making path integral formula, we need lattice action for quarks and gluons. Because of discretization, normal covariant derivative form does not satisfy gauge invariance exactly. Thus, it is difficult to use gluon field as variable. Instead, we introduce link variable as a gauge transporter. Then, fermion action becomes,

$$\begin{aligned} S_F[\psi,\bar{\psi},U] \quad = \quad & a^4\sum_{f=1}^{N_f}\sum_{\boldsymbol{n}\in\Lambda}\left(\bar{\psi}^{(f)}(\boldsymbol{n})\sum_{\mu=1}^{4}\gamma_\mu\frac{U_\mu(n)\psi^{(f)}(n+\hat{\mu}) - U_{-\mu}(n)\psi^{(f)}(n-\hat{\mu})}{2a}\right. \\ & \left. + m^{(f)}\bar{\psi}^{(f)}(n)\psi^{(f)}(n)\right) + \text{ additional terms} \end{aligned} \tag{1.60}$$

where, link variable, $U_\mu(n)$, links between site $\boldsymbol{n}$ and $\boldsymbol{n}+\mu$ and make the term gauge invariant,

$$\begin{aligned}&\bar{\psi}'(n)U'_\mu(n)\psi'(n+\mu) = \bar{\psi}(n)\Omega(n)^\dagger U'_\mu(n)\Omega(n+\mu)\psi(n+\mu) = \bar{\psi}(n)U_\mu(n)\psi(n+\mu),\\ &U_\mu(n) \to U'_\mu(n) = \Omega(n)U_\mu(n)\Omega(n+\mu)^\dagger, \quad U_{-\mu}(n) = U_\mu(n-\mu)^\dagger\end{aligned} \tag{1.61}$$

Explicit form of link and gauge field can be thought as

$$U_\mu(n) = \exp(iaA_\mu(n)), \tag{1.62}$$

which corresponds to the covariant derivative in continuum limit and make sure fermion bilinear becomes gauge invariant.

Another gauge invariant term is a closed loop, $L[U]$,

$$L[U] = \mathrm{tr}\left[U_{\mu_0}(n_0)U_{\mu_1}(n_0+\mu_0)\dots U_{-\mu_N}(n_0)\right] = \mathrm{tr}\left[\prod_{(n,\mu)\in \text{ loop}} U_\mu(n)\right] \tag{1.63}$$

We can construct lattice gauge action in terms of plaquette such that

$$S_G[U] = \frac{2}{g^2}\sum_{n\in\Lambda}\sum_{\mu<\nu}\mathrm{Re}\left[\mathrm{tr}[I - U_{\mu\nu}(n)]\right] = \frac{a^4}{2g^2}\sum_{n\in\Lambda}\sum_{\mu,\nu}\mathrm{tr}[F_{\mu\nu}(n)^2] + \mathcal{O}(a^2). \tag{1.64}$$

where, plaquette is a product of 4 links,

$$U_{\mu\nu}(n) = U_\mu(n)U_\nu(n+\mu)U_\mu(n+\nu)^\dagger U_\nu(n)^\dagger = \exp(ia^2F_{\mu\nu}(n) + \mathcal{O}(a^3)). \tag{1.65}$$

Gauge invariance/fixing/Integration

Because the guage link is a matrix, it is necessary to specify how to integrate over elements, $\int dU_\mu(\boldsymbol{n})$, in Lie algebra. Also, it is important to make the measure gauge invariant. Such measure is known as Harr measure.

The Harr measure satisfies the properies,

$$\begin{aligned} dU &= d(UV) = d(VU), \quad V \in G,\\ \int dU\ 1 &= 1.\end{aligned} \tag{1.66}$$

It can be defined as

$$\begin{aligned} dU &= c\sqrt{\det[g(\omega)]}\prod_k d\omega^{(k)},\\ g(\omega)_{nm} &= \mathrm{tr}\left[\frac{\partial U(\omega)}{\partial\omega^{(n)}}\frac{\partial U(\omega)^\dagger}{\partial\omega^{(m)}}\right].\end{aligned} \tag{1.67}$$

where, ω are real parameters for compact Lie group. [2] We can fix gauge in many ways in lattice. Simpliest might be the temporal gauge,

$$U_4(n) = 1, \quad \forall n. \tag{1.69}$$

[2] some of basic integrals for SU(3) are

$$\begin{aligned}&\int_{SU(3)} dU U_{ab} = 0,\\ &\int_{SU(3)} dU U_{ab}U_{cd} = 0,\\ &\int_{SU(3)} dU U_{ab}(U^\dagger)_{cd} = \frac{1}{3}\delta_{ad}\delta_{bc},\\ &\int_{SU(3)} dU U_{ab}U_{cd}U_{ef} = \frac{1}{6}\epsilon_{ace}\epsilon_{bdf}.\end{aligned} \tag{1.68}$$

1.7 Gaussian integration in D-dimension

The most basic integral in field theory is the Gaussian integration,

$$\int_{-\infty}^{\infty} dv^{-\frac{1}{2}av^2} = \left(\frac{2\pi}{a}\right)^{\frac{1}{2}}. \tag{1.70}$$

For a D-dimensional vectors v, ρ and $D \times D$ real symmetric matrix A,

$$\int d^D v e^{-\frac{1}{2}v^T Av} = (2\pi)^{D/2} e^{-\frac{1}{2}\mathrm{Tr}\ln A} = (2\pi)^{D/2} (\det A)^{-\frac{1}{2}} \tag{1.71}$$

$$\int d^D v e^{-\frac{1}{2}v^T Av + \rho^T v} = (2\pi)^{D/2} e^{-\frac{1}{2}\mathrm{Tr}\ln A} e^{\frac{1}{2}\rho^T A^{-1}\rho} \tag{1.72}$$

a slight modification gives [3]

$$\int d^D v\ e^{-\frac{1}{2}v^T Av} v_{k_1} \dots v_{k_n} = (2\pi)^{D/2} e^{-\frac{1}{2}\mathrm{Tr}\ln A} \left(A^{-1}_{k_1 k_2} \dots A^{-1}_{k_{n-1} k_n} + \text{permut.} \right) \tag{1.74}$$

This relation can be used later for the introduction of auxiliary particle field.
Another useful form may be

$$\int \mathcal{D}v e^{-\frac{1}{2}v^T Av + \rho^T Bv} = (2\pi)^{D/2} e^{-\frac{1}{2}\mathrm{Tr}\ln A} e^{\frac{1}{2}\rho^T X^{-1}\rho}, \quad X^{-1} = BA^{-1}B^T. \tag{1.75}$$

When A is a positive definite hermitian matrix and z is a complex vector,

$$\int dz_1 dz_1^* \dots dz_D dz_D^* e^{-z^\dagger Az} = (2\pi)^D e^{-\mathrm{Tr}\ln A} \tag{1.76}$$

where complex measure is defined as

$$\int dz dz^*\ f(z, z^*) = 2 \int d\mathrm{Re}z \int d\mathrm{Im}z\ f(z, z^*) \tag{1.77}$$

In many case, we need the integration of continuous fields. Let us define, scalar products for continuum.

$$\begin{aligned} (\phi, \psi) &= \int d^4x \phi(x)\psi(x), \\ (\phi, A\psi) &= \int d^4x \int d^4x' \phi(x) A(x, x') \psi(x') \end{aligned} \tag{1.78}$$

Then, we can use similar expressions for integration over continuous fields by replacing, $v^T Av \to (\phi^\dagger, A\phi)$

an example of auxiliary field

Let us consider a simple case of auxiliary particle. We will show

[3] This is an analogy of

$$\int_{-\infty}^{+\infty} dx e^{-cx^2 \pm ibx} = \sqrt{\frac{\pi}{c}} e^{-b^2/4c}, \tag{1.73}$$

$$: \exp\left(-\frac{c\alpha_t}{2}\rho^2\right) := \sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty} ds : \exp\left(-\frac{1}{2}s^2 + \sqrt{-c\alpha_t}s\rho\right) : \tag{1.79}$$

This can be proved from eq. (1.72), with $D = 1$, $A^{-1} = -c\alpha_t$ and rename $v \to \sqrt{-c\alpha_t}s$,

$$\begin{aligned} & \int dv e^{-\frac{1}{2}v^2\frac{1}{-c\alpha_t}+\rho v} = \sqrt{-c\alpha_t}\int ds e^{-\frac{1}{2}s^2+\sqrt{-c\alpha_t}\rho s} \\ = \quad & (2\pi)^{1/2}e^{-\frac{1}{2}\ln(\frac{1}{-c\alpha_t})}e^{-\frac{c\alpha_t}{2}\rho^2} = (2\pi)^{1/2}\sqrt{-c\alpha_t}e^{-\frac{c\alpha_t}{2}\rho^2} \end{aligned} \tag{1.80}$$

where $e^{-\frac{1}{2}\ln(\frac{1}{-c\alpha_t})} = \sqrt{-c\alpha_t}$.

an example of auxiliary field for Non-local interaction

Let us consider a non-local interaction, with $f_{s_L}(\boldsymbol{n}' - \boldsymbol{n}) = f_{s_L}(|\boldsymbol{n}' - \boldsymbol{n}|)$,

$$\begin{aligned} & \exp(-\frac{c_0\alpha_t}{2}\sum_{n',n,n''} : \rho_{NL}(n')f_{s_L}(n'-n)f_{s_L}(n-n'')\rho_{NL}(n'') :) \\ = \quad & : \exp(-\frac{c_0\alpha_t}{2}\sum_n \left(\sum_{n'}\rho_{NL}(n')f_{s_L}(n'-n)\right)\left(\sum_{n''}f_{s_L}(n-n'')\rho_{NL}(n'')\right)) : \\ = \quad & : \exp(-\frac{c_0\alpha_t}{2}\sum_n \tilde{\rho}_{NL}(n)\tilde{\rho}_{NL}(n)) : \end{aligned} \tag{1.81}$$

From eq. (1.72) , with $A^{-1}(n,n') = -c_0\delta_{nn'}$,

$$\begin{aligned} & \exp(-\frac{c_0\alpha_t}{2}\sum_{n',n,n''} : \rho_{NL}(n')f_{s_L}(n'-n)f_{s_L}(n-n'')\rho_{NL}(n'') :) \\ \propto \quad & \int [ds]\exp\left(-\frac{1}{2}\sum_n s(n)^2 + \sqrt{-c_0\alpha_t}\sum_{nn'}\rho_{NL}(n)f_{s_L}(n-n')s(n')\right) \end{aligned} \tag{1.82}$$

Note here that there is no α_t in kinetic part of auxiliary action.(With scale $s(\boldsymbol{n}) \to \sqrt{\alpha_t}s(\boldsymbol{n})$, we get α_t factor in all action.)

Also note the sign of the coupling gives potential,

$$V_s = -\sqrt{-c_0\alpha_t}\sum_{nn'}\rho_{NL}(n)f_{s_L}(n-n')s(n'). \tag{1.83}$$

This has opposite sign with the paper , PRL119,222505. I think PRL119,222505 have a typo.

an example of auxiliary field for one-pion exchange

Consider a pion field and its derivative $\nabla_S\pi_I(\boldsymbol{n})$ using DFT,

$$\begin{aligned} \pi_I(\boldsymbol{n}) &= \frac{1}{L^3}\sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{n}}\hat{\pi}(\boldsymbol{q}), \quad \hat{\pi}(\boldsymbol{q}) = \sum_{\boldsymbol{n}} e^{-i\boldsymbol{q}\cdot\boldsymbol{n}}\pi_I(\boldsymbol{n}), \\ \nabla_S\pi_I(\boldsymbol{n}) &= \frac{1}{L^3}\sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{n}}(i\boldsymbol{q})_S\hat{\pi}(\boldsymbol{q}) \end{aligned} \tag{1.84}$$

One may introduce a function ("qhop" function $\Delta_S(\boldsymbol{n})$ or $f_S^\pi(\boldsymbol{n})$) such that

$$\begin{aligned}
\nabla_S \pi_I(\boldsymbol{n}) &= \frac{1}{L^3}\sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot\boldsymbol{n}}(i\boldsymbol{q})_S \sum_{\boldsymbol{n}'} e^{-i\boldsymbol{q}\cdot\boldsymbol{n}'}\pi_I(\boldsymbol{n}') = \frac{1}{L^3}\sum_{\boldsymbol{n}'}\pi_I(\boldsymbol{n}')\sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot(\boldsymbol{n}-\boldsymbol{n}')}(i\boldsymbol{q})_S \\
&= \sum_{\boldsymbol{n}'}\pi_I(\boldsymbol{n}')\Delta_S(\boldsymbol{n}'-\boldsymbol{n}) = \sum_{\boldsymbol{n}'}\pi_I(\boldsymbol{n}+\boldsymbol{n}')\Delta_S(\boldsymbol{n}'), \\
\Delta_S(\boldsymbol{n}-\boldsymbol{n}') &= \frac{1}{L^3}\sum_{\boldsymbol{q}} e^{-i\boldsymbol{q}\cdot(\boldsymbol{n}-\boldsymbol{n}')}(i\boldsymbol{q})_S = -\Delta_S(\boldsymbol{n}'-\boldsymbol{n}).
\end{aligned} \tag{1.85}$$

This function can be further simplified in cubic lattice as 1-D function,

$$\Delta_S(\boldsymbol{n}-\boldsymbol{n}') = \delta_{n_i,n_i'}\delta_{n_j,n_j'}\Delta_S(n_S - n_S'), \quad (i,j)\neq S. \tag{1.86}$$

Thus, we can write the πN coupling term,

$$\begin{aligned}
V_{\pi N} &= \frac{g_A}{2f_\pi}\sum_{\boldsymbol{n}}\sum_{SI}\nabla_S\pi_I(\boldsymbol{n})\rho_{SI}(\boldsymbol{n}) \\
&= \frac{g_A}{2f_\pi}\sum_{\boldsymbol{n},\boldsymbol{n}'}\sum_{SI}\pi_I(\boldsymbol{n}')f_S(\boldsymbol{n}'-\boldsymbol{n})\rho_{SI}(\boldsymbol{n}) \\
&= -\frac{g_A}{2f_\pi}\sum_{\boldsymbol{n},\boldsymbol{n}'}\sum_{SI}\rho_{SI}(\boldsymbol{n})f_S(\boldsymbol{n}-\boldsymbol{n}')\pi_I(\boldsymbol{n}')
\end{aligned} \tag{1.87}$$

For the free pion action, we may introduce $f_{\pi\pi}(\boldsymbol{n})$,

$$f_{\pi\pi}(\boldsymbol{n},\boldsymbol{n}') = \frac{1}{L^3}\sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot(\boldsymbol{n}-\boldsymbol{n}')}\hat{f}_{\pi\pi}(\boldsymbol{q}) = \frac{1}{L^3}\sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot(\boldsymbol{n}-\boldsymbol{n}')}\exp(b_\pi\boldsymbol{q}^2)(\boldsymbol{q}^2+m_\pi^2) \tag{1.88}$$

and its inverse matrix

$$f_{\pi\pi}^{-1}(\boldsymbol{n},\boldsymbol{n}') = \frac{1}{L^3}\sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot(\boldsymbol{n}-\boldsymbol{n}')}\frac{\exp(-b_\pi\boldsymbol{q}^2)}{\boldsymbol{q}^2+m_\pi^2}. \tag{1.89}$$

Thus, the Path integral with pion and coupling becomes, (Note that the sign change according to the arguments of pion and qhop function.)[4]

$$\begin{aligned}
I &\equiv \int [d\pi]\exp\left(-S_{\pi\pi}-S_{\pi N}\right) \\
&= \int [d\pi]\exp\left(-\frac{1}{2}\sum_{\boldsymbol{n},\boldsymbol{n}'}\pi_I(\boldsymbol{n})f_{\pi\pi}(\boldsymbol{n}-\boldsymbol{n}')\pi_I(\boldsymbol{n}') - \frac{g_A}{2f_\pi}\sum_{\boldsymbol{n},\boldsymbol{n}'}\sum_{SI}\pi_I(\boldsymbol{n}')f_S(\boldsymbol{n}'-\boldsymbol{n})\rho_{SI}(\boldsymbol{n})\right) \\
&= \int [d\pi]\exp\left(-\frac{1}{2}\sum_{\boldsymbol{n},\boldsymbol{n}'}\pi_I(\boldsymbol{n})f_{\pi\pi}(\boldsymbol{n}-\boldsymbol{n}')\pi_I(\boldsymbol{n}') + \frac{g_A}{2f_\pi}\sum_{\boldsymbol{n},\boldsymbol{n}'}\sum_{SI}\rho_{SI}(\boldsymbol{n})f_S(\boldsymbol{n}-\boldsymbol{n}')\pi_I(\boldsymbol{n}')\right)
\end{aligned} \tag{1.90}$$

Then from analogy with eq. (1.72), $v\to\pi_I$, $A\to f_{\pi\pi}$,

$$\begin{aligned}
-\frac{1}{2}v^TAv &\to -\frac{1}{2}\sum_{\boldsymbol{n},\boldsymbol{n}'}\pi_I(\boldsymbol{n})f_{\pi\pi}(\boldsymbol{n},\boldsymbol{n}')\pi_I(\boldsymbol{n}'), \\
+\rho^Tv &\to +\sum_{\boldsymbol{n},\boldsymbol{n}'}\frac{g_A}{2f_\pi}\rho_{SI}(\boldsymbol{n})f_S(\boldsymbol{n}-\boldsymbol{n}')\pi_I(\boldsymbol{n}')
\end{aligned} \tag{1.91}$$

[4] The numerical code uses the first form when computing pion derivative using qhop function.

Then,

$$
\begin{aligned}
I &= (2\pi)^{L^3/2}\exp\left(-\frac{1}{2}\mathrm{Tr}\ln f_{\pi\pi}\right) \\
&\quad\times\exp\left(\frac{1}{2}\left(\frac{g_A}{2f_\pi}\right)^2\sum_{\boldsymbol{n}_1\boldsymbol{n}_2,\boldsymbol{n}',\boldsymbol{n}''}\sum_{S_1,S_2,I}\rho_{S_1I}(\boldsymbol{n}')f_{S_1}(\boldsymbol{n}',\boldsymbol{n}_1)f^{-1}_{\pi\pi}(\boldsymbol{n}_1-\boldsymbol{n}_2)f^T_{S_2}(\boldsymbol{n}_2,\boldsymbol{n}'')\rho_{S_2I}(\boldsymbol{n}'')\right)
\end{aligned}
$$

By doing sum over $\boldsymbol{n}_1,\boldsymbol{n}_2$, we can define

$$
\begin{aligned}
f_{S_1S_2}(\boldsymbol{n}'-\boldsymbol{n}'') &\equiv \sum_{\boldsymbol{n}_1,\boldsymbol{n}_2} f_{S_1}(\boldsymbol{n}',\boldsymbol{n}_1)f^{-1}_{\pi\pi}(\boldsymbol{n}_1-\boldsymbol{n}_2)f^T_{S_2}(\boldsymbol{n}_2,\boldsymbol{n}'') \\
&= \left(\frac{1}{L^3}\right)^3\sum_{\boldsymbol{n}_1,\boldsymbol{n}_2}\sum_{\boldsymbol{q}_1\boldsymbol{q}\boldsymbol{q}_2} e^{i\boldsymbol{q}_1\cdot(\boldsymbol{n}'-\boldsymbol{n}_1)}(-i\boldsymbol{q}_1)_{S_1}e^{i\boldsymbol{q}\cdot(\boldsymbol{n}_1-\boldsymbol{n}_2)}\frac{e^{-b_\pi q^2}}{(\boldsymbol{q}^2+m_\pi^2)}e^{-i\boldsymbol{q}_2\cdot(\boldsymbol{n}_2-\boldsymbol{n}'')}(-i\boldsymbol{q}_2)_{S_2} \\
&= \frac{1}{L^3}\sum_{\boldsymbol{q}} e^{i\boldsymbol{q}\cdot(\boldsymbol{n}'-\boldsymbol{n}'')}\frac{q_{S_1}q_{S_2}e^{-b_\pi q^2}}{(\boldsymbol{q}^2+m_\pi^2)} = \frac{1}{L^3}\sum_{\boldsymbol{q}} e^{-i\boldsymbol{q}\cdot(\boldsymbol{n}'-\boldsymbol{n}'')}\frac{q_{S_1}q_{S_2}e^{-b_\pi q^2}}{(\boldsymbol{q}^2+m_\pi^2)}
\end{aligned}
\tag{1.92}
$$

Thus, we get

$$
I\propto\exp\left(+\frac{1}{2}\left(\frac{g_A}{2f_\pi}\right)^2\sum_{\boldsymbol{n}',\boldsymbol{n},S,S',I}\rho_{SI}(\boldsymbol{n}')f_{SS'}(\boldsymbol{n}'-\boldsymbol{n})\rho_{S'I}(\boldsymbol{n})\right) \tag{1.93}
$$

Thus, we get the OPE potential

$$
V_{OPE} = -\frac{g_A^2}{8f_\pi^2}\sum_{n'n,S',S,I}:\rho_{S',I}(n')f_{SS'}(n'-n)\rho_{S,I}(n): \tag{1.94}
$$

Note that this has different sign with paper, PRL119,222505. I think PRL119,222505 have typo by mistaking order of π_I field and qhop function.

1.7.1 Example: analytic calculation of quadratic functional

For free scalar field, we have the functional as,

$$
\begin{aligned}
W_0^E[J] &= \mathcal{N}_E\int\mathcal{D}\phi e^{-\frac{1}{2}(\phi,A\phi)+(\rho,\phi)} \\
&= \mathcal{N}_E(\det A)^{-\frac{1}{2}}e^{\frac{1}{2}(\rho,A^{-1}\rho)}
\end{aligned}
\tag{1.95}
$$

where, [5]

$$
\begin{aligned}
\mathcal{L}_E &= -\frac{1}{2}\left(\partial_\mu^E\phi\partial_\mu^E\phi+m^2\phi^2\right) = -\frac{1}{2}\phi\left(-\partial_E^2+m^2\right)\phi, \\
A(x_E,x'_E) &= (-\partial_E^2+m^2)\delta^4(x'_E-x_E), \quad \rho(x_E)=J(x_E).
\end{aligned}
\tag{1.97}
$$

If matrix $A(x,x')$ only depends on the difference, we can Fourier transform,

$$
A(x,x')=\int\frac{dk}{2\pi}e^{-ik(x'-x)}A(k). \tag{1.98}
$$

[5] In a similar way, Grassmann integration

$$
\int\mathcal{D}v^*\mathcal{D}v e^{(v^*,Av)+(v^*,\eta)+(\eta^*,v)} = [\det A]e^{-(\eta^*,A^{-1}\eta)} \tag{1.96}
$$

In a similar way, any function of matrix A, only depending on the difference, also can be F.T. ,

$$f(A)(x,x') = \int \frac{dk}{2\pi} e^{-ik(x'-x)} f(A(k)) \tag{1.99}$$

In other words, with $A(p_E) = (p_E^2 + m^2)$,(here p_E are 4-dimensional)

$$\begin{aligned} \text{Tr } \ln A(x,x') &= \int d^4x_E (\ln A)(x_E, x_E) = \int d^4x_E \int \frac{d^4p_E}{(2\pi)^4} (\ln A(p_E)) \\ &= \int d^4x_E \int \frac{d^4p_E}{(2\pi)^4} \ln(p_E^2 + m^2) \end{aligned} \tag{1.100}$$

and

$$\begin{aligned} A^{-1}(x_E, x'_E) &= \int \frac{d^4p_E}{(2\pi)^4} e^{-ip_E\cdot(x'_E - x_E)} A^{-1}(p_E) = \int \frac{d^4p_E}{(2\pi)^4} e^{-ip_E\cdot(x'_E - x_E)} \frac{1}{p_E^2 + m^2} \\ &= \Delta_F^E(x'_E - x_E) \end{aligned} \tag{1.101}$$

This implies that free two point Green's function, in Minkowski space,

$$\begin{aligned} G_0^{(2)}(x_1, x_2) &= (\frac{\hbar}{i})^2 \frac{\delta^2 W_0[J]}{\delta J(x_1)\delta J(x_2)}|_{J=0} = i\hbar \Delta_F(x_1 - x_2) \\ &= i\hbar A^{-1}(x_1, x_2) = \int \frac{d^4p}{(2\pi)^4} e^{-ip\cdot(x'-x)} \frac{i}{p^2 - m^2 + i\epsilon} \end{aligned} \tag{1.102}$$

Also, we can change

$$e^{\frac{1}{2}(\rho, A^{-1}\rho)} = (\det A)^{\frac{1}{2}} \int \mathcal{D}\phi \; e^{-\frac{1}{2}(\phi, A\phi) + (\rho,\phi)} \tag{1.103}$$

For example, we can rewrite the original action into auxiliary formalism form as,

$$\begin{aligned} & Z \propto \int \mathcal{D}\bar{N}\mathcal{D}N e^{\int d^4x \mathcal{L}_E(\bar{N}, N)}, \\ & \mathcal{L}_E(\bar{N}, N) = -\bar{N}[\partial_4 - \frac{\nabla^2}{2m} + (m - \mu)]N - \frac{1}{2}C_1 \bar{N}N\bar{N}N - \frac{1}{2}C_2 \bar{N}\vec{\tau}N \cdot \bar{N}\vec{\tau}N, \\ \rightarrow \quad & Z \propto \int \mathcal{D}\bar{N}\mathcal{D}N\mathcal{D}f\mathcal{D}\vec{\phi} e^{\int d^4x \mathcal{L}(\bar{N}, N, f, \vec{\phi})}, \\ & \mathcal{L}_E(\bar{N}, N, f, \vec{\phi}) = -\bar{N}[\partial_4 - \frac{\nabla^2}{2m} + (m - \mu)]N - \frac{1}{2} f \frac{1}{-C_1} f + \bar{N}Nf - \frac{1}{2}\vec{\phi}\frac{1}{-C_2}\vec{\phi} + \bar{N}\vec{\tau}N \cdot \vec{\phi} \\ & \simeq -\bar{N}[\partial_4 - \frac{\nabla^2}{2m} + (m - \mu)]N - \frac{1}{2} f' f' + \sqrt{-C_1}\bar{N}Nf' - \frac{1}{2}\vec{\phi}' \cdot \vec{\phi}' + \sqrt{-C_2}\bar{N}\vec{\tau}N \cdot \vec{\phi}' \end{aligned} \tag{1.104}$$

6

[6] **(ref. nucl-th/0407088)** Note here, if $C_1 < 0$, the interaction between f and Nucleon is real and if $C_1 > 0$, the interaction between f and Nucleon is complex. On the other hand, if $C_2 > 0$, the matrix $M = \exp(\mathcal{L}_E \Delta_t)$ becomes real because $\tau_2 M \tau_2 = M^*$ despite the appearance of i . However, $C_2 < 0$ makes the M to be complex.

Thus, to avoid sign problem it is better to use a form of $C_2 > 0$. Thus, though formally equivalent, $: \bar{N}N\bar{N}N := -\frac{1}{2} : \bar{N}\vec{\sigma}N \cdot \bar{N}\vec{\sigma}N : -\frac{1}{2}\bar{N}\vec{\tau}N \cdot \bar{N}\vec{\tau}N :$, it is better to use a form of

$$-\frac{1}{2}C_1 \bar{N}N\bar{N}N - \frac{1}{2}C_2 \bar{N}\vec{\tau}N \cdot \bar{N}\vec{\tau}N \tag{1.105}$$

instead of

$$-\frac{1}{2}C'_1 \bar{N}N\bar{N}N - \frac{1}{2}C'_2 \bar{N}\vec{\sigma}N \cdot \bar{N}\vec{\sigma}N \tag{1.106}$$

because $C'_1 < 0, C'_2 < 0$ but $C_2 = -C'_2 > 0, C_1 = C'_1 - 2C'_2 < 0$.

Chapter 2

Numerical method: Basic

In case of fermion integration, the basic steps to compute the lattice action and compute observables are as follows.

- Euclidean action is converted into auxiliary action

$$Z = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi e^{-S[\psi^\dagger,\psi]} \to \int \mathcal{D}\phi \mathcal{D}\psi^\dagger \mathcal{D}\psi \rho[\phi] e^{-S[\phi,\psi^\dagger,\psi]} \tag{2.1}$$

- fermion action is integrated analytically,

$$Z = \int \mathcal{D}\phi \mathcal{D}\psi^\dagger \mathcal{D}\psi \rho[\phi] e^{-S[\phi,\psi^\dagger,\psi]} \to \int \mathcal{D}\phi \rho[\phi] \det K[\phi] = \int \mathcal{D}\phi P[\phi] \tag{2.2}$$

  where, kinetic and interaction terms in action may be written as

$$S[\phi,\psi^\dagger,\psi] = \frac{1}{b_\tau} \sum_{\tau,\tau'} \psi^\dagger_{\tau'} [K(\phi)]_{\tau',\tau} \psi_\tau \tag{2.3}$$

- observable can be approximated as

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}\phi P[\phi] \mathcal{O}[\phi] \to \frac{1}{N_{cf}} \sum_n^{N_{cf}} \mathcal{O}(\phi_n) \tag{2.4}$$

  where, configurations of ϕ_n is selected according to the probability $P[\phi]$. This selection or update of ϕ_n can be done by **determinantal Monte Carlo**(Metropolis sampling), or **Hybrid Monte Carlo** method.

- one way to compute the determinant or compute integration over Grassman number is to use transfer matrix.

Basic numerical technique to compute path integral is Importance sampling Monte Carlo integration, or Metropolis algorithm,

$$\begin{aligned} \langle O \rangle &= \int D[U] P[U] O[U], \text{ with } P[U] = \frac{e^{-S[U]}}{Z}, \quad Z = \int D[U] e^{-S[U]} \\ &\simeq \frac{1}{N} \sum_{U_n \text{ with probability } P[U_n]}^{N} O[U_n] \end{aligned} \tag{2.5}$$

In general,

$$\langle\langle \Gamma[x] \rangle\rangle = \frac{\int \mathcal{D}x(t)\ \Gamma[x] e^{-S[x]}}{\int \mathcal{D}x(t)\ e^{-S[x]}} \tag{2.6}$$

With N_{cf} **number of random paths or configurations**, $x^{(\alpha)}$, if the configuration is chosen with probability $P[x^{(\alpha)}] \propto e^{-S[x^{(\alpha)}]}$, above integral can be expressed as unweighted average over path,

$$\langle\langle \Gamma[x] \rangle\rangle \simeq \bar{\Gamma} \equiv \frac{1}{N_{cf}} \sum_{\alpha=1}^{N_{cf}} \Gamma[x^{(\alpha)}]. \tag{2.7}$$

$\bar{\Gamma}$ is a MC estimation of integral. Uncertainty in MC estimation can be thought as

$$\sigma_{\bar{\Gamma}}^2 \simeq \frac{1}{N_{cf}} \left\{ \frac{1}{N_{cf}} \sum_{\alpha=1}^{N_{cf}} \Gamma^2[x^{(\alpha)}] - \bar{\Gamma}^2 \right\} \tag{2.8}$$

Updating path can be done by using Markov process in metropolis algorithm. Instead of updating path as a whole, it updates paths at each sites by the difference in action at each sites. Algorithm for randomizing x_j at j-th site is :

- generate a random number ζ with probability uniformly distributed between $-\epsilon$ and $+\epsilon$.
- replace $x_j \to x_j + \zeta$ and compute the change ΔS in the action caused by this replacement. $\Delta S = S_{new} - S_{old}$
- if $\Delta S < 0$, retain new value for x_j and proceed to next site.
- if $\Delta S > 0$, generate random number η uniformly distributed between 0 and 1; retain the new value x_j if $\exp(-\Delta S) > \eta$, otherwise restore old value;
- proceed to the next site. If this is done for all sites, it is called as one **sweep**. A random walk parameter ϵ have to be tuned so that the acceptance rate around 50% for one sweep.
- However, not every sweep will be used in the calculation. To remove correlation between sweeps, only one path per every N_{cor} sweep will be used in the calculation. The optimal value of N_{cor} depends on lattice spacing, $N_{cor} \propto 1/a^2$.

The procedure to start the algorithm, we need thermalization.

- Initialization Path
- Update $5N_{corr} - 10N_{corr}$ times to thermalize it.
- Update the path N_{corr} times, then compute $\Gamma[x]$ and save it; repeat N_{cf} times.
- average N_{cf} values of $\Gamma[x]$ saved in the previous step to obtain Monte Carlo estimate $\bar{\Gamma}$ for $\langle\langle \Gamma[x] \rangle\rangle$. Compute statistical error.

To compute **statistical error** without too large N_{cf}, we can use 'boot strap' and 'binning' method. Suppose we obtained N_{cf} values of $\{\Gamma^{(\alpha)}, \alpha = 1 \dots N_{cf}\}$. Then,

- bootstrap: generate N_{bts} copies of $\Gamma^{(\alpha)}$'s by selecting random configurations while allowing duplication and omission. Then compute statistical error from each bootstrap copies to compute uncertainty. This is only for statistical error estimates, not average estimates.
- Binning: When N_{cf} is very large, it is difficult to store all results, $\Gamma^{(\alpha)}$'s Instead, we can store average of $\Gamma^{(\alpha)}$'s with several number of configurations, $\bar{\Gamma}^{(\beta)} = \frac{1}{N_{bin}} \sum_{n=1}^{N_{bin}} \Gamma^{(\alpha)_n}$. The final results can be stored as $50 - 100\bar{\Gamma}^{(\beta)}$ results.

2.1 A simple example of MC calculation

This example shows how the world line method can be used to compute path integral.

Problem: Suppose there exists three possible states $|1\rangle, |2\rangle, |3\rangle$ and the transition probability between them at finite time interval is known, M_{ij} as

$$M = \begin{pmatrix} 1.1 & 0.1 & 0.1 \\ 0.1 & 0.8 & 0.1 \\ 0.1 & 0.1 & 0.8 \end{pmatrix}, \tag{2.9}$$

$f(n) \equiv \langle 1|M^n|1\rangle$ is a probability of getting state $|1\rangle$ after n-time interval started from $|1\rangle$ state. Compute $\frac{f(20)}{f(19)}$ by using Metropolis Monte Carlo.

Here M corresponds to the transfer matrix $e^{-H\Delta t}$. Note that this example does not involve lattice representation of states. The exact solution can be obtained easily by doing matrix product. But, how can we do this with Monte Carlo?

We may consider many possible way way to reach state $|1\rangle$. For example, series of matrix elements $M_{12}M_{22}\ldots M_{11}M_{12}M_{21}$ represent one possible path(or configuration). If we sum over every possible configuration, we get exact result. In MC, we sample only several possible configuration randomly.

$$\begin{aligned} f(n) &= \sum_{i_1 i_2 \ldots i_n = 1} M_{1 i_{n-1}} M_{i_{n-1} i_{n-2}} \ldots M_{i_1 1} \\ &= \sum_{\text{all path}} [M \cdots M]_{path} \end{aligned} \tag{2.10}$$

Here total number of possible path is $3^{(n-1)}$. Let us denote product for a path c for n-steps as $W^{(n)}[c]$ then,

$$f(n) = \sum_c W^{(n)}[c] \tag{2.11}$$

If we choose path c randomly every time, it is a simple Monte Carlo. If we update new path c_{i+1} from previous path c_i according, with a certain probability, it is a Markov chain Monte Carlo.

Suppose old path gives $W^{(20)}(old)$ and new choice of path gives $W^{(20)}(new)$. By choosing random number r and accept the update when $r \leq \frac{W^{(20)}(new)}{W^{20}(old)}$. While doing this, one also can keep track of $W^{(19)}$.

If the state at step 19 is $k(k = 1, 2, 3)$ for one path, then

$$\frac{W^{(19)}}{W^{(20)}} = \begin{cases} 1/M_{11} & \text{if k=1} \\ 0 & \text{if k=2} \\ 0 & \text{if k=3} \end{cases} \tag{2.12}$$

Because $W^{19} = 0$ if state at step 19 is not $k = 1$. This acts as an observable(or operator) to be averaged.

Average $\frac{W^{(19)}}{W^{(20)}}$ over all twenty-step paths gives $\frac{f(19)}{f(20)}$. If we sample path according to $W^{(20)}$,

$$\frac{f(19)}{f(20)} = \frac{\sum_{paths} W^{(20)} \left(\frac{W^{(19)}}{W^{(20)}}\right)}{\sum_{paths} W^{(20)}} = \frac{\sum_{sampling} \left(\frac{W^{(19)}}{W^{(20)}}\right)}{\sum_{sampling} 1} \tag{2.13}$$

Chapter 3

Fermion Path integral: Transfer Matrix formalism

How one can treat Fermion in path integral? As we can see later, the path integral of fermion field requires Grassmann variables. But, it would be difficult to realize Grassmann number integration numerically. Then how one can proceed? Let us separate the average of any operator into fermion part and boson part.

$$\langle O \rangle = \langle \, \langle O \rangle_F \rangle_G. \tag{3.1}$$

And fermion part

$$\begin{aligned} \langle A \rangle_F &= \frac{1}{Z_F[U]} \int \mathcal{D}[\psi, \bar{\psi}] \; e^{-S_F[\psi, \bar{\psi}, U]} A[\psi, \bar{\psi}, U] \\ Z_F[U] &= \int \mathcal{D}[\psi, \bar{\psi}] \; e^{-S_F[\psi, \bar{\psi}, U]} \end{aligned} \tag{3.2}$$

boson part

$$\langle B \rangle_G = \frac{1}{Z} \int \mathcal{D}[U] \; e^{-S_G[U]} Z_F[U] B[U] \tag{3.3}$$

In practice, computation of $Z_F[U]$ or $\langle O \rangle_F$ requires analytic methods or transfer matrix formalism. Once they are calculated, one can numerically compute bosonic path integral for $\langle \langle O \rangle_F \rangle_G$.

3.1 Grassmann integral

The Grassmann variables anti-commutes with each other, fermion field operators satisfy the equal time anti-commutation relations. Thus, the correspondence between fermion field and Grassmann variables are not obvious. We might introduce path integral over Grasmann variables in several different ways

Fermion operators satisfy equaltime anti-commutation relation,

$$\{\hat{a}_n, \hat{a}_m^\dagger\} = \delta_{nm}, \quad \{\hat{a}_n, \hat{a}_m\} = \{\hat{a}_n^\dagger, \hat{a}_m^\dagger\} = 0. \tag{3.4}$$

On the other hand, we introduce Grasmann numbers such that that Grassmann number χ, $\chi^\dagger$ anti-commutes with each others.

$$\{\chi_i, \chi_j^\dagger\}_+ = \{\chi_i, \chi_j\}_+ = \{\chi_i^\dagger, \chi_j^\dagger\}_+ = 0. \tag{3.5}$$

Then, Grasman integration is defined as

$$\int d\chi\ 1 = 0, \quad \int d\chi\ \chi = 1, \quad d\eta_i d\eta_j = -d\eta_j d\eta_i \tag{3.6}$$

Several basic integrals are

$$\eta_i' = \sum_{j=1}^{N} M_{ij}\eta_j \quad \rightarrow \quad d^N\eta = \det[M] d^N\eta' \tag{3.7}$$

$$\int d\eta_N d\bar{\eta}_N \dots d\eta_1 d\bar{\eta}_1 \exp\left(\sum_{i,j=1}^{N} \bar{\eta}_i M_{ij}\eta_j\right) = \det[M]. \tag{3.8}$$

$$\begin{aligned} & \int \prod_{i=1}^{N} d\eta_i d\bar{\eta}_i \exp\left(\sum_{k,l=1}^{N} \bar{\eta}_k M_{kl}\eta_l + \sum_{k=1}^{N} \bar{\theta}_k\eta_k + \sum_{k=1}^{N} \bar{\eta}_k\theta_k\right) \\ = \quad & \det[M] \exp\left(-\sum_{n,m=1}^{N} \bar{\theta}_n (M^{-1})_{nm}\theta_m\right). \end{aligned} \tag{3.9}$$

$$\begin{aligned} \langle \eta_{i_1}\bar{\eta}_{j_1} \dots \eta_{i_n}\bar{\eta}_{j_n}\rangle_F &= \frac{1}{Z_F}\int [\prod_{k=1}^{N} d\eta_k d\bar{\eta}_k]\ \eta_{i_1}\bar{\eta}_{j_1} \dots \eta_{i_n}\bar{\eta}_{j_n} \exp\left(\sum_{l,m=1}^{N} \bar{\eta}_l M_{lm}\eta_m\right) \\ &= (-1)^n \sum_{P(1,2,\dots,n)} \mathrm{sign}(P)(M^{-1})_{i_1 j_{P_1}}(M^{-1})_{i_2 j_{P_2}} \dots (M^{-1})_{i_n j_{P_n}} \end{aligned} \tag{3.10}$$

As we can see, we often need the inverse of matrix M, M^{-1}. When M_{nm} is a position space matrix, it is convenient to use its F.T. expression , M_{pq} in momentum space because this matrix is diagonal in many case. So, $M_{pq} = \delta_{pq}D(p)$ and inverse can be easily obtainable $M_{pq}^{-1} = \delta_{pq}D^{-1}(p)$. Then we can obtain $(M^{-1})_{nm}$ by Fourier transformation of M_{pq}^{-1}. (Fermion doubling occurs when the $D^{-1}(p)$ have additional poles because of lattice Fourier transformation. For example, $D^{-1}(p) \sim 1/\sin(pa)^2$ have physical pole $p = 0$ and unphysical poles $p = n\pi a$.)

3.2 Anti-periodicity of Fermion field

The periodic boundary condition in time is necessary in path integral, because we are interested in the trace of operators. In case of scalar field, it is easy to see why we impose periodic boundary condition, $\phi(T) = \phi(0)$. However, it is not easy to see why anti-periodic boundary condition is necessary for fermion. On the other hand, in path integral formalism, for fermion states, $|0\rangle$ and $|1\rangle = a^\dagger|0\rangle$, trace means

$$\mathrm{Tr}\ \hat{O} = \langle 0|\hat{O}|0\rangle + \langle 1|\hat{O}|1\rangle \tag{3.11}$$

One way to see is to compute thermal average of correlators. Thermal average is defined as

$$\langle\hat{A}\rangle_\beta = \mathrm{Tr}\ e^{-\beta\hat{H}}\hat{A}, \quad \text{with nomarlization Tr } e^{-\beta\hat{H}} = 1. \tag{3.12}$$

Then,

$$\begin{aligned} \langle\hat{\psi}(x,\tau_1)\hat{\psi}(y,0)\rangle_\beta &= \mathrm{Tr}[e^{-\beta\hat{H}}\hat{\psi}(x,\tau_1)\hat{\psi}(y,0)] = \mathrm{Tr}[\hat{\psi}(y,0)e^{-\beta\hat{H}}\hat{\psi}(x,\tau_1)] \\ &= \mathrm{Tr}[e^{-\beta\hat{H}}e^{\beta\hat{H}}\hat{\psi}(y,0)e^{-\beta\hat{H}}\hat{\psi}(x,\tau_1)] \\ &= \mathrm{Tr}[e^{-\beta\hat{H}}\hat{\psi}(y,\beta)\hat{\psi}(x,\tau_1)] \\ &= \langle\hat{\psi}(y,\beta)\hat{\psi}(x,\tau_1)\rangle_\beta \\ &= \pm\langle\hat{\psi}(x,\tau_1)\hat{\psi}(y,\beta)\rangle_\beta \end{aligned} \tag{3.13}$$

Thus, we impose $\hat{\psi}(y,\beta) = \pm\hat{\psi}(y,0)$ for *bosonic* and fermionic field operators. This is also the reason for introducing Matsubara frequency in thermal theory because the two particle Green's function is periodic(anti-periodic). So the frequency have to be $\omega_n = \frac{2n\pi}{\beta}$ for boson and $\omega_n = \frac{(2n+1)\pi}{\beta}$ for fermion.

3.3 Coherent state formalism

First, let us define coherent states

$$|\psi\rangle \equiv e^{-\psi\hat{a}^\dagger}|0\rangle = |0\rangle - \psi|1\rangle. \tag{3.14}$$

We may assume Grasman number and fermion operators anti-commutes,

$$\begin{aligned} \{\chi,\hat{a}\}_+ &= \{\chi,\hat{a}^\dagger\}_+ = 0, \\ (\psi\hat{a}^\dagger)^\dagger &= \hat{a}\psi^*, \\ |1\rangle\psi &= \hat{a}^\dagger|0\rangle\psi = -\psi|1\rangle, \\ \hat{a}|\psi\rangle &= \psi|\psi\rangle. \end{aligned} \tag{3.15}$$

Then, we define bra-states as

$$\langle\phi| \equiv \langle 0|e^{-\hat{a}\phi^*} = \langle 0| + \phi^*\langle 1| = (|\phi\rangle)^\dagger \tag{3.16}$$

Then, the scalar product of coherent states becomes

$$\langle\psi|\phi\rangle = (\langle 0| + \psi^*\langle 1|)(|0\rangle - \phi|1\rangle) = 1 - \psi^*\langle 1|\phi|1\rangle = 1 + \psi^*\phi = e^{\psi^*\phi} \tag{3.17}$$

We can see coherent states are not normlaized. So completeness relation requires compensation factor,

$$\int d\psi^* d\psi \; |\psi\rangle e^{-\psi^*\psi}\langle\psi| = I. \tag{3.18}$$

where factors $e^{-\psi^*\psi}$ enters as a kind of measure in Grasmann integrations. We can check above completeness relation,

$$\begin{aligned} \int d\psi^* d\psi e^{-\psi^*\psi}|\psi\rangle\langle\psi|\psi'\rangle &= \int d\psi^* d\psi e^{-\psi^*\psi}e^{\psi^*\psi'}|\psi\rangle = \int d\psi^* d\psi e^{-\psi^*(\psi-\psi')}|\psi\rangle \\ &= \int d\psi\delta(\psi-\psi')|\psi\rangle = |\psi'\rangle \end{aligned} \tag{3.19}$$

where the delta function is defined as

$$\delta(\psi-\psi') = \int d\chi e^{\chi(\psi-\psi')} \tag{3.20}$$

[1] Then, let us consider matrix elements for bosonic operator $\hat{O}$,

$$\begin{aligned} \langle\eta|\hat{O}|\chi\rangle &= (\langle 0| + \eta^*\langle 1|)\hat{O}(|0\rangle - \chi|1\rangle) = \langle 0|\hat{O}|0\rangle + \eta^*\langle 1|\hat{O}|0\rangle - \langle 0|\hat{O}\chi|1\rangle - \eta^*\langle 1|\hat{O}\chi|1\rangle \\ &= \langle 0|\hat{O}|0\rangle + \eta^*\chi\langle 1|\hat{O}|1\rangle. \end{aligned} \tag{3.22}$$

[1] Careful that, in case of many particle states,

$$e^{-\sum\chi_i} = \sum_n \frac{1}{n!}(-\sum\chi_i)^n \neq 1 - \sum_i \chi_i \tag{3.21}$$

[2] Note that $\langle\eta|\hat{O}|\chi\rangle$ is not a c-number. Then, we can see that

$$\begin{aligned}\int d\eta^* d\eta \langle\eta|\hat{O}|\eta\rangle e^{-\eta^*\eta} &= \langle 0|\hat{O}|0\rangle - \langle 1|\hat{O}|1\rangle, \\ \int d\eta^* d\eta \langle -\eta|\hat{O}|\eta\rangle e^{-\eta^*\eta} &= \langle 0|\hat{O}|0\rangle + \langle 1|\hat{O}|1\rangle \end{aligned} \tag{3.24}$$

Thus, the Euclidean partition function in fermion path integral have to be defined as

$$\langle\hat{O}\rangle_T = \mathrm{Tr}\ e^{-T\hat{H}}\hat{O} = \int d\eta^* d\eta \langle -\eta|e^{-T\hat{H}}\hat{O}|\eta\rangle e^{-\eta^*\eta}. \tag{3.25}$$

This implies that we need anti-periodic-time boundary condition for Grasmann variable. $\eta(T) = -\eta(0)$.

3.4 Transfer matrix formalism 1

Ref: M.Lüscher, Commun.math.Phys. 54(1977)283. (Is this reference correct? Probably, it have to be replaced with M.Creutz, Phys.Rev.D38(1988)1228 .)

As similar as coherent states, we can use isomorphism between Fock space vectors

$$|k_1, k_2, \dots k_j\rangle = \hat{a}^\dagger_{k_1}\hat{a}^\dagger_{k_2}\dots\hat{a}^\dagger_{k_j}|0\rangle \leftrightarrow \chi^*_{k_1}\chi^*_{k_2}\dots\chi^*_{k_j}.$$

From now on, let us use χ represent set of Grassman numbers $\{\chi_1, \chi_2 \dots\}$. And represent general Fock space vector $|X\rangle = X(\hat{a}^\dagger)|0\rangle \leftrightarrow X(\chi^*)$. [3]

Also use notation for short, for n-dimensional Grassmann numbers,

$$\begin{aligned}\chi^*\eta &\equiv \sum_j \chi^*_j\eta_j, \\ \int [d\eta] &\equiv \int d\eta_n \dots d\eta_1, \quad [d\eta^*][d\eta] = (-1)^n [d\eta][d\eta^*] \\ \int [d\eta^* d\eta] &\equiv \int d\eta^*_n d\eta_n \dots d\eta^*_1 d\eta_1 = (-1)^n \int [d\eta d\eta^*] = (-1)^{n-1}\int [d\eta^*][d\eta] \end{aligned} \tag{3.26}$$

Then, we wiil assoicitaes the scalar product $\langle X|Y\rangle$ as [4]

$$\langle X|Y\rangle = \int d\eta^*_n d\eta_n \dots d\eta^*_1 d\eta_1 e^{-\sum_{j=1}^n \eta^*_j\eta_j} (X(\eta^*))^\dagger Y(\eta^*) \tag{3.28}$$

Here, note that the integration with $e^{-\sum_{j=1}^n \eta^*_j\eta_j}$ factor is introduced to be consistent with normalization.(Unlike previous coherent formalism.)

Representation of operators in Grassmann number can be associated from matrix elements of operators $\hat{A}(\hat{a}^\dagger, \hat{a})$ as

$$A(k_1, \dots, k_j|l_1, \dots l_i) \equiv \langle k_1, \dots, k_j|\hat{A}|l_1, \dots l_i\rangle = \langle 0|\hat{a}_{k_j}\dots\hat{a}_{k_1}\hat{A}\hat{a}^\dagger_{l_1}\dots\hat{a}^\dagger_{l_i}|0\rangle \tag{3.29}$$

[2] If $\hat{O} = c_0 + c_2\hat{a}^\dagger\hat{a}$, then $\langle 0|\hat{O}|0\rangle = c_0$ and $\langle 1|\hat{O}|1\rangle = c_0 + c_2$ and

$$\langle\eta|\hat{O}|\eta'\rangle = c_0 + \eta^*\eta'(c_0 + c_2) = (1 + \eta^*\eta')c_0 + \eta^*\eta' c_2 = e^{+\eta^*\eta'}(c_0 + \eta^*\eta' c_2) \tag{3.23}$$

[3] for example, $|0\rangle \leftrightarrow 0,\ |k_1\rangle \leftrightarrow \chi^*_{k_1}$.

[4]

$$\begin{aligned}\langle k_1|k_1\rangle &= \int d\eta^*_1 d\eta_1 e^{-\eta^*_1\eta_1}(\eta^*_1)^*\eta^*_1, \\ \langle k_1, k_2|k_1 k_2\rangle &= \int d\eta^*_1 d\eta^*_2 d\eta_1 d\eta_2 e^{-\eta^*_1\eta_1 - \eta^*_2\eta_2}\eta_2\eta_1\eta^*_1\eta^*_2 \end{aligned} \tag{3.27}$$

$$\bar{A}(\chi^*,\chi) \equiv \sum_{\{k\},\{l\}} \frac{1}{j!i!}\chi^*_{k_1}\dots\chi^*_{k_j}A(k_1,\dots,k_j|l_1,\dots l_i)\chi_{l_1}\dots\chi_{l_i} \tag{3.30}$$

This definition of $A(\chi^*,\chi)$ satisfies

$$(\bar{A}X)(\chi^*) = \int db^*_n db_n \dots db^*_1 db_1 e^{-\sum_{j=1}^n b^*_j b_j}\bar{A}(\chi^*,b)X(b^*) \tag{3.31}$$

similar to integral kernel.

Product of two operators,

$$(\bar{A}\cdot\bar{B})(\chi^*,\chi) = \int db^*_n db_n \dots db^*_1 db_1 e^{-\sum_{j=1}^n b^*_j b_j}\bar{A}(\chi^*,b)\bar{B}(b^*,\chi) \tag{3.32}$$

And the trace of operator is given by

$$\begin{aligned}
\text{Tr } \bar{A} &= \int d\chi^*_n \dots d\chi_1 e^{-\sum_{j=1}^n \chi^*_j\chi_j}\bar{A}(\chi^*,-\chi) \\
\text{Tr } \overline{AB} &= \int [d\chi^* d\chi] e^{-\chi^*\chi}\overline{AB}(\chi^*,-\chi) \\
&= \int [d\chi^* d\chi] e^{-\chi^*\chi}\int [d\eta^* d\eta] e^{-\eta^*\eta}\bar{A}(\chi^*,\eta)\bar{B}(\eta^*,-\chi)
\end{aligned} \tag{3.33}$$

For example, (1) if there is only two states, $|0\rangle$ and $|1\rangle$,

$$\begin{aligned}
&: \hat{A} := c_0 + c_2\hat{a}^\dagger\hat{a} \\
\leftrightarrow\quad &\bar{A}(\chi^*,\chi) = c_0 + (c_0+c_2)\chi^*\chi = e^{\chi^*\chi}(c_0 + c_2\chi^*\chi)
\end{aligned} \tag{3.34}$$

One can verify the equivalence $\text{Tr} : \hat{A} := \int d\chi^*_n \dots d\chi_1 e^{-\sum_{j=1}^n \chi^*_j\chi_j}\bar{A}(\chi^*,-\chi)$. In a similar way, (2) if there are four states $|0\rangle, |1_1\rangle, |1_2\rangle, |1_1 1_2\rangle$,

$$\begin{aligned}
&: \hat{A} := c_{00} + c_{20}\hat{a}^\dagger_1\hat{a}_1 + c_{02}\hat{a}^\dagger_2\hat{a}_2 + c_{22}\hat{a}^\dagger_1\hat{a}_1\hat{a}^\dagger_2\hat{a}_2 \\
\leftrightarrow\quad &\bar{A}(\chi^*,\chi) = e^{\chi^*_1\chi_1+\chi^*_2\chi_2}(c_{00} + c_{20}\chi^*_1\chi_1 + c_{02}\chi^*_2\chi_2 + c_{22}\chi^*_1\chi_1\chi^*_2\chi_2)
\end{aligned} \tag{3.35}$$

Another examples are

$$\hat{A} = e^{\sum_{k,l}\hat{a}^\dagger_k M_{kl}\hat{a}_l} \quad\leftrightarrow\quad \bar{A}(\chi^*,\chi) = e^{\sum_{kl}\chi^*_k(e^M)_{kl}\chi_l}, \tag{3.36}$$

$$\hat{A} = e^{\sum_{k,l}\hat{a}^\dagger_k M_{kl}\hat{a}_l}e^{\sum_{k,l}\hat{a}^\dagger_k N_{kl}\hat{a}_l} \quad\leftrightarrow\quad \bar{A}(\chi^*,\chi) = e^{\sum_{kl}\chi^*_k(e^M e^N)_{kl}\chi_l}. \tag{3.37}$$

Under change of variables, $\eta_k = \sum_l A_{kl}\chi_l$ and $\eta^*_k = \sum_l A^*_{kl}\chi^*_l$,

$$\int d\chi^*_n \dots d\chi_1 f(\chi,\chi^*) = |\text{det}A|^2 \int d\eta^*_n \dots d\eta_1 f(A^{-1}\eta, (A^*)^{-1}\eta^*) \tag{3.38}$$

3.5 Transfer matrix formalism 2

However, previous definition of A operator is not convenient to use because of additional factor. If we use convention Grassmann functional corresponding to operator as

$$\hat{A}(\hat{a}^\dagger,\hat{a}) \leftrightarrow A(\chi^*,\chi) \tag{3.39}$$

Previous Grassmann functional becomes

$$: \hat{A}(\hat{a}^\dagger,\hat{a}) :\to \bar{A}(\chi^*,\chi) \to e^{\chi^*\chi}A(\chi^*,\chi) \tag{3.40}$$

Then we can write

$$\begin{aligned} \mathrm{Tr}\ :A: &= \int [d\chi^* d\chi]\ e^{-2\chi^*\chi} A(\chi^*, -\chi) \\ &= \int [d\chi d\chi^*]\ e^{2\chi^*\chi} A(\chi^*, \chi) \end{aligned} \tag{3.41}$$

where, we changed variable and orders of $d\chi^* d\chi$ in second line.

In other way, if there is a periodic condition $c(1) = -c(0)$, we can rewrite as

$$\mathrm{Tr}\ :f(a, a^\dagger): = \int [dc(0)dc^*(0)]\ e^{c^*(0)(c(0)-c(1))} A(c(0), c^*(0)) \tag{3.42}$$

In a similar way, product of operators can be rewritten in a similar form .

$$\begin{aligned} \mathrm{Tr}\ :A::B: &= \int [d\chi^* d\chi] e^{-\chi^*\chi} \int [d\eta^* d\eta] e^{-\eta^*\eta} e^{\chi^*\eta} e^{-\eta^*\chi} A(\chi^*, \eta) B(\eta^*, -\chi) \\ &= \int [d\chi^*][d\chi][d\eta^*][d\eta] e^{-\chi^*\chi} e^{-\eta^*\eta} e^{\chi^*\eta} e^{-\eta^*\chi} A(\chi^*, \eta) B(\eta^*, -\chi) \\ &= \int [d\eta][d\chi^*][d\chi][d\eta^*] e^{\chi^*\chi} e^{-\eta^*\eta} e^{\chi^*\eta} e^{\eta^*\chi} A(\chi^*, \eta) B(\eta^*, \chi). \end{aligned} \tag{3.43}$$

Let us rename $\chi^* \to \chi_1^*$, $\eta \to \chi_1$, $\eta^* \to \chi_2^*$ and $\chi \to \chi_2$. Then

$$\begin{aligned} \mathrm{Tr}\ :A::B: &= \int [d\chi_1 d\chi_1^*][d\chi_2 d\chi_2^*] e^{\chi_1^*\chi_2} e^{-\chi_2^*\chi_1} e^{\chi_1^*\chi_1} e^{\chi_2^*\chi_2} A(\chi_1^*, \chi_1) B(\chi_2^*, \chi_2) \\ &= \int [d\chi_1 d\chi_1^*][d\chi_2 d\chi_2^*] e^{\chi_1^*(\chi_1+\chi_2)} e^{\chi_2^*(\chi_2-\chi_1)} A(\chi_1^*, \chi_1) B(\chi_2^*, \chi_2) \\ &= \int [d\chi_1 d\chi_1^*][d\chi_0 d\chi_0^*] e^{\chi_1^*(\chi_1+\chi_0)} e^{\chi_0^*(\chi_0-\chi_1)} A(\chi_1^*, \chi_1) B(\chi_0^*, \chi_0) \end{aligned} \tag{3.44}$$

Now the general relation between trace of operators and Grassman path integral is

$$\begin{aligned} &\mathrm{Tr}\left\{ :F_{L_t-1}[a^\dagger(\boldsymbol{n}'), a(\boldsymbol{n})] : \times \cdots \times : F_0[a^\dagger(\boldsymbol{n}'), a(\boldsymbol{n})] : \right\} \\ = &\int DcDc^* \exp\left[\sum_{n_t=0}^{L_t-1} \sum_{\boldsymbol{n},i} c_i^*(\boldsymbol{n}, n_t)[c_i(\boldsymbol{n}, n_t) - c_i(\boldsymbol{n}, n_t+1)] \right] \prod_{n_t=0}^{L_t-1} F_{n_t}[c_{i'}^*(\boldsymbol{n}', n_t), c_i(\boldsymbol{n}, n_t)]. \\ &\text{with } c_i(\boldsymbol{n}, L_t) = -c_i(\boldsymbol{n}, 0) \end{aligned} \tag{3.45}$$

There are several characteristic and implication of this equation.

- This implies that one can replace the path integral over Grassman variable into an operator relation.
- Though it is possible to compute right-hand side analytically in a perturbation theory, the left-hand side can be done even in non-perturvative case by explicitly computing action of creation and annihilation operators.
- Note that the Trace implies the sum of results of actions of operators on all possible states.

- In right side, Grassman numbers have time dependence. In left side, operator themselves have no time dependence.

If we define new Matrix $\mathcal{F}$, above product of normal ordered operators can be considered as a standard form,

$$\int [DcDc^*]\ e^{c^*\mathcal{F}c} = \det[\mathcal{F}], \tag{3.46}$$

with $\mathcal{F}$ have matrix elements

$$c^*\mathcal{F}c = \sum_{n_t=0}^{L_t-1}\sum_{\boldsymbol{n},i} c^*(\boldsymbol{n},n_t)[c_i(\boldsymbol{n},n_t) - c_i(\boldsymbol{n},n_t+1)] + \log\left(\prod_{n_t=0}^{L_t-1} F_{n_t}[c^*_{i'}(\boldsymbol{n}',n_t), c_i(\boldsymbol{n},n_t)]\right) \tag{3.47}$$

In other words, the standard form of path integral can be recovered if we choose

$$\log\left(\prod_{n_t=0}^{L_t-1} F_{n_t}[c^*_{i'}(\boldsymbol{n}',n_t), c_i(\boldsymbol{n},n_t)]\right) \to \sum_{n_t=0}^{L_t-1} \hat{H}[c^*(n,n_t), c(n,n_t)] \tag{3.48}$$

Thus, if we choose transfer matrix, we can write partition function as

$$\begin{aligned} Z &= \mathrm{Tr}(M^{L_t}), \\ M &= :\exp\left[-\alpha_t \hat{H}(a^\dagger, a)\right]: \end{aligned} \tag{3.49}$$

Note here the trace is for any multi particle states and M is an operator acting on states. This is equivalent to the ordinary form

$$Z = \int DcDc^* \exp[-S(c,c^*)] \tag{3.50}$$

Note that though the action $S(c,c^*)$ in path integral have time derivative but the action $M = e^{-H\alpha_t}$ in transfer matrix does not have time derivative.

In a more general case of auxiliary field or bosons, only fermion part of path integral is converted into transfer matrix form and path integral over auxiliary particle or bosons is done numerically. Roughly speaking, the actual numerical calculation is done with

$$Z = \int Dse^{-S(s)}\mathrm{Tr}[M_A^{L_t}(s)] \tag{3.51}$$

3.5.1 Another derivation of Creutz(?) formula

Consider one component fermion $|0\rangle$ and $|1\rangle = a^\dagger|0\rangle$. For $|i\rangle = |0\rangle$ or $|1\rangle$, we can prove following identity,

$$\langle i| : f(a,a^\dagger) : |j\rangle = f_{ij} = \overrightarrow{\left(\frac{\partial}{\partial c^*}\right)^i}\left[e^{c^*c} f(c,c^*)\right]\overleftarrow{\left(\frac{\partial}{\partial c}\right)^j}\Big|_{c=0,c^*=0}. \tag{3.52}$$

by considering four possible cases, $f(a,a^\dagger) = 1$, a, $a^\dagger$, $a^\dagger a$. (For example, if $f = a$, $f_{ij} = \delta_{i0}\delta_{j1}$ in both expression.)

Then, we can express trace of operators as

$$\begin{aligned} \mathrm{Tr} : f(a,a^\dagger) : &= \sum_{i=0,1}\langle i| : f(a,a^\dagger) : |i\rangle = \sum_{i=0,1}\overrightarrow{\left(\frac{\partial}{\partial c^*}\right)^i}\left[e^{c^*c} f(c,c^*)\right]\overleftarrow{\left(\frac{\partial}{\partial c}\right)^i}\Big|_{c=0,c^*=0} \\ &= \int dcdc^* e^{c^*c} f(c,c^*) \end{aligned} \tag{3.53}$$

Because of the equivalence between derivative and integration of Grassman number,

$$\int dc \leftrightarrow \frac{\partial}{\partial c}, \quad \int dc^* \leftrightarrow \frac{\partial}{\partial c^*}. \tag{3.54}$$

$$\int dc\ 1 = 0 = \int dc^*\ 1 \tag{3.55}$$

$$\int dc_a\ c_b = \delta_{ab} = \int dc_a^*\ c_b^* \tag{3.56}$$

On the other hand , matrix product is

$$\sum_{i=0,1} f(a)|i\rangle\langle i|g(a^\dagger) = f(c')\overleftarrow{\left(\frac{\partial}{\partial c'}\right)^i}\overrightarrow{\left(\frac{\partial}{\partial c^*}\right)^i} g(c^*)\Big|_{c=0,c^*=0} = \int (-1)dc'dc^* e^{-c^*c} f(c')g(c^*) \tag{3.57}$$

Then,

$$\begin{aligned}
&\mathrm{Tr} : f_{L_t-1}(a,a^\dagger) :: f_{L_t-2}(a,a^\dagger) : \cdots : f_0(a,a^\dagger) : \\
&= \sum_{i_{L_t-1}, i_{L_t-2} \ldots i_0} \langle i_0| : f_{L_t-1}(a,a^\dagger) : |i_{L_t-1}\rangle\langle i_{L_t-1}| : f_{L_t-2}(a,a^\dagger) : |i_{L_t-2}\rangle \ldots \langle i_1| : f_0(a,a^\dagger) : |i_0\rangle \\
&= \int dc(0)dc^*(L_t-1) e^{c^*(L_t-1)c(0)} e^{c^*(L_t-1)c(L_t-1)} f_{L_t-1}(c,c^*) \\
&\quad \times(-1)dc(L_t-1)dc^*(L_t-2) e^{-c^*(L_t-2)c(L_t-1)} \times \ldots \\
&\quad \times(-1)dc(1)dc^*(0) e^{-c^*(0)c(1)} e^{c^*(0)c(0)} f_0(c(0),c^*(0))
\end{aligned} \tag{3.58}$$

change order in measure,

$$\begin{aligned}
& dc(0)dc^*(L_t-1)(-1)dc(L_t-1)dc^*(L_t-2)\ldots(-1)dc(1)dc^*(0) \\
= \quad & dc(L_t-1)dc^*(L_t-1)\ldots dc(0)dc^*(0) = DcDc^*
\end{aligned} \tag{3.59}$$

Thus,

$$\begin{aligned}
&\mathrm{Tr} : f_{L_t-1}(a,a^\dagger) :: f_{L_t-2}(a,a^\dagger) : \cdots : f_0(a,a^\dagger) : \\
&= \int DcDc^* \exp\left(\sum_{n_t=0}^{L_t-1} c^*(n_t)[c(n_t)-c(n_t+1)]\right) f_{L_t-1}(c(L_t-1),c^*(L_t-1))\ldots f_0(c(0),c^*(0)) \\
&\quad \text{with} \quad c(L_t) = -c(0)
\end{aligned} \tag{3.60}$$

3.6 Auxiliary Field

Let us consider the simple action,

$$Z = \int DcDc^* \exp[-S(c,c^*)], \quad S(c,c^*) = S_{free}(c,c^*) + C\alpha_t \sum_{\boldsymbol{n},n_t} \rho_\uparrow(\boldsymbol{n},n_t)\rho_\downarrow(\boldsymbol{n},n_t). \tag{3.61}$$

with

$$\begin{aligned}
S_{free}(c,c^*) \quad = \quad & \sum_{\boldsymbol{n},n_t,i=\uparrow,\downarrow} [c_i^*(\boldsymbol{n},n_t)c_i(\boldsymbol{n},n_t+1) - c_i^*(\boldsymbol{n},n_t)c_i(\boldsymbol{n},n_t)] \\
& +h \sum_{\boldsymbol{n},n_t,i=\uparrow,\downarrow} 3\cdot 2c_i^*(\boldsymbol{n},n_t)c_i(\boldsymbol{n},n_t) \\
& -h \sum_{\boldsymbol{n},n_t,i=\uparrow,\downarrow} \sum_{l=1,2,3} [c_i^*(\boldsymbol{n},n_t)c_i(\boldsymbol{n}+\hat{l},n_t) + c_i^*(\boldsymbol{n},n_t)c_i(\boldsymbol{n}-\hat{l},n_t)]
\end{aligned} \tag{3.62}$$

When the interaction involves more than two fermion field, we can not do integration manually because it is not in Gaussian integral form. In that case, we can use auxiliary field to make the interaction to be linear in two fermion field.

$$\begin{aligned} Z &= \prod_{\boldsymbol{n},n_t} \left[\int d_A s(\boldsymbol{n},n_t) \right] \int DcDc^* \exp[-S_A(c,c^*,s)], \\ S_A(c,c^*,s) &= S_{free}(c,c^*) - \sum_{\boldsymbol{n},n_t} A[s(\boldsymbol{n},n_t)]\rho(\boldsymbol{n},n_t) \end{aligned} \tag{3.63}$$

such that[5]

$$\begin{aligned} \int d_A s(\boldsymbol{n},n_t)\ 1 &= 1, \\ \int d_A s(\boldsymbol{n},n_t) A[s(\boldsymbol{n},n_t)] &= 0, \\ \int d_A s(\boldsymbol{n},n_t) A^2(s(\boldsymbol{n},n_t)) &= -C\alpha_t. \end{aligned} \tag{3.65}$$

This is equivalent to previous fermion partition function after integration over $s(\boldsymbol{n},n_t)$.

In a similar way, we can introduce auxiliary field in transfer matrix form,

$$Z = \prod_{\boldsymbol{n},n_t} [\int d_A s(\boldsymbol{n},n_t)] \mathrm{Tr}\{M_A(s,L_t-1)\dots M_A(s,0)\}, \tag{3.66}$$

$$M_A(s,n_t) =: \exp\left[-\alpha_t \hat{H}_{free} + \sum_{\boldsymbol{n}} A[s(\boldsymbol{n},n_t)]\rho(\boldsymbol{n}) \right] : \tag{3.67}$$

where $\hat{H}_{free}$ have kinetic energy part of fermion and all interactions are described by the coupling of auxiliary field and nucleon density. (Time derivatives are already included in the formalism and $\hat{H}_{free}$ only have spatial derivatives) And $d_A s(n,n_t)$ includes actions of auxiliary particles.

As we can see now the transfer matrix is a function of auxiliary field, but it is linear in fermion density. Thus, the transfer matrix acts each nucleon separately linked by auxiliary field.

Now the numerical calculation is done roughly

- setup auxiliary filed configuration $s(n_t,\boldsymbol{n})$ for every time and lattice points.
- compute the fermion trace for transfer matrix **(How to compute this is explained later)**
- update auxiliary field configuration according to the probability distribution(which is calculated using previous transfer matrix elements) **(How to update the configuration is explained in section about Metropolis or hybrid Monte carlo algorithm.)**
- repeat the above procedure with many configurations

[5] Exact form of auxiliary field measure varies as long as they satisfy conditions. Some example is

$$\begin{aligned} \int d_A s(\boldsymbol{n},n_t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds(\boldsymbol{n},n_t) e^{-\frac{1}{2}s^2(\boldsymbol{n},n_t)}, \\ A[s(\boldsymbol{n},n_t)] &= \sqrt{-C\alpha_t}\, s(\boldsymbol{n},n_t) \end{aligned} \tag{3.64}$$

- take average over all configurations
- In many case, we have to test dependence on L_t. Thus, repeat the above steps to obtain $\mathcal{O}(L_t)$ functions and extrapolate to get physical values.

This part requires further explanation. More detailed treatment of auxiliary field is already introduce in the first chapter.

3.7 chemical potential

For the case of chemical potential or any operators, we can use following relation to make it normal ordered.

$$e^{\alpha a^\dagger a} = 1 + (e^\alpha - 1)a^\dagger a =: e^{(e^\alpha - 1)a^\dagger a} :, \tag{3.68}$$

Because, for any parameter α,

$$e^{\alpha a^\dagger a}|0\rangle = 1|0\rangle, \quad e^{\alpha a^\dagger a}|1\rangle = e^\alpha|1\rangle. \tag{3.69}$$

Thus, any operator should be written as normal ordered as

$$\exp[a_i^\dagger X_{ij} a_j] = :\exp[a_i^\dagger (e^X - 1)_{ij} a_j]: \tag{3.70}$$

3.8 Long range interaction in auxiliary field formalism

In previous subsection we rewrote the 4-fermion contact interaction in terms of auxiliary field. Then how can we represent the long range interaction among fermions or smeared contact interaction in terms of auxiliary field?

$$\Delta S = \sum_{\boldsymbol{n},\boldsymbol{n}',n_t} \rho(\boldsymbol{n}) V(\boldsymbol{n} - \boldsymbol{n}') \rho(\boldsymbol{n}', n_t) \tag{3.71}$$

One example can be found in the first chapter.

3.9 Fermion transfer amplitude calculation

Let us consider fermion transfer matrix with auxiliary field. By the introduction of auxiliary field, all operators in the action becomes one-body operators.

$$M_A(s, n_t) =: \exp\left[-\alpha_t \hat{H}_{free} + \sum_{\boldsymbol{n}} A[s(\boldsymbol{n}, n_t)]\rho(\boldsymbol{n})\right] : \tag{3.72}$$

Then, physical spectrum of N-body fermion system can be obtained by computing,

$$Z_\Psi = \prod_{\boldsymbol{n},n_t} [\int d_A s(\boldsymbol{n}, n_t)] \langle\Psi|\{M_A(s, L_t - 1)\dots M_A(s, 0)\}|\Psi\rangle, \tag{3.73}$$

with proper N-body state $|\Psi\rangle$ which have quantum number of system of interests. We will use following identity,

For N free fermion states with momentum $\boldsymbol{k}$'s($\boldsymbol{k}_{i=1,N}$), $|\Psi\rangle$ is a slater determinant ground state wave function on lattice.

For $\Psi = |\phi_{\boldsymbol{k}1}, \dots \phi_{\boldsymbol{k}N}\rangle$,

$$\langle\Psi|M(s, L_t - 1)\dots M(s, 0)|\Psi\rangle = \det X(s) \tag{3.74}$$

where

$$X_{\boldsymbol{k},\boldsymbol{k}'}(s) = \langle\phi_{\boldsymbol{k}}|M(s, L_t - 1)\dots M(s, 0)|\phi'_{\boldsymbol{k}}\rangle \tag{3.75}$$

with single particle state $\phi_{\boldsymbol{k}}$ have momentum $\boldsymbol{k}$.

This means that we can compute the amplitude as

$$Z_\Psi(t) = \int D\pi Ds \exp[-S_{\pi\pi} - S_{ss}] \det X(\pi, s, ; t). \tag{3.76}$$

and X_{ij} matrix ,$i, j = 1, \dots A$ can be calculated by only computing single particle operators.

In other words, we don't even need to construct slater determinant wave function $|\Psi\rangle$ itself. Only prepare N different single particle wave functions and compute all $X_{k,k'}(s)$ separately. Then, one can compute the action by $\det X$. Thus actual numerical calculation only involves computing $X_{kk'}(s)$ using operators.

3.9.1 proof

We can create a single-nucleon state using creation operators acting on the vacuum with coefficient function $f(\boldsymbol{n})$. $f(\boldsymbol{n})$ is written as a column vector in the space of nucleon spin and isospin components, and the single-nucleon state can be

$$|f\rangle = \sum_{\boldsymbol{n}} a^\dagger(\boldsymbol{n}) f(\boldsymbol{n})|0\rangle. \tag{3.77}$$

View identical nucleons as having a hidden index $j = 1, \dots A$ that makes all of the nucleons distinguishable. If we anti-seymmetrize all physical states over this extra index then all physical observables are exactly recovered. (Actually this is the slater determinant of single particle wave functions.) So, A-body initial state to be a slater determinant of single nucleon states,(thus, actually the index is for state index of single particle wave function, not a particle index.)

$$\begin{aligned}
|f_1, \dots, f_A\rangle &= \left[\sum_{\boldsymbol{n}} a^\dagger(\boldsymbol{n}) f_1(\boldsymbol{n})\right] \cdots \left[\sum_{\boldsymbol{n}} a^\dagger(\boldsymbol{n}) f_A(\boldsymbol{n})\right] |0\rangle \\
&= \frac{1}{\sqrt{A!}} \sum_P \left[\sum_{\boldsymbol{n}} a^\dagger_{P(1)}(\boldsymbol{n}) f_1(\boldsymbol{n})\right] \cdots \left[\sum_{\boldsymbol{n}} a^\dagger_{P(A)}(\boldsymbol{n}) f_A(\boldsymbol{n})\right] |0\rangle \\
&= \frac{1}{\sqrt{A!}} \sum_{P'} \mathrm{sgn}(P') \left[\sum_{\boldsymbol{n}} a^\dagger_{[1]}(\boldsymbol{n}) f_{P'(1)}(\boldsymbol{n})\right] \cdots \left[\sum_{\boldsymbol{n}} a^\dagger_A(\boldsymbol{n}) f_{P'(A)}(\boldsymbol{n})\right] |0\rangle.
\end{aligned} \tag{3.78}$$

where the summations are over all permutations P. With these hidden indices, (the Hamiltonian also have to be changed with index J, $a_i^\dagger,\ a_i \to a_{i,J}^\dagger,\ a_{i,J}$) normal-ordered auxiliary-field transfer

matrix $M^{(n_t)}(s)$ becomes

$$\begin{aligned} M_A^{(n_t)}(s) &= :\exp\left[\sum_J\left(-\alpha_t\hat{H}^J_{free}+\sum_{\boldsymbol{n}}A[s(\boldsymbol{n},n_t)]\rho^J(\boldsymbol{n})\right)\right]: \\ &= \prod_J :\exp\left[-\alpha_t\hat{H}^J_{free}+\sum_{\boldsymbol{n}}A[s(\boldsymbol{n},n_t)]\rho^J(\boldsymbol{n})\right] := \prod_J M_J(s) \\ &= \left[1-H^{(n_t)}(a^\dagger_{[1]},a_{[1]},s)\alpha_t\right]\cdots\left[1-H^{(n_t)}(a^\dagger_{[A]},a_{[A]},s)\alpha_t\right] \end{aligned} \tag{3.79}$$

where $M_J(s)$ only acts on $|\phi\rangle_J$. Thus, transfer matrix is factorized into product of one-particle operators. Thus,

$$Z(n_t) = \langle f_1\dots f_A|M^{(n_t-1)}(s)\dots M^{(0)}(s)|f_1\dots f_A\rangle \tag{3.80}$$

can be calculated as

$$\frac{1}{\sqrt{N!}}\sum_{j'_n}\frac{1}{\sqrt{N!}}\sum_{j_n}\epsilon_{j'_1\dots j'_n}\epsilon_{j_1\dots j_n}\langle\phi_{j'_1}|M_1(s,L_t-1)\dots M_1(s,0)|\psi_{j_1}\rangle_1\cdots\langle\phi_{j'_N}|M_N(s,L_t-1)\dots M_N(s,0)|\psi_{j_N}\rangle_N \tag{3.81}$$

Because the matrix elements are all equivalent for 'hidden' index, we can define matrix X such that

$$X_{j'j}(s)=\langle\phi_{j'}|M(s,L_t-1)\dots M(s,0)|\phi_j\rangle, \tag{3.82}$$

and

$$\langle\Psi|M(s,L_t-1)\dots M(s,0)|\Psi\rangle=\frac{1}{N!}\sum_{j'_n}\sum_{j_n}\epsilon_{j'_1\dots j'_n}\epsilon_{j_1\dots j_n}X_{j'_1j_1}(s)\dots X_{j'_Nj_N}(s)=\det X(s) \tag{3.83}$$

3.9.2 example in 2-body case.

As an illustrative example, consider anti-symmetric two fermion states $|k_1k_2\rangle$ and only one transfer matrix. Let us consider general action as $\sum_{ij}a^\dagger_ia_jA_{ij}$,

$$M =: \exp(\sum_{ij}a^\dagger_ia_jA_{ij}): \tag{3.84}$$

Then, we have amplitude

$$\begin{aligned} \langle k_1k_2|M|k_1k_2\rangle &= \langle k_1k_2|:\left(1+(\sum a^\dagger aA)+\frac{1}{2}(\sum a^\dagger aA)^2\right):|k_1k_2\rangle \\ &= 1+A_{k_1k_1}+A_{k_2k_2}+A_{k_1k_1}A_{k_2k_2}-A_{k_1k_2}A_{k_2k_1} \end{aligned} \tag{3.85}$$

On the other hand,

$$\begin{aligned} &X_{k'k}=\langle k'|M|k\rangle=\delta_{k'k}+A_{k'k}, \\ &\det X=1+A_{k_1k_1}+A_{k_2k_2}+A_{k_1k_1}A_{k_2k_2}-A_{k_1k_2}A_{k_2k_1} \end{aligned} \tag{3.86}$$

3.9.3 Application of the theorem for observables

In fact, during the derivation of the theorem, the explicit form of transfer matrix M was not used except that it can be expanded in powers of density operator $\rho(\boldsymbol{n})$ and only the one power of $\rho(\boldsymbol{n})$ is need to be evaluated for a single particle state. Thus, if we replace the transfer matrix with other observables, we may evaluate matrix element of a operator as

$$\langle\Psi|M\dots\hat{\mathcal{O}}\dots M|\Psi\rangle=\det X(s,\hat{\mathcal{O}}) \tag{3.87}$$

where

$$X_{ij}(s,\hat{\mathcal{O}}) = \langle\phi_i|M\ldots\hat{\mathcal{O}}\ldots M|\phi_j\rangle \tag{3.88}$$

with single particle states.

Note that even though the $X_{ij}(s,\hat{\mathcal{O}})$ looks linear to $\hat{\mathcal{O}}$, the full matrix element $\det X(s,\hat{\mathcal{O}})$ is not linear to $\hat{\mathcal{O}}$.

Also, note that because what we actually wants to measure is a expectation value of operator for ground state, we divides with $Z_\Psi(L_t)$ or $Z_\Psi(L_t-1)$

$$\langle 0|\hat{O}|0\rangle = \lim_{L_t\to\infty}\frac{\langle\Psi|M\ldots\hat{O}\ldots M|\Psi\rangle}{\langle\Psi|M^{L_t}|\Psi\rangle} = \lim_{L_t\to\infty}\frac{\langle\Psi|M\ldots\hat{O}\ldots M|\Psi\rangle}{\langle\Psi|M^{L_t-1}|\Psi\rangle} \tag{3.89}$$

3.9.4 In lattice code

We can express the trasnfer matrix elements for any $n_t \le L_t$ as

$$\langle\Psi_0|M^{L_t}|\Psi_0\rangle = \langle\Phi(n_t)|\Phi(n_t)\rangle = \langle\Phi(n_t+1)|M^{(n_t)}|\Phi(n_t)\rangle, \tag{3.90}$$

where vector and dual vector are defined as

$$\begin{aligned}|\Phi(n_t)\rangle &= M^{(n_t-1)}\ldots M^{(0)}|\Psi_0\rangle = M^{(n_t-1)}|\Phi(n_t-1)\rangle,\\ \langle\Phi(n_t+1)| &= \langle\Psi_0|M^{(L_t-1)}\ldots M^{(n_t+1)} = \langle\Phi(n_t)|M^{(n_t+1)}.\end{aligned} \tag{3.91}$$

Thus, any observable $\mathcal{O}(n_t)$, we get

$$\langle\Psi_0|M^{(L_t-1)}\cdots M^{(n_t)}\mathcal{O}^{(n_t)}\cdots M^{(0)}|\Psi_0\rangle = \langle\Phi(n_t)|\mathcal{O}^{(n_t)}|\Phi(n_t)\rangle \tag{3.92}$$

In lattice code 'zvecs(nx,ny,nz,nt,ns,ni,np)' corresponds to $\Phi(n_t)\rangle$,

$$|zvecs_i^{(n_t)}\rangle = M^{(n_t-1)}(s)|zvecs_i^{(n_t-1)}\rangle \tag{3.93}$$

, starting from $|zvecs_i^{(0)}\rangle = |zvecs_i\rangle$ where $i = (ns, nt, ni, np)$. In a similar way, 'zdualvecs(nt)' corresponds to $\langle\Phi(n_t)$,

$$\langle zdualvecs_i^{(n_t-1)}| = \langle zdualvecs_i^{(n_t)}|M^{(n_t-1)} \tag{3.94}$$

3.9.5 Coulomb correction

We expect the Coulomb potential can be treated perturbatively. Thus, with perturbative approximation, At a certain time

$$M_{full}^{(n_t)}(s,\pi) = \exp(-H_0\alpha_t - H_{int}\alpha_t - V_c\alpha_t) \simeq 1 - H_0\alpha_t - H_{int}\alpha_t - V_c\alpha_t = M^{(n_t)} - V_c\alpha_t. \tag{3.95}$$

Then, we may think

$$\begin{aligned}Z_\Psi(L_t) &= \langle M_{LO}^{(n_t)}\rangle \sim e^{-E_{LO}L_t\alpha_t},\\ \langle M_{full}^{(n_t)}\rangle &\sim e^{-E_{LO}L_t\alpha_t}(1-\langle V_c\rangle\alpha_t),\\ \langle V_c\rangle &\sim -\frac{1}{\alpha_t}\left(\frac{\langle M_{full}^{(n_t)}\rangle - \langle M_{LO}^{(n_t)}\rangle}{Z_\Psi(L_t)}\right)\end{aligned} \tag{3.96}$$

3.10 Exact method to solve lattice Hamiltonian?

For a few body case(2 or 3 fermions), one can solve the problem exactly on the lattice. I am not sure whether this is the way used in the MATLAB code

We would like to obtain the energy spectrum of the lattice Hamiltonian.

One way to solve the problem is to diagonalize the Hamiltonian.

One-body case it is simple. Suppose we list states $|\boldsymbol{n}\rangle = a^\dagger(\boldsymbol{n})|0\rangle$ and obtain the matrix elements $\langle \boldsymbol{n}'|\hat{H}|\boldsymbol{n}\rangle$. By computing this matrix elements with lattice Hamiltonian, one can diagonalize the matrix $\langle \boldsymbol{n}'|\hat{H}|\boldsymbol{n}\rangle$ to obtain s.p. eigen states $|f\rangle = \sum_n c_n|\boldsymbol{n}\rangle$ and energy levels.

In a similar way, if one prepare a complete set of two nucleon states $|\boldsymbol{n}_1\boldsymbol{n}_2\rangle$ and diagonalize $\langle \boldsymbol{n}_1'\boldsymbol{n}_2'|\hat{H}|\boldsymbol{n}_1\boldsymbol{n}_2\rangle$ with lattice Hamiltonian one can get the full solutions.

Another way is to compute the Euclidiean time evolution without using MC samplings. This may be possible with transfer matrix formalism without auxiliary field. With two-body interactions, the transfer matrix can be constructed such as

$$M =: \exp\{-H_{free}\alpha_t - \sum V(\boldsymbol{n}_1,\boldsymbol{n}_2)\rho(\boldsymbol{n}_1)\rho(\boldsymbol{n}_2)\} : \tag{3.97}$$

Computing the action of transfer matrix operator on two- or three-body initial states $|\Psi_2\rangle$, Ψ_3 in center of mass frame, one can compute the discrete Euclidean time evolution exactly without using MC samplings.

As for example, two nucleon ${}^1S_0$ or ${}^3S_1$ state in CM frame may be written as

$$\begin{aligned} |f,{}^1S_0\rangle &\propto \sum_{\boldsymbol{n}_1\boldsymbol{n}_2}\sum_{\alpha\beta} f(\boldsymbol{n}_1-\boldsymbol{n}_2)P_{\alpha\beta}a^\dagger_\alpha(\boldsymbol{n}_1)a^\dagger_\beta(\boldsymbol{n}_2)|0\rangle, \\ |f,{}^3S_1,s\rangle &\propto \sum_{\boldsymbol{n}_1\boldsymbol{n}_2}\sum_{\alpha\beta} f(\boldsymbol{n}_1-\boldsymbol{n}_2)P^s_{\alpha\beta}a^\dagger_\alpha(\boldsymbol{n}_1)a^\dagger_\beta(\boldsymbol{n}_2)|0\rangle \end{aligned} \tag{3.98}$$

where, α,β are spin and isospin index and $P_{\alpha\beta}, P^s_{\alpha\beta}$ are matrix elements of ${}^1S_0$, ${}^3S_1$ projection operators. (For example, $P=\sigma_2\tau_2\tau_3$ for ${}^1S_0$, $P^s=\sigma_2\sigma_s\tau_2$ for ${}^3S_1$ up to complex constant.) (In CM frame, only relative coordinate is relevant. And complete sets of two nucleon states in ${}^1S_0$ can be thought as $|\boldsymbol{n}_1\boldsymbol{n}_2,{}^1S_0\rangle = a^\dagger_\alpha(\boldsymbol{n}_1)a^\dagger_\beta(\boldsymbol{n}_2)P_{\alpha\beta}|0\rangle$.)

More generally, initial nucleon state may be expressed with some wave function F such that

$$|F\rangle = \sum_{\{\boldsymbol{n}_i\}}\sum_{\{\alpha_i\}} F_{\{\alpha_i\}}(\{\boldsymbol{n}_i\})\prod_i a^\dagger_{\alpha_i}(\boldsymbol{n}_i)|0\rangle \tag{3.99}$$

Thus, by computing action of lattice Hamiltonian on this states, one can compute the $Z(\tau)$ exactly without using MC sampling. Though, it will be impractical for more than 3-body.

3.11 Pinhole algorithm

Let us review the Lattice calculation. From the path integral, we convert

$$\begin{aligned} Z_\Psi(L_t) &= \langle\Psi|e^{-\int d\tau H(\tau)}|\Psi\rangle = \int \mathcal{D}s\mathcal{D}\pi\mathcal{D}\psi^\dagger\psi e^{-S_{ss}-S_{\pi\pi}-S_\psi} \\ &= \int \mathcal{D}s\mathcal{D}\pi e^{-S_{ss}-S_{\pi\pi}}\langle\Psi|M^{(L_t)}(s,\pi)|\Psi\rangle \\ &= \int \mathcal{D}s\mathcal{D}\pi e^{-S_{ss}-S_{\pi\pi}}\det X(s,\pi) \\ &\simeq \frac{1}{N_{cf}}\sum_{i=1}^{N_{cf}} P(s_i,\pi_i)e^{i\theta_i}, \quad P(s_i,\pi_i) = e^{-S_{ss}-S_{\pi\pi}+\ln|\det X(s_i,\pi_i)|} \\ &\simeq \frac{1}{N_{cf}}\sum_{i\in P_i}{}' e^{i\theta_i} = \langle e^{i\theta}\rangle \end{aligned} \tag{3.100}$$

where θ is a phase of $\det X(s,\pi)$.

In the first line, one express the correlation $Z_\Psi(L_t)$ into a path integral. However, this is not easy to solve numerically. Thus, one converts the fermion path integral into a matrix element of a transfer operator. This transfer matrix elements can be expressed as a determinant of a correlation matrix $X(s,\pi)$ which can be solved numerically from operator relations. Then the bosonic path integral can be done using MC samplings or metropolis MC samplings according to the probability $P(s_i,\pi_i)$.

In a similar way, a expectation value of a operator $\mathcal{O}$ can be computed as

$$\begin{aligned}
\langle\Psi|\hat{\mathcal{O}}|\Psi\rangle(L_t) &= \langle\Psi_0|e^{-H\tau}\hat{\mathcal{O}}(t)e^{-H\tau}|\Psi_0\rangle = \int \mathcal{D}s\mathcal{D}\pi e^{-S_{ss}-S_{\pi\pi}}\langle\Psi_0|M^{(L_t/2)}(s,\pi)\hat{\mathcal{O}}M^{(L_t/2)}(s,\pi)|\Psi_0\rangle \\
&= \int \mathcal{D}s\mathcal{D}\pi e^{-S_{ss}-S_{\pi\pi}}\det X(s,\pi,\mathcal{O}) \\
&\simeq \frac{1}{N_{cf}}\sum_i P(s_i,\pi_i)e^{-\ln|\det X(s,\pi)|+\ln\det X(s,\pi,\mathcal{O})} \\
&= \frac{1}{N_{cf}}\sum_i P(s_i,\pi_i)e^{-\ln|\det X(s,\pi)|+\ln|\det X(s,\pi,\mathcal{O})|+i\theta(s,\pi,\mathcal{O})} \\
&= \langle e^{-\ln|\det X(s,\pi)|+\ln|\det X(s,\pi,\mathcal{O})|+i\theta(s,\pi,\mathcal{O})}\rangle
\end{aligned} \tag{3.101}$$

where $\theta(s,\pi,\mathcal{O})$ is a phase of $\det X(s,\pi,\mathcal{O})$. In other words, $\langle\Psi|\hat{\mathcal{O}}|\Psi\rangle(L_t)$ is the same as a average of $e^{-\ln|\det X(s,\pi)|+\ln|\det X(s,\pi,\mathcal{O})|+i\theta(s,\pi,\mathcal{O})}$ over configurations. For $\mathcal{O}=I$, $\langle\Psi|\hat{\mathcal{O}}|\Psi\rangle(L_t)=\langle e^{i\theta(s,\pi)}\rangle = Z_\Psi(L_t)$. Thus, the expectation value of an operator which depends on configurations can be obtained from

$$\frac{\langle\Psi|\mathcal{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \lim_{L_t\to\infty}\frac{\langle\mathcal{O}e^{+i\theta(L_t)}\rangle}{\langle e^{+i\theta(L_t)}\rangle}. \tag{3.102}$$

Thus, if $P(s_i,\pi_i)$ is already available and once $\det X(s,\pi,\mathcal{O})$ is calculated, one can compute the expectation value $\langle\Psi|\hat{\mathcal{O}}|\Psi\rangle(L_t)$. From the Euclidean time evolution, we can extract the contribution from ground state or excited states.

Let us consider A-body density operator,

$$\rho_{i_1j_1\cdots i_Aj_A}(\boldsymbol{n}_1,\cdots,\boldsymbol{n}_A) =: \rho_{i_1j_1}(\boldsymbol{n}_1)\cdots\rho_{i_Aj_A}(\boldsymbol{n}_A):, \tag{3.103}$$

where i is a spin index, j is a isospin index. We have identity,

$$\sum_{i_1j_1\cdots i_Aj_A}\sum_{\boldsymbol{n}_1,\cdots,\boldsymbol{n}_A}\rho_{i_1j_1\cdots i_Aj_A}(\boldsymbol{n}_1,\cdots,\boldsymbol{n}_A) = A!. \tag{3.104}$$

Then, for following amplitude

$$Z_{f,i}(i_1,j_1,\cdots,i_A,j_A;\boldsymbol{n}_1,\cdots\boldsymbol{n}_A;L_t) = \langle\Psi_f|M_*^{L_t'}M^{L_t/2}\rho_{i_1j_1\cdots i_Aj_A}(\boldsymbol{n}_1,\cdots,\boldsymbol{n}_A)M^{L_t/2}M_*^{L_t'}|\Psi_i\rangle \tag{3.105}$$

In other words, roughly speaking

$$Z_{f,i}(i_1,j_1,\cdots,i_A,j_A;\boldsymbol{n}_1,\cdots\boldsymbol{n}_A;L_t) \simeq |c_0|^2e^{-E_0L_t\alpha_t}\langle\Psi_0|\rho_{i_1j_1\cdots i_Aj_A}(\boldsymbol{n}_1,\cdots,\boldsymbol{n}_A)|\Psi_0\rangle \tag{3.106}$$

We have identity,

$$Z_{fi}(L_t) = \frac{1}{A!}\sum_{i_1j_1\cdots i_Aj_A}\sum_{\boldsymbol{n}_1,\cdots,\boldsymbol{n}_A} Z_{f,i}(i_1,j_1,\cdots,i_A,j_A;\boldsymbol{n}_1,\cdots\boldsymbol{n}_A;L_t) \tag{3.107}$$

In other words, with summation over pinholes in MC samplings, we can do the lattice calculation by using amplitudes $Z_{f,i}(i_1,j_1,\cdots,i_A,j_A;\boldsymbol{n}_1,\cdots\boldsymbol{n}_A;L_t)$. In other words, we may extend the meaning of a configuration to include both pinhole configuration and (auxiliary) boson field configurations.

While doing MC samplings, if we count the number of configurations for a distribution of nucleons, we may get the density distribution of a ground state.

To do this, for given configuration of pinholes, extract the center of mass position. Then, compute the number of nucleons in radial distance from the c.m. Then, taking average over pinhole configurations will give the average number of nucleons in radial distance. In other words, density distribution.

In summary, denoting pinhole configurations as $[i_x, j_x, \boldsymbol{n}_x]$, boson configurations $[s_i, \pi_i]$ and both configuration as $[cf_i]$,

$$\begin{aligned}
\langle\Psi|\mathcal{O}|\Psi\rangle(L_t) &= \frac{1}{A!}\sum_{[i_x,j_x,\boldsymbol{n}_x]}\int \mathcal{D}s\mathcal{D}\pi e^{-S_{ss}-S_{\pi\pi}}\det X(s,\pi,[i_x,j_x,\boldsymbol{n}_x],\mathcal{O},L_t) \\
&= \frac{1}{A!}\sum_{[i_x,j_x,\boldsymbol{n}_x]}\sum_{[s_i,\pi_i]} P(s_i,\pi_i,[i_x,j_x,\boldsymbol{n}_x]) \\
&\quad \times e^{-\ln|\det X(s_i,\pi_i,[i_x,j_x,\boldsymbol{n}_x],L_t)|+\ln|\det X(s_i,\pi_i,[i_x,j_x,\boldsymbol{n}_x],\mathcal{O},L_t)|+i\theta(s_i,\pi_i,[i_x,j_x,\boldsymbol{n}_x],\mathcal{O},L_t)} \\
&\propto \langle e^{-\ln|\det X([cf_i],L_t)|+\ln|\det X([cf_i],\mathcal{O},L_t)|+i\theta([cf_i],\mathcal{O},L_t)}\rangle \qquad (3.108)
\end{aligned}$$

where average is over the all configurations $[cf_i]$ of pinholes and bosons . If $\mathcal{O}$ is the same as density operator, we only have $\langle e^{+i\theta([cf_i],L_t)}\rangle$.

In other words, we obtains the expectation value of an operator which depends on configurations of pinholes and bosons as

$$\frac{\langle\Psi|\mathcal{O}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \lim_{L_t\to\infty}\frac{\langle\mathcal{O}[cf_i]e^{+i\theta([cf_i],L_t)}\rangle}{\langle e^{+i\theta([cf_i],L_t)}\rangle}. \qquad (3.109)$$

Chapter 4

Lattice actions and the form of Transfer matrix operators

4.1 Background material: Discrete Fourier Transformation

(For a DFT of general lattice, FCC and BCC, look at the Zheng and Gu, J. Math. Imaging. Vis.(2014), 49:530-550.)

4.1.1 Relation between discretization and continuum limit

First, let us make it clear for the terms. For harmonic system, Period T, frequency $\nu = \frac{1}{T}$, angular frequency $\omega = 2\pi\nu = \frac{2\pi}{T}$, and Energy $E = \hbar\omega$. Wave length λ, angular wave number $k = \frac{2\pi}{\lambda}$, momentum $p = \hbar k$. Then, we have relations,

$$\exp(-i\frac{Et}{\hbar})\exp(i\frac{px}{\hbar}) = \exp(-i\omega t)\exp(ikx) \tag{4.1}$$

continuum	x	$p = \hbar k$	$\int dx$	$\int \frac{dp}{2\pi\hbar}$	$\delta(x)$	$\delta(k)$	e^{ikx}
discrete	$x_n = an$	$k_m = \frac{2\pi}{L}m$	$a\sum_n$	$\frac{1}{L}\sum_m$	$\frac{1}{a}\delta_{n0}$	$\frac{L}{2\pi}\delta_{m0}$	$e^{i2\pi\frac{mn}{N}}$

And delta function (orthogonality) relation

$$\begin{aligned} & \int dx e^{ikx} = 2\pi\delta(k) \\ \rightarrow \quad & a\sum_n e^{i(\frac{2\pi}{L}m)\cdot(an)} = a\sum_n e^{i2\pi\frac{mn}{N}} = (2\pi)\frac{L}{2\pi}\delta_{m0} = Na\delta_{m0}, \\ \rightarrow \quad & \sum_n e^{i2\pi\frac{mn}{N}} = N\delta_{m0} \end{aligned} \tag{4.2}$$

Discretization of Fourier transformation,

$$\begin{aligned} & f(x) = \int \frac{dp}{2\pi\hbar} e^{ikx}\hat{f}(k) \\ \rightarrow \quad & f(x_n) = \frac{1}{L}\sum_m e^{ik_m x_n}\hat{f}(k_m) = \frac{1}{N}\sum_m e^{i2\pi\frac{mn}{N}}\frac{\hat{f}(k_m)}{a} = \frac{1}{N}\sum_m e^{i2\pi\frac{mn}{N}}\hat{f}_m \end{aligned} \tag{4.3}$$

implies the momentum component $\hat{f}_m = \frac{1}{a}\hat{f}(k_m)$ have different dimension with $\hat{f}(k_m)$ though $f(x_n)$ and f_n have the same dimension.

And its reverse is

$$\hat{f}(k) = \int dx e^{-ikx} f(x)$$
$$\rightarrow \quad \hat{f}(k_m) = a\hat{f}_m = a\sum_n e^{-i2\pi\frac{mn}{N}} f_n \tag{4.4}$$

4.1.2 DFT

Let us consider equally spaced N points. $x_j = ja$, $j = 0, \ldots N-1$. Thus, it covers $x \in [0, L = Na]$ if it is considered to be periodic. Then, a (periodic) function can be expressed in DFT as

$$\begin{aligned} \hat{f}_m &= \hat{f}(k_m) = \sum_{n=0}^{N-1} e^{-ix_n \cdot k_m} f_n, \\ f_n &= f(x_n) = \frac{1}{N}\sum_{m=0}^{N-1} e^{ix_n \cdot k_m} \hat{f}_m, \end{aligned} \tag{4.5}$$

with angular wave number $k_m = \frac{2\pi m}{L} = \frac{2\pi m}{Na}$,

$$\exp(i\boldsymbol{x}_n \cdot \boldsymbol{p}_m) \rightarrow \exp\left(ina \times \frac{2\pi m}{L}\right) = \exp\left(i2\pi\frac{nm}{N}\right) \tag{4.6}$$

(In fact, in analogy of $i\omega t = i\frac{2\pi}{T}t = i2\pi\nu t$, we may call $\nu \rightarrow \frac{m}{Na}$ frequency.) In fact the definition or dimension of $\hat{f}$ depends on the convention.

For given equal spaced points, $t_k = k\Delta$, $k = 0, \ldots, N-1$ and function values $f(t_k)$

$$F_n = \sum_{k=0}^{N-1} f_k e^{-\frac{2\pi i}{N}nk} \quad \leftrightarrow \quad f_k = \frac{1}{N}\sum_{n=0}^{N-1} F_n e^{\frac{2\pi i}{N}nk}. \tag{4.7}$$

In other words, basic equation is

$$\frac{1}{N}\sum_{k=0}^{N-1} e^{-i\frac{2\pi}{N}k(n-n')} = \delta_{nn'} \tag{4.8}$$

In symmetric convention, complex valued function a defined on a subset $[N] := \{0, 1, 2, \ldots, N-1\}$ can be DFT to function $\hat{a}$ on $k \in [N]$,

$$\hat{a}(k) = \frac{1}{\sqrt{N}}\sum_{j\in[N]} a(j)e^{-2\pi i\frac{jk}{N}}. \tag{4.9}$$

For general dimension, by using generators of a basis of Lattice L, one can construct

$$L := \Big\{\sum_{i=1}^{d} k_i \boldsymbol{u}_i : k_i \in Z \text{ for } i = 1, 2, \ldots d\Big\}. \tag{4.10}$$

If there is a sub-lattice L_0, (in other words, if there is a periodicity
we have

$$\begin{aligned} \hat{a}(\bar{s}) &= \frac{1}{\sqrt{|G|}}\sum_{\bar{r}\in G} a(\bar{r}) \cdot e^{-2\pi i\langle \boldsymbol{r}\cdot\boldsymbol{s}\rangle}, \\ a(\bar{r}) &= \frac{1}{\sqrt{|G|}}\sum_{\bar{s}\in \hat{G}} \hat{a}(\bar{s}) \cdot e^{2\pi i\langle \boldsymbol{r}\cdot\boldsymbol{s}\rangle} \end{aligned} \tag{4.11}$$

Or

$$\hat{f}(n) = \sum_{m=1}^{L} f_{in}(m) e^{-2\pi i \boldsymbol{r}_m^T \cdot \boldsymbol{s}_n} \tag{4.12}$$

where $\boldsymbol{r}_m$ is a point in S_Ω and $\boldsymbol{s}_n$ is a point in $S^A_\Omega = (V_{bs}^{-1})^T S^A_{\Omega,coef}$. It is equivalent to

$$\hat{f}(n) = \sum_{m=1}^{L} f_{in}(m) e^{-2\pi i [c]_m^T \cdot (M^{-1})^T \cdot [s]_n} \tag{4.13}$$

where $[c]_m$ is a point in $S_{\Omega,coef}$ and $[s]_n$ is a point in $S^A_{\Omega,coef}$

$$\langle \boldsymbol{r}_m, \boldsymbol{s}_n \rangle = \boldsymbol{r}^T \cdot \boldsymbol{s} = [\boldsymbol{c}]_m^T \cdot (M^{-1})^T \cdot [s]_n \tag{4.14}$$

When using numerical FFT, one have to keep in mind that

- In MATLAB and FORTRAN, the index of an array usually starts from 1. However, the FFT routine treats first element of f, $f(1)$ is at $x = 0$. Thus, in explicit indexing $f(x_i)$, $x_i = (i-1)$,

$$\hat{f}(m) = \sum_{l=1}^{L} f_{in}(l) \exp\left(-i \frac{2\pi}{L} \cdot (m-1)(l-1)\right) \tag{4.15}$$

  In a similar way, 2-dimensional FFT is

$$\hat{f}(m,n) = \sum_{i=1}^{L}\sum_{j=1}^{L} f_{in}(i,j) \exp\left[-2\pi i \left(\frac{(i-1)(m-1)}{L} + \frac{(j-1)(n-1)}{L}\right)\right] \tag{4.16}$$

- Depending on the code, the normalization of $\hat{f}$ can be different and also inverse transformation. For example, MATLAB fftn have $1/N$ factor for inverse transformation, on the other hand, FFTW routine does not have $1/N$ factor. Thus, successive FFT and iFFT does not give original f_{in} but $L * f_{in}$.

- FFTW use standard ordering of frequency k/n. It can be interpreted as the positive frequency in the first half of the output and the negative frequencies are stored in backward order in the second half of the output. ($-k/n$ is equivalent to $(n-k)/n$).

$$\begin{aligned} Y_k &= \sum_{j=0}^{n-1} X_j e^{-2\pi i \frac{jk}{n}} \quad \text{forward FFT}, \\ Y_k &= \sum_{j=0}^{n-1} X_j e^{2\pi i \frac{jk}{n}} \quad \text{backward FFT}. \end{aligned} \tag{4.17}$$

- in other words, the 1-dimensional lattice and its momentum(frequency) index are

$$\begin{aligned} x &= a\left[0, 1, 2, \ldots \frac{N}{2}, \frac{N}{2}+1, \ldots N-1\right], \\ p &= \frac{2\pi}{L}\left[0, 1, 2, \ldots, -\frac{N}{2}, -\frac{N}{2}+1, \ldots, -1\right] \end{aligned} \tag{4.18}$$

  Or, $p_k = \frac{2\pi}{L} k$ for $k < \frac{N}{2}$, $p_k = \frac{2\pi}{L}(k-N)$ for $k \geq \frac{N}{2}$. (this may be written in Fortran as $\frac{2\pi}{L}(k - N \times \text{int}(\frac{k}{N/2}))$)

- In case DFT of real function, $X_j^* = X_j$ one can use the symmetry,

$$Y_k = Y_{-k}^* = Y_{n-k}^*. \tag{4.19}$$

  FFTW of r2c and c2r use this symmetry.(the real array has length n, but complex array has length $n/2+1$.)

4.1.3 Derivative calculation using DFT

One may obtain the numerical derivative of function by approximating finite difference,

$$f'(x_i) \simeq \frac{f(x_{i+1}) - f(x_{i-1})}{2a}, \quad f''(x_i) \simeq \frac{f(x_{i+1}) + f(x_{i-1}) - 2f(x_i)}{a^2}. \tag{4.20}$$

But, for periodic function in range, we can also use DFT and inverse DFT to compute derivative.

$$f'(x_n) = \frac{1}{N}\sum_m e^{i2\pi\frac{mn}{N}}(i\frac{2\pi m}{Na})\hat{f}_m, \quad f''(x_n) = \frac{1}{N}\sum_m e^{i2\pi\frac{mn}{N}}(i\frac{2\pi m}{Na})^2\hat{f}_m. \tag{4.21}$$

This will give exact results if the function is periodic $f(x+L) = f(x)$.

On the other hand, previous numerical derivative expression corresponds to

$$\frac{f(x_{n+1}) + f(x_{n-1}) - 2f(x_n)}{a^2} = \frac{1}{N}\sum_m e^{i2\pi\frac{mn}{N}}\frac{1}{a^2}\left(e^{i\frac{2\pi m}{N}} + e^{-i\frac{2\pi m}{N}} - 2\right)\hat{f}_m. \tag{4.22}$$

In fact, there is an ambiguity using the DFT for differentiation. Any periodic shift in momentum (aliasing) will also give the same spatial function values but will have significant difference in derivative. One convention is to use "minimal-oscillation" trigonometric interpolation for iFFT :

$$f(x) = \hat{f}_0 + \sum_{0<k<N/2}\left(\hat{f}_k e^{i\frac{2\pi}{L}kx} + \hat{f}_{N-k}e^{-i\frac{2\pi}{L}kx}\right) + \hat{f}_{N/2}\cos(\frac{\pi}{L}Nx), \tag{4.23}$$

where the Nyquist term ($k = \frac{N}{2}$) is absent for odd N.

However, if the function is not periodic, the derivative calculation by using DFT will gives errors. One way to improve the problem is to sample data in $x \in [-1, 1]$ at the points $x_n = \cos(n\pi/N)$ for n=0,... N and then to use Chevyshev interpolation. $f(x) = \sum_{n=0}^{N} a_n T_n(x)$ with Chevyshev polynomial $T_n(x)$. This is essentially the Fourier series with change of variable $x = \cos\theta$.

$$T_n(\cos\theta) = \cos n\theta, \quad T_{2n+1}(\sin\theta) = (-1)^n \sin((2n+1)\theta). \tag{4.24}$$

4.2 Lattice notation

Let us denote a_t and a as a lattice interval in time and space respectively and L is the length of the cubic spatial lattice in each direction such as

$$L_t = N_t a_t, \quad L = Na, \tag{4.25}$$

And $\alpha_t \equiv \frac{a_t}{a}$ is a ratio of lattice intervals. To discretize coordinate and momentum, we replace

$$\boldsymbol{x} \to a\boldsymbol{n}, \quad \boldsymbol{p} \to \hbar\frac{2\pi}{L}\boldsymbol{m}, \quad (\boldsymbol{n}, \boldsymbol{m} \text{ are sets of 3 integers }) \tag{4.26}$$

such that

$$\int dt d\boldsymbol{x} \to a_t a^3 \sum_{\boldsymbol{n}, n_t}, \quad i\frac{\boldsymbol{x}\cdot\boldsymbol{p}}{\hbar} \to i\frac{2\pi}{N} \times \boldsymbol{n}\cdot\boldsymbol{m}. \tag{4.27}$$

with $n_i, m_i = 0, 1, \ldots L-1$. We can consider $\frac{\boldsymbol{m}}{N}$ as a frequency. Because of periodicity, all integers are up to modular N. (For frequency, one can use $m_i = -N/2, \ldots N/2-1$).

- $\vec{n}$ represents integer-valued lattice vectors on a three-dimensional spatial lattice
- $\vec{p}, \vec{q}, \vec{k}$ represent integer-valued momentum lattice vectors.

- $\hat{l} = \hat{1}, \hat{2}, \hat{3}$ are unit lattice vectors in the spatial directions
- n_t labels the number of time steps.
- Everything will be written in a **dimensionless parameters** and operators which can be converted to physical dimension by appropriate power of a.
- $\hat{a}$ and $\hat{a}^\dagger$ are annihilation and creation operators.
- spin and isospin indices are used as

$$\begin{aligned} a_{0,0} &= a_{\uparrow,p}, \quad a_{0,1} = a_{\uparrow,n}, \\ a_{1,0} &= a_{\downarrow,p}, \quad a_{1,1} = a_{\downarrow,n} \end{aligned} \tag{4.28}$$

- $\tau_{I=1,2,3}$ and $\sigma_{S=1,2,3}$ are Pauli matrices in isospin and spin.

For a creation and annihilation operator for states p, $a_p^\dagger$ and a_p, one can define position space operator

$$a(x) = \frac{1}{L}\sum_p e^{ip\cdot x} a_p, \quad a^\dagger(x) = \frac{1}{L}\sum_p e^{-ip\cdot x} a_p^\dagger. \tag{4.29}$$

$$\int_0^L dx a^\dagger(x) a(x) \quad = \quad \sum_p a_p^\dagger a_p \tag{4.30}$$

Note that these operator does not have (energy) state index.

4.2.1 Discrete Fourier transformation

Because lattice size acts as a momentum cutoff, in actual calculation we choose size of a such that

$$m_\pi < \frac{\pi}{a} < \Lambda_\chi. \tag{4.31}$$

And because we will use periodic boundary condition in space, range of k values are

$$-\Lambda < \frac{2\pi}{L} k_{1,2,3} \leq (\Lambda = \frac{\pi}{a}) \ \rightarrow \ -\frac{N}{2} < k_{1,2,3} \leq \frac{N}{2} \tag{4.32}$$

Let us consider **4-dimensional** F.T., [1] [2]

$$\begin{aligned} \tilde{f}(\boldsymbol{k}) &= \frac{1}{\sqrt{L_t L^3}} \sum_{\boldsymbol{n}_*} e^{i\boldsymbol{k}_*\cdot\boldsymbol{n}_*} f(\boldsymbol{n}), \\ f(\boldsymbol{n}) &= \frac{1}{\sqrt{L_t L^3}} \sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}_*\cdot\boldsymbol{n}_*} \tilde{f}(\boldsymbol{k}), \end{aligned} \tag{4.34}$$

[1] Normalization factors $L_t L^3$ depends on the convention.

[2] Though I use k_*, n_* to distinguish dimensional quantity and dimension less quantity, we can always replace them as dimensionless qunatities keeping in mind above conevntion. So, $\boldsymbol{n}_* = a\boldsymbol{n}$,

$$\sum_k e^{i\boldsymbol{k}_*\cdot(\boldsymbol{n}_* - \boldsymbol{n}'_*)} = N^3 \delta_{\boldsymbol{n}\boldsymbol{n}'} \tag{4.33}$$

with

$$\begin{aligned}\boldsymbol{k}_* &= \left(\frac{2\pi}{N_t}k_0, \frac{2\pi}{N}k_1, \frac{2\pi}{N}k_2, \frac{2\pi}{N}k_3\right), \quad k_i \text{ are integers,} \\ \sum_{\boldsymbol{n}_*} e^{i\boldsymbol{k}_*\cdot\boldsymbol{n}_*} &= N_t N^3 \delta_{\boldsymbol{k}0} \end{aligned} \tag{4.35}$$

Then F.T. of some typical operators are[3]

$$\begin{aligned}&\sum_{\boldsymbol{n}} c_i^*(\boldsymbol{n})c_i'(\boldsymbol{n}+\hat{0}) = \sum_{\boldsymbol{k}}\sum_{\boldsymbol{k}'} \tilde{c}_i^*(\boldsymbol{k}')\tilde{c}_i'(\boldsymbol{k})\frac{1}{L_t L^3}\sum_{\boldsymbol{n}} e^{-i\boldsymbol{k}'\cdot\boldsymbol{n}}e^{-i\boldsymbol{k}\cdot\boldsymbol{n}}e^{-i\boldsymbol{k}\cdot\hat{0}} = \sum_{\boldsymbol{k}} \tilde{c}_i^*(-\boldsymbol{k})\tilde{c}_i'(\boldsymbol{k})e^{-i\boldsymbol{k}\cdot\hat{0}}, \\ &\sum_{\boldsymbol{n}} c_i^*(\boldsymbol{n})c_i'(\boldsymbol{n}) = \sum_{\boldsymbol{k}} \tilde{c}_i^*(-\boldsymbol{k})\tilde{c}_i'(\boldsymbol{k}), \quad \sum_{\boldsymbol{n}} c_i^*(\boldsymbol{n})c_i'(\boldsymbol{n}+\hat{l}_s) = \sum_{\boldsymbol{k}} \tilde{c}_i^*(-\boldsymbol{k})\tilde{c}_i'(\boldsymbol{k})e^{-i\boldsymbol{k}\cdot\hat{l}_s}, \\ &\sum_{\boldsymbol{n}} [c_i^*(\boldsymbol{n})c_i'(\boldsymbol{n}+\hat{l}_s) + c_i^*(\boldsymbol{n})c_i'(\boldsymbol{n}-\hat{l}_s)] = \sum_{\boldsymbol{k}} \tilde{c}_i^*(-\boldsymbol{k})\tilde{c}_i'(\boldsymbol{k})[e^{-i\boldsymbol{k}\cdot\hat{l}_s} + e^{+i\boldsymbol{k}\cdot\hat{l}_s}] = \sum_{\boldsymbol{k}} \tilde{c}_i^*(-\boldsymbol{k})\tilde{c}_i'(\boldsymbol{k})[2\cos(\boldsymbol{k}\cdot\hat{l}_s)]\end{aligned} \tag{4.36}$$

4.2.2 Spatial derivatives

We approximate the derivative of a function in terms of hopping operators in lattice.

For each spatial direction $l = 1, 2, 3$ and any lattice function $f(\boldsymbol{n})$, let

$$\Delta_l f(\boldsymbol{n}) \equiv \frac{1}{4}\sum_{\nu_{1,2,3}=0,1} (-1)^{\nu_l+1} f(\boldsymbol{n}+\vec{\nu}), \quad \vec{\nu} = \nu_1\hat{1} + \nu_2\hat{2} + \nu_3\hat{3}. \tag{4.37}$$

Explicit expression for $l = 1$ case is

$$\begin{aligned}\Delta_1 f(\boldsymbol{n}) &= \frac{1}{4}\Big[f(\boldsymbol{n}+\hat{1}) - f(\boldsymbol{n}) + f(\boldsymbol{n}+\hat{1}+\hat{2}) - f(\boldsymbol{n}+\hat{2}) \\ &\quad + f(\boldsymbol{n}+\hat{1}+\hat{3}) - f(\boldsymbol{n}+\hat{3}) + f(\boldsymbol{n}+\hat{1}+\hat{2}+\hat{3}) - f(\boldsymbol{n}+\hat{2}+\hat{3})\Big]\end{aligned} \tag{4.38}$$

This can be thought as average of 1-direction derivative of values at $\boldsymbol{n}$, $\boldsymbol{n}+\hat{2}$,$\boldsymbol{n}+\hat{3}$,$\boldsymbol{n}+\hat{2}+\hat{3}$.

Double spatial derivative along direction l,

$$\nabla_l^2 f(\boldsymbol{n}) = f(\boldsymbol{n}+\hat{l}) + f(\boldsymbol{n}-\hat{l}) - 2f(\boldsymbol{n}). \tag{4.39}$$

4.3 local densities and currents

We define

$$\begin{aligned}\rho^{a^\dagger,a}(\boldsymbol{r}) &= \sum_{i,j=0,1} a_{i,j}^\dagger(\boldsymbol{r})a_{ij}(\boldsymbol{r}), \\ \rho_S^{a^\dagger,a}(\boldsymbol{r}) &= \sum_{i,j,i'=0,1} a_{ij}^\dagger(\boldsymbol{r})[\boldsymbol{\sigma}_S]_{ii'}a_{i'j}(\boldsymbol{r}), \quad S = 1,2,3 \\ \rho_I^{a^\dagger,a}(\boldsymbol{r}) &= \sum_{i,j,j'=0,1} a_{ij}^\dagger(\boldsymbol{r})[\tau_I]_{jj'}a_{ij'}(\boldsymbol{r}), \quad I = 1,2,3 \\ \rho_{SI}^{a^\dagger,a}(\boldsymbol{r}) &= \sum_{iji'j'=0,1} a_{ij}^\dagger(\boldsymbol{r})[\boldsymbol{\sigma}_S]_{ii'}[\tau_I]_{jj'}a_{i'j'}(\boldsymbol{r}).\end{aligned} \tag{4.40}$$

where, each are local density, local spin density, local isospin densitym local spin-isospin density.

[3] If we use other convention, there will be $\frac{1}{L_t L^3}$ factors to operators.

For each static density, we also have an associated current density. Using definition $\vec{\nu}$ and $\vec{\nu}(-l)$, which is a reflecting l-th component of $\vec{\nu}$ about the center of the cube,

$$\begin{aligned} \vec{\nu} &= \nu_1\hat{1} + \nu_2\hat{2} + \nu_3\hat{3}, \quad \nu_{1,2,3} = 0, 1, \\ \vec{\nu}(-l) &= \vec{\nu} + (1 - 2\nu_l)\hat{l}, \quad l = 1, 2, 3 \end{aligned} \tag{4.41}$$

Omitting factors of i and m[4], SU(4) invariant current density,(with a discretization of derivative)

$$\Pi_l^{a^\dagger,a}(\boldsymbol{n}) = \frac{1}{4}\sum_{\nu_{1,2,3}=0,1}\sum_{i,j=0,1}(-1)^{\nu_l+1}a_{i,j}^\dagger(\boldsymbol{n}+\vec{\nu}(-l))a_{i,j}(\boldsymbol{n}+\vec{\nu}). \tag{4.42}$$

Explicit form for $l = 1$ case,[5]

$$\begin{aligned} \Pi_1^{a^\dagger,a}(\boldsymbol{n}) = \frac{1}{4}\sum_{i,j=0,1}\Big[& a_{ij}^\dagger(\boldsymbol{n})a_{ij}(\boldsymbol{n}+\hat{1}) - a_{ij}^\dagger(\boldsymbol{n}+\hat{1})a_{ij}(\boldsymbol{n}) \\ & + a_{ij}^\dagger(\boldsymbol{n}+\hat{2})a_{ij}(\boldsymbol{n}+\hat{1}+\hat{2}) - a_{ij}^\dagger(\boldsymbol{n}+\hat{1}+\hat{2})a_{ij}(\boldsymbol{n}+\hat{2}) \\ & + a_{ij}^\dagger(\boldsymbol{n}+\hat{3})a_{ij}(\boldsymbol{n}+\hat{1}+\hat{3}) - a_{ij}^\dagger(\boldsymbol{n}+\hat{1}+\hat{3})a_{ij}(\boldsymbol{n}+\hat{3}) \\ & + a_{ij}^\dagger(\boldsymbol{n}+\hat{2}+\hat{3})a_{ij}(\boldsymbol{n}+\hat{2}+\hat{3}) - a_{ij}^\dagger(\boldsymbol{n}+\hat{1}+\hat{2}+\hat{3})a_{ij}(\boldsymbol{n}+\hat{2}+\hat{3})\Big] \end{aligned} \tag{4.43}$$

In a similar way, we can define spin current density, isospin current density and spin-isospin current density as

$$\begin{aligned} \Pi_{l,S}^{a^\dagger,a}(\boldsymbol{n}) &= \frac{1}{4}\sum_{\nu_{1,2,3}=0,1}\sum_{i,j,i'=0,1}(-1)^{\nu_l+1}a_{i,j}^\dagger(\boldsymbol{n}+\vec{\nu}(-l))[\sigma_S]_{ii'}a_{i',j}(\boldsymbol{n}+\vec{\nu}), \\ \Pi_{l,I}^{a^\dagger,a}(\boldsymbol{n}) &= \frac{1}{4}\sum_{\nu_{1,2,3}=0,1}\sum_{i,j,j'=0,1}(-1)^{\nu_l+1}a_{i,j}^\dagger(\boldsymbol{n}+\vec{\nu}(-l))[\tau_I]_{jj'}a_{i,j'}(\boldsymbol{n}+\vec{\nu}), \\ \Pi_{l,SI}^{a^\dagger,a}(\boldsymbol{n}) &= \frac{1}{4}\sum_{\nu_{1,2,3}=0,1}\sum_{i,j,i',j'=0,1}(-1)^{\nu_l+1}a_{i,j}^\dagger(\boldsymbol{n}+\vec{\nu}(-l))[\sigma_S]_{ii'}[\tau_I]_{jj'}a_{i',j'}(\boldsymbol{n}+\vec{\nu}), \end{aligned} \tag{4.44}$$

4.4 Explicit form of lattice action

Until now, we have not used any specific expression for lattice action. Let us write the lattice action explicitly in case of chiral EFT.

4.4.1 Example: complex scalar field on a circle of length L

Momentum space

$$|p\rangle = a_p^\dagger|0\rangle \tag{4.45}$$

Non-interacting Hamiltonian,

$$\sum_p \frac{p^2}{2m}a_p^\dagger a_p \tag{4.46}$$

Total number of particle,

$$\sum_p a_p^\dagger a_p \tag{4.47}$$

[4] Exactly? $\frac{1}{2im}$?

[5] $a^\dagger(\boldsymbol{x})\nabla a(\boldsymbol{x}) - \nabla a^\dagger(\boldsymbol{x})a(\boldsymbol{x}) \to a^\dagger(\boldsymbol{n})[a(\boldsymbol{n}+1) - a(\boldsymbol{n})] - [a^\dagger(\boldsymbol{n}+1) - a(\boldsymbol{n})]a(\boldsymbol{n}) = a^\dagger(\boldsymbol{n})a(\boldsymbol{n}+1) - a^\dagger(\boldsymbol{n}+1)a(\boldsymbol{n})$

Position operator

$$a(x) = \frac{1}{\sqrt{L}} \sum_p e^{ipx} a_p, \quad a^\dagger(x) = \frac{1}{\sqrt{L}} \sum_p e^{-ipx} a_p^\dagger \tag{4.48}$$

Local density operator $a^\dagger(x)a(x)$

$$\int_0^L dx a^\dagger(x)a(x) = \sum_p a_p^\dagger a_p \tag{4.49}$$

Space discretization

$$\begin{aligned} &\int_0^L dx \to a \sum_{n=0}^{N-1}, \quad a = \frac{L}{N}, \\ &a(x) \to a(n), \quad a(N) = a(0), \quad [a(n), a^\dagger(n')] = \delta_{n,n'}, \\ &\psi(x) \to \psi(n). \end{aligned} \tag{4.50}$$

The momentum eigen-state may be written as

$$|p\rangle = a_p^\dagger |0\rangle = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} e^{ipn} a^\dagger(n)|0\rangle, \quad p = \frac{2\pi}{N} k \tag{4.51}$$

We may approximate free Hamiltonian as

$$H^{free} = -\frac{1}{2m}\frac{a}{a^2} \sum_{n=0}^{N-1} [a^\dagger(n+1)a(n) + a^\dagger(n)a(n+1) - 2a^\dagger(n)a(n)] \tag{4.52}$$

This gives dispersion relation,

$$E(p) = \frac{1}{m}(1 - \cos p) = \frac{p^2}{2m} + \mathcal{O}(p^4) \tag{4.53}$$

The action of free transfer matrix can be calculated exactly for one-body system,

$$M_{free} =: \exp[-H_{free}\alpha_t] :=: 1 - H_{free}\alpha_t \cdots : \tag{4.54}$$

And one nucleon state $|p\rangle$, we have

$$M_{free}|p = \frac{2\pi}{L}k\rangle = \left(1 + \frac{\alpha_t}{m}(\cos\frac{2\pi}{L}k - 1)\right)|p\rangle = e^{-E(k)\alpha_t}|p\rangle \tag{4.55}$$

with

$$E(k) = -\frac{1}{\alpha_t} \ln\left(1 + \frac{\alpha_t}{m}(\cos\frac{2\pi}{L}k - 1)\right) \tag{4.56}$$

For two nucleon state $|k,\uparrow;k',\downarrow\rangle$, exponential of transfer matrix have to be expanded up to 2nd order,

$$\begin{aligned} M_{free}|k,\uparrow;k',\downarrow\rangle &= \left[1 + \frac{\alpha_t}{2m}\sum_n (a^\dagger(n+1)a(n) + a^\dagger(n)a(n+1) - 2a^\dagger(n)a(n))\right]_\uparrow \\ &\quad \times \left[1 + \frac{\alpha_t}{2m}\sum_n (a^\dagger(n+1)a(n) + a^\dagger(n)a(n+1) - 2a^\dagger(n)a(n))\right]_\downarrow |k,\uparrow;k',\downarrow\rangle \\ &= e^{-E_\uparrow(k)\alpha_t} e^{-E_\downarrow(k')\alpha_t} |k,\uparrow;k',\downarrow\rangle \end{aligned} \tag{4.57}$$

4.5 3-d free nucleon Hamiltonian

Approximate action

Consider fermion action

$$\begin{aligned} -S_E[\psi,\psi^\dagger] &= -\int dt_E \int d^3x \left[\psi^\dagger \partial_t \psi + \mathcal{H}_{free} + \mathcal{H}_{int}\right], \\ \mathcal{H}_{free} &= -\frac{1}{2m}\psi^\dagger \nabla^2 \psi \end{aligned} \tag{4.58}$$

[6] For one small time slap, a simple discretization[7] gives

$$\begin{aligned} &\int_t^{t+a_t} dt_E \int d^3x \left[\psi^\dagger \partial_t \psi + \mathcal{H}_{free}\right] \\ \to\ & a_t a^3 \sum_{\boldsymbol{n}} \frac{1}{a_t}(a^\dagger(\boldsymbol{n},n_t)a(\boldsymbol{n},n_t+1) - a^\dagger(\boldsymbol{n},n_t)a(\boldsymbol{n},n_t)) \\ & +(-\frac{\alpha_t}{2m}\frac{a^3}{a})\sum_{\boldsymbol{n}}\sum_{\boldsymbol{l}}(a^\dagger(\boldsymbol{n},n_t)a^\dagger(\boldsymbol{n}+\boldsymbol{l},n_t) + a^\dagger(\boldsymbol{n},n_t)a^\dagger(\boldsymbol{n}-\boldsymbol{l},n_t) - 2a^\dagger(\boldsymbol{n},n_t)a^\dagger(\boldsymbol{n},n_t)) \end{aligned}$$

where $\boldsymbol{l}$ if for 3-direction and gives $\hat{H}_{free}$ for transfer matrix operator $M^{(n_t)} =: \exp(-\hat{H}_{free}\alpha_t) :$.

If we use 'improved action', we get (set $a = 1$)

$$\begin{aligned} \hat{H}_{free} &= \frac{1}{2m}3\cdot 2\omega_0 \sum_{\boldsymbol{n}}\sum_{i,j} a^\dagger_{ij}(\boldsymbol{n})a_{ij}(\boldsymbol{n}) \\ &\quad -\frac{1}{2m}\omega_1 \sum_{\hat{l}=1,2,3}\sum_{\boldsymbol{n}}\sum_{i,j}[a^\dagger_{ij}(\boldsymbol{n})a_{ij}(\boldsymbol{n}+\hat{l}) + a^\dagger_{ij}(\boldsymbol{n})a_{ij}(\boldsymbol{n}-\hat{l})] \\ &\quad +\frac{1}{2m}\omega_2 \sum_{\hat{l}=1,2,3}\sum_{\boldsymbol{n}}\sum_{i,j}[a^\dagger_{ij}(\boldsymbol{n})a_{ij}(\boldsymbol{n}+2\hat{l}) + a^\dagger_{ij}(\boldsymbol{n})a_{ij}(\boldsymbol{n}-2\hat{l})] + \cdots \end{aligned} \tag{4.60}$$

where i, j are spin and isospin index.

Following expressions are not clear....(note that this is a 4-dimensional momentum not 3-dimensional)

In momentum space, .

$$S^E_{NN} \to \sum_{\boldsymbol{k},ij}\tilde{c}^\dagger_{ij}(-\boldsymbol{k})\tilde{c}_{ij}(\boldsymbol{k})[e^{-ik_0} - e^{-6h} - 2h\sum_{l_s}\cos(\boldsymbol{k}\cdot\hat{l}_s)] \tag{4.61}$$

This corresponds to free neutron propagator as

$$D_N(\boldsymbol{k}) = \frac{1}{e^{-ik_0} - e^{-6h} - 2h\sum_{l_s}\cos(\boldsymbol{k}\cdot\hat{l}_s)}. \tag{4.62}$$

And, the free nucleon correlation,

$$\langle c'_i(\boldsymbol{n})c^*_i(0)\rangle = \frac{\int Dc'Dc^* c'_i(\boldsymbol{n})c^*(0)\exp[-S_{NN}]}{\int Dc'Dc^*\exp[-S_{NN}]} = \frac{1}{L_t L^3}\sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}_*\cdot\boldsymbol{n}} D_N(\boldsymbol{k}) \tag{4.63}$$

[6] Later it will be useful to define h

$$h = \frac{\alpha_t}{2m}. \tag{4.59}$$

[7] Use $f'' = \frac{f_{+h}-2f_0+f_{-h}}{h^2}$. But, more improved action can be used.

Momentum space expression(?)

Another way to compute the transfer matrix is to use DFT.

$$\begin{aligned}
&\int_t^{t+a_t} dt_E \int d^3x \mathcal{H}_{free} \\
\to\ & a_t a^3 \sum_{\boldsymbol{n}} a^\dagger(\boldsymbol{n}, n_t) \widehat{\left(-\frac{\nabla^2}{2m}\right)} a(\boldsymbol{n}, n_t) = a_t a^3 \sum_{\boldsymbol{n}} a^\dagger(\boldsymbol{n}, n_t) \widehat{\left(-\frac{\nabla^2}{2m}\right)} \frac{1}{N^3} \sum_{\boldsymbol{m}} \hat{a}(\boldsymbol{m}, n_t) e^{i\boldsymbol{n}\cdot\boldsymbol{k}_m} \\
=\ & a_t a^3 \sum_{\boldsymbol{n}} \frac{1}{N^3} \sum_{\boldsymbol{m}} a^\dagger(\boldsymbol{n}, n_t) \left(\frac{\boldsymbol{k}_m^2}{2m}\right) \hat{a}(\boldsymbol{m}, n_t) e^{i\boldsymbol{n}\cdot\boldsymbol{k}_m} \\
=\ & a_t a^3 \sum_{\boldsymbol{n}} a^\dagger(\boldsymbol{n}, n_t) \frac{1}{N^3} \sum_{\boldsymbol{m}} \hat{b}(\boldsymbol{m}, n_t) e^{i\boldsymbol{n}\cdot\boldsymbol{k}_m} = a_t a^3 \sum_{\boldsymbol{n}} a^\dagger(\boldsymbol{n}, n_t) b(\boldsymbol{n}, n_t)
\end{aligned} \tag{4.64}$$

where $\boldsymbol{k}_m = 2\pi(\frac{m_1}{N}, \frac{m_2}{N}, \frac{m_3}{N})$ and

$$\begin{aligned}
&\hat{a}(\boldsymbol{k}_m, n_t) = \underbrace{\sum_{\boldsymbol{n}} a(\boldsymbol{n}, n_t) e^{-i\boldsymbol{n}\cdot\boldsymbol{k}_m}}_{FFT}, \quad a(\boldsymbol{n}, n_t) = \frac{1}{N^3} \sum_{\boldsymbol{m}} \hat{a}(\boldsymbol{m}, n_t) e^{i\boldsymbol{n}\cdot\boldsymbol{k}_m} \\
&b(\boldsymbol{n}, n_t) = \frac{1}{N^3} \underbrace{\sum_{\boldsymbol{m}} \left(\frac{\boldsymbol{k}_m^2}{2m}\right) \hat{a}(\boldsymbol{m}, n_t) e^{i\boldsymbol{n}\cdot\boldsymbol{k}_m}}_{iFFT}
\end{aligned} \tag{4.65}$$

4.6 instantaneous free pion lattice action

Instantaneous pion action is

$$\begin{aligned}
-S_E[\pi_I] &= -\int d\tau \int d^3x \left[\frac{1}{2}(\nabla\pi_I)^2 + \frac{1}{2}m_\pi^2 \pi_I^2 + V(\pi_I)\right] \\
&= -\int d\tau \int d^3x \left[\frac{1}{2}\pi_I(-\nabla^2)\pi_I + \frac{1}{2}m_\pi^2 \pi_I^2 + V(\pi_I)\right]
\end{aligned} \tag{4.66}$$

Then free pion action for small time slap is

$$\begin{aligned}
H_{\pi\pi} a_t &= \int_t^{t+a_t} d\tau \int d\boldsymbol{x} \frac{1}{2} \vec{\pi}(-\nabla^2 + m_\pi^2)\vec{\pi} \\
&\to a_t a^3 \sum_{\boldsymbol{n}, j} \frac{1}{2} \pi_j(\boldsymbol{n}, n_t) [\widehat{(-\nabla^2)} + m_\pi^2] \pi_j(\boldsymbol{n}, n_t)
\end{aligned} \tag{4.67}$$

Approximate action

If we use a simple approximation for Laplacian, we get

$$\begin{aligned}
\to\ & a_t a^3 \sum_{\boldsymbol{n}} \frac{1}{2} m_\pi^2 \pi_j(\boldsymbol{n}, n_t)\pi_j(\boldsymbol{n}, n_t) + a_t a^3 \sum_{\boldsymbol{n}} \sum_{\boldsymbol{l}} \frac{1}{2} \frac{1}{a^2} \pi_j(\boldsymbol{n}, n_t)[2\pi_j(\boldsymbol{n}, n_t) - \pi_j(\boldsymbol{n}+\boldsymbol{l}, n_t) - \pi_j(\boldsymbol{n}-\boldsymbol{l}, n_t)] \\
=\ & \alpha_t a^4 \sum_{\boldsymbol{n}} \frac{1}{2} \left(m_\pi^2 + \frac{6}{a^2}\right) \pi_j(\boldsymbol{n}, n_t)\pi_j(\boldsymbol{n}, n_t) \\
& + \alpha_t(-\frac{a^4}{a^2}) \sum_{\boldsymbol{n}} \sum_{\boldsymbol{l}} \frac{1}{2} \pi_j(\boldsymbol{n}, n_t)[\pi_j(\boldsymbol{n}+\boldsymbol{l}, n_t) + \pi_j(\boldsymbol{n}-\boldsymbol{l}, n_t)] \\
=\ & \alpha_t a^4 \sum_{\boldsymbol{n}} \frac{1}{2} \left(m_\pi^2 + \frac{6}{a^2}\right) \pi_j(\boldsymbol{n}, n_t)\pi_j(\boldsymbol{n}, n_t) + \alpha_t(-\frac{a^4}{a^2}) \sum_{\boldsymbol{n}} \sum_{\boldsymbol{l}} \pi_j(\boldsymbol{n}, n_t)\pi_j(\boldsymbol{n}+\boldsymbol{l}, n_t)
\end{aligned} \tag{4.68}$$

where the last line uses the fact that π is a real scalar.

We may rescale pion field to simplify the action,

$$\pi'_I(\boldsymbol{n}) = \sqrt{q_\pi}\pi_I(\boldsymbol{n}), \quad q_\pi = \alpha_t(m_\pi^2 + 6). \tag{4.69}$$

This position space action as (set $a = 1$)

$$\boxed{S^E_{\pi\pi}(\pi') = \frac{1}{2}\sum_{\boldsymbol{n},j}\pi'_j(\boldsymbol{n},n_t)\pi'_j(\boldsymbol{n},n_t) - \frac{\alpha_t}{q_\pi}\sum_{\boldsymbol{n},\boldsymbol{l},j}\pi'_j(\boldsymbol{n},n_t)\pi'_j(\boldsymbol{n}+\boldsymbol{l},n_t)} \tag{4.70}$$

Following expressions need clarification.. (here only 3-d DFT is used)

On the other hand, if we convert approximate action into momentum space action for original pion, it can be written as

$$S^E_{\pi\pi}(\pi) \to \frac{1}{L^3}\sum_{\boldsymbol{k},j}\frac{1}{2}\tilde{\pi}_j(-\boldsymbol{k},n_t)\tilde{\pi}_j(\boldsymbol{k},n_t)\alpha_t\left[(m_\pi^2+6) - \sum_{\boldsymbol{l}} 2\cos(\frac{2\pi}{L}\boldsymbol{k}\cdot\boldsymbol{l})\right] \tag{4.71}$$

or for rescaled pion

$$S^E_{\pi\pi}(\pi') \quad = \quad \frac{1}{L^3}\sum_{\boldsymbol{k},I}\frac{1}{2}\pi'_I(-\boldsymbol{k},n_t)\pi'_I(\boldsymbol{k},n_t)\left[1 - \frac{2\alpha_t}{q_\pi}\sum_{l_s}\cos(\frac{2\pi k_{l_s}}{L})\right], \tag{4.72}$$

[8] This corresponds to the pion propagator

$$D_\pi(\boldsymbol{k}) = \frac{1}{2\left[(\frac{m_\pi^2}{2}+3)\alpha_t - \alpha_t\sum_{\boldsymbol{l}_s}\cos(\boldsymbol{k}\cdot\boldsymbol{l}_s)\right]}. \tag{4.73}$$

$$\langle\pi(\boldsymbol{n})\pi(0)\rangle = \frac{\int D\pi\pi(\boldsymbol{n})\pi(0)\exp[-S_{\pi\pi}]}{\int D\pi\exp[-S_{\pi\pi}]} = \frac{1}{L_tL^3}\sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}_*\cdot\boldsymbol{n}}D_\pi(\boldsymbol{k}) \tag{4.74}$$

Thus, for rescaled pion,

$$\langle\pi'(\boldsymbol{n})\pi'(0)\rangle = \frac{1}{L_tL^3}\sum_{\boldsymbol{k}} e^{-i\frac{2\pi}{L_t}k_t\cdot n_t}e^{-i\frac{2\pi}{L}\boldsymbol{k}_s\cdot\boldsymbol{n}_s}D_\pi(\boldsymbol{k}_s), \tag{4.75}$$

$$D_\pi(\boldsymbol{k}_s) = \frac{1}{1 - \frac{2\alpha_t}{q_\pi}\sum_{l_s=1,2,3}\cos(\frac{2\pi k_{l_s}}{L})} \tag{4.76}$$

Note here

$$\begin{aligned}(\frac{\alpha_t}{q_\pi}D(\boldsymbol{k}_s))^{-1} \quad &= \quad \frac{q}{\alpha_t} - 2\sum_{l_s}\cos(\frac{2\pi k_{l_s}}{L}) \simeq m_\pi^2 + 6 - 2\sum_{l_s=1,2,3}\left[1 - \frac{1}{2}(\frac{2\pi k_{l_s}}{L})^2 + \frac{1}{24}(\frac{2\pi k_{l_s}}{L})^4 + \cdots\right] \\ &\simeq \quad m_\pi^2 + k_{*1}^2 + k_{*2}^2 + k_{*3}^2 - \frac{1}{12}(k_{*1}^4 + k_{*2}^4 + k_{*3}^4) + \ldots \end{aligned} \tag{4.77}$$

It is useful to define the two-derivative pion correlator,

$$\begin{aligned}G_{S_1S_2}(\boldsymbol{n}) \quad &= \quad \langle\Delta_{S_1}\pi'_I(\boldsymbol{n},n_t)\Delta_{S_2}\pi'_I(\vec{0},n_t)\rangle \quad \text{(no sum on I)} \\ &= \quad \frac{1}{16}\sum_{\nu_{1,2,3}=0,1}\sum_{\nu'_{1,2,3}=0,1}(-1)^{\nu_{S_1}}(-1)^{\nu'_{S_2}}\langle\pi'_I(\boldsymbol{n}+\vec{\nu}-\vec{\nu}',n_t)\pi'_I(\vec{0},n_t)\rangle. \end{aligned} \tag{4.78}$$

[8] where, from $\sum_{\boldsymbol{k}}\tilde{\pi}_j(-\boldsymbol{k})\tilde{\pi}_j(\boldsymbol{k})f(\boldsymbol{k}) = \sum_{\boldsymbol{k}}\tilde{\pi}_j(-\boldsymbol{k})\tilde{\pi}_j(\boldsymbol{k})f(-\boldsymbol{k})$, we can replace $e^{i\boldsymbol{k}\cdot\boldsymbol{l}} \to = \frac{1}{2}(e^{i\boldsymbol{k}\cdot\boldsymbol{l}} + e^{-i\boldsymbol{k}\cdot\boldsymbol{l}}) = \cos(\boldsymbol{k}\cdot\boldsymbol{l})$ for pion.

with

$$\begin{aligned}\langle \pi_I'(\boldsymbol{n}, n_t)\pi_I'(0, n_t)\rangle &= \frac{1}{L^3}\sum_{\boldsymbol{k}} e^{-i\frac{2\pi}{L}\boldsymbol{k}\cdot\boldsymbol{n}} D_\pi(\boldsymbol{k}), \\ D_\pi(\boldsymbol{k}) &= \frac{1}{1-\frac{2\alpha_t}{q_\pi}\sum_l \cos(k_l)}, \quad k_l = \frac{2\pi}{L}\boldsymbol{k}\cdot\boldsymbol{l}. \end{aligned} \tag{4.79}$$

We may further simplify the free pion action by rescaling pion field in momentum space,

$$\begin{aligned}\pi_I'(-\boldsymbol{k}, n_t) &= \pi_I(-\boldsymbol{k}, n_t)\sqrt{m_\pi^2 + 6 - \sum_l 2\cos(\frac{2\pi}{L}\boldsymbol{k}\cdot\boldsymbol{l})}, \\ \pi_I'(\boldsymbol{k}, n_t) &= \pi_I(\boldsymbol{k}, n_t)\sqrt{m_\pi^2 + 6 - \sum_l 2\cos(\frac{2\pi}{L}\boldsymbol{k}\cdot\boldsymbol{l})} \end{aligned} \tag{4.80}$$

so that the free pion action becomes in configuration space and momentum space as

$$S_{\pi\pi}(\pi') = \frac{1}{2}\sum_{\boldsymbol{n},I}\pi_I'(\boldsymbol{n})\pi_I'(\boldsymbol{n}) = \frac{1}{L^3}\frac{1}{2}\sum_{\boldsymbol{k},I}\pi_I'(-\boldsymbol{k})\pi_I'(\boldsymbol{k}) \tag{4.81}$$

Momentum space expression

If we set pions as real valued, we have $\hat{\pi}(\boldsymbol{m}) = \hat{\pi}^*(-\boldsymbol{m})$,

$$H_{\pi\pi}a_t \;\to\; a_t a^3 \sum_j \sum_{\boldsymbol{n}} (\frac{1}{N^3})^2 \sum_{\boldsymbol{m},\boldsymbol{m}'} \frac{1}{2}\hat{\pi}_j(-\boldsymbol{m}')\hat{\pi}(\boldsymbol{m})(m_\pi^2 + \boldsymbol{q}_m^2)e^{i(\boldsymbol{q}_m - \boldsymbol{q}_{m'})\cdot\boldsymbol{n}}. \tag{4.82}$$

If we define

$$\hat{\phi}(\boldsymbol{m}) = \sqrt{m_\pi^2 + \boldsymbol{q}_m^2}\hat{\pi}(\boldsymbol{m}), \quad \hat{\phi}(-\boldsymbol{m}) = \sqrt{m_\pi^2 + \boldsymbol{q}_m^2}\hat{\pi}(-\boldsymbol{m}) \tag{4.83}$$

Then, from iFFT of $\hat{\phi}(\boldsymbol{m})$, we get simple free action,

$$\begin{aligned}&\phi(\boldsymbol{n}) = \frac{1}{N^3}\sum_{\boldsymbol{m}}\hat{\phi}(\boldsymbol{m})e^{i\boldsymbol{q}_m\cdot\boldsymbol{n}} = \frac{1}{N^3}\sum_{\boldsymbol{m}}\hat{\phi}(-\boldsymbol{m})e^{-i\boldsymbol{q}_m\cdot\boldsymbol{n}}, \\ &H_{\pi\pi}a_t \to a_t a^3 \sum_j \sum_{\boldsymbol{n}} \frac{1}{2}\phi_j(\boldsymbol{n})\phi_j(\boldsymbol{n}). \end{aligned} \tag{4.84}$$

4.7 Lattice action for Cold atom

Consider a cold atom system which interacts each other with short range interaction. Cold atom can have spins. Then, we can write the effective Hamiltonian at leading order as

$$\begin{aligned} H_{LO} &= H_{free} + V_{LO}, \\ H_{free} &= \frac{1}{2m} \sum_{i=\uparrow,\downarrow} \int d^3\boldsymbol{r} \nabla a_i^\dagger(\boldsymbol{r}) \cdot \nabla a_i(\boldsymbol{r}), \\ V_{LO} &= \frac{C}{2} \int d^3\boldsymbol{r} : [\rho^{a^\dagger,a}(\boldsymbol{r})]^2 :, \end{aligned} \tag{4.85}$$

Then, we will have discretized lattice action,

$$\mathcal{Z} = \mathrm{Tr}[M^{L_t}], \tag{4.86}$$

where,

$$M =: \exp\left\{ -H_{free}\alpha_t - \frac{1}{2} C\alpha_t \sum_{\boldsymbol{n}} [\rho^{a^\dagger,a}(\boldsymbol{n})]^2 \right\} : \tag{4.87}$$

Note the auxiliary coupling is not introduced yet.

If we introduce auxiliary field $s(\boldsymbol{n})$, we get

$$\mathcal{Z} = \int \mathcal{D}s e^{-\frac{1}{2}\sum_{\boldsymbol{n}} s(\boldsymbol{n})^2} \mathrm{Tr}[M(s)^{L_t}] \tag{4.88}$$

where

$$M(s) =: \exp\left\{ -H_{free}\alpha_t + \sqrt{-C\alpha_t} \sum_{\boldsymbol{n}} \rho^{a^\dagger,a}(\boldsymbol{n}) s(\boldsymbol{n}) \right\} : \tag{4.89}$$

4.8 Lattice action for Pionless EFT

In case of pionless EFT, we have to consider isospin too. If we denote spins $i = 0, 1$ as spin up and down and isospin $j = 0, 1$ as isospin up and down, we can think of following local density operators.

Then, pionless EFT interaction becomes

$$\begin{aligned} H_{LO} &= H_{free} + V_{LO}, \\ H_{free} &= \frac{1}{2m} \sum_{ij=0,1} \int d^3\boldsymbol{r} \nabla a_{ij}^\dagger(\boldsymbol{r}) \cdot \nabla a_{ij}(\boldsymbol{r}), \\ V_{LO} &= V + V_{I^2} + V^{3N}, \\ V &= \frac{C}{2} \int d^3\boldsymbol{r} : [\rho(\boldsymbol{r})]^2 :, \\ V_{I^2} &= \frac{C_{I^2}}{2} \sum_{I=1,2,3} \int d^3\boldsymbol{r} : [\rho_I(\boldsymbol{r})]^2 :, \\ V^{(3N)} &= \frac{D}{6} \int d^3\boldsymbol{r} : \rho(\boldsymbol{r})^3 : \end{aligned} \tag{4.90}$$

Note that here V^{3N} is required at leading order.

Then, the discretized lattice action becomes

$$\mathcal{Z} = \mathrm{Tr}[M^{L_t}], \tag{4.91}$$

where,

$$M =: \exp\left\{-H_{free}\alpha_t - \frac{1}{2}C\alpha_t\sum_{\boldsymbol{n}}[\rho^{a^\dagger,a}(\boldsymbol{n})]^2 - \frac{1}{2}C_{I^2}\alpha_t\sum_{\boldsymbol{n},I}[\rho_I^{a^\dagger,a}(\boldsymbol{n})]^2 - \frac{1}{6}D\alpha_t\sum_{\boldsymbol{n}}[\rho^{a^\dagger,a}(\boldsymbol{n})]^3\right\} \quad (4.92)$$

Can we introduce auxiliary field ? D-term may be problematic. Refer next section for other terms with auxiliary field.

4.9 Lattice action of LO Chiral EFT

4.9.1 Continuum limit

The LO chiral Lagrangian is,

$$\begin{aligned}\mathcal{L} &= \frac{1}{2}\partial_\mu\vec{\pi}\cdot\partial^\mu\vec{\pi} - \frac{1}{2}m_\pi^2\vec{\pi}^2 + N^\dagger i\partial_0 N + N^\dagger\frac{\nabla^2}{2m}N \\ &\quad -\frac{g_A}{2f_\pi}N^\dagger\boldsymbol{\tau}\boldsymbol{\sigma}N\cdot\nabla\boldsymbol{\pi} - \frac{1}{2}C(N^\dagger NN^\dagger N) - \frac{1}{2}C_I(N^\dagger\boldsymbol{\tau}N)\cdot(N^\dagger\boldsymbol{\tau}N),\end{aligned} \quad (4.93)$$

which give rise the LO NN potential,

$$V_{LO} = C + C_I\tau_1\cdot\tau_2 - (\frac{g_A}{2f_\pi})^2\tau_1\cdot\tau_2\frac{\boldsymbol{\sigma}_1\cdot\boldsymbol{q}\boldsymbol{\sigma}_2\cdot\boldsymbol{q}}{\boldsymbol{q}^2+m_\pi^2}. \quad (4.94)$$

Treating pions instantaneously[9] we have continuum LO action with instantaneous pion as

$$\begin{aligned}-S_E &= \int d\tau d^3x\mathcal{L}_E, \\ \mathcal{L}_E &= -\frac{1}{2}\nabla\vec{\pi}\nabla\vec{\pi} - \frac{1}{2}m_\pi^2\vec{\pi}^2 - N^\dagger\partial_t^E N + N^\dagger\frac{\nabla^2}{2m}N \\ &\quad -\frac{g_A}{2f_\pi}N^\dagger\boldsymbol{\tau}\boldsymbol{\sigma}N\cdot\nabla\boldsymbol{\pi} - \frac{1}{2}C(N^\dagger NN^\dagger N) - \frac{1}{2}C_I(N^\dagger\boldsymbol{\tau}N)\cdot(N^\dagger\boldsymbol{\tau}N).\end{aligned} \quad (4.95)$$

The detailed procedure for the discretization will be continued on following sections.

We may use two different method to write the transfer matrix. By integrating out pions, we would get pure nucleon-nucleon interactions. This form can be used to obtain $Z_\Psi = \langle\Psi|M^{L_t}|\Psi\rangle$. However, this form will be too complicate to be used for many nucleons. Thus, we may keep pions as auxiliary fields and also introduce other auxiliary fields to remove contact interactions from the transfer matrix, so that $Z_\Psi = \int D\pi Dse^{-S_\pi - S_s}\langle\Psi|M^{L_t}(\pi,s)|\Psi\rangle$.

4.9.2 pion-nucleon term in approximate derivative form

Interacting Hamiltonian for pion-nucleon term is

$$H_{\pi NN} = \frac{g_A}{2f_\pi}\int d\boldsymbol{x}N^\dagger\boldsymbol{\tau}_I\boldsymbol{\sigma}_S N\cdot\nabla_S\pi_I \quad (4.96)$$

We get

$$H_{\pi NN}\alpha_t \rightarrow \frac{g_A}{2f_\pi}\alpha_t a^4\sum_{\boldsymbol{n}}\sum_{S,i,j}\sum_{I,i',j'}c_{i,i'}^\dagger(\boldsymbol{n},n_t)(\boldsymbol{\sigma}_S)_{ij}(\tau_I)_{i'j'}c_{j,j'}(\boldsymbol{n},n_t)\times\hat{\nabla}_S\pi_I(\boldsymbol{n},n_t). \quad (4.97)$$

[9] In other words, pion does not have time derivative terms and acts as an auxiliary field which reproduce the leading order OPE potential.

One may approximate the derivative as

$$\hat{\nabla}_S \pi_I(\boldsymbol{n}, n_t) \to \frac{1}{2a}[\pi_I(\boldsymbol{n}+\hat{l}_s) - \pi_I(\boldsymbol{n}-\hat{l}_s)]. \tag{4.98}$$

However, this form has disadvantage by computing derivative coarsely with two points values in two step size. It is not necessary for pions to be defined at the same lattice position as nucleons. Instead if we define pions at shifted positions(If there is no terms like πNN, pion does not need to be evaluated at the same point of nucleons.)

$$\boldsymbol{n}_{pion} = \boldsymbol{n}_{nul} - \frac{1}{2}\hat{1} - \frac{1}{2}\hat{2} - \frac{1}{2}\hat{3}, \tag{4.99}$$

then, One way to approximate $\Delta_S \pi(\boldsymbol{n})$ is, to average surrounding pions near $\boldsymbol{n}_{nuc}$[10] , thus have approximation

$$\Delta_S \pi'_I(\boldsymbol{n}_{nuc}) \to \frac{1}{4} \sum_{\nu_1,\nu_2,\nu_3=0,1} (-1)^{\nu_S+1} \pi'_I(\boldsymbol{n}_{pion}+\boldsymbol{\nu}), \quad \boldsymbol{\nu} = \nu_1\hat{1} + \nu_2\hat{2} + \nu_3\hat{3}. \tag{4.101}$$

Thus, with scaled pion,

$$\begin{aligned} S^E_{\pi N} &\to \frac{g_A \alpha_t}{2 f_\pi \sqrt{q_\pi}} \sum_{\boldsymbol{n}} \sum_{S,I} \Delta_S \pi'_I(\boldsymbol{n}) \rho_{S,I}(\boldsymbol{n}), \\ \rho_{S,I}(\boldsymbol{n}) &= \sum_{i,j,i',j'} c^\dagger_{i,i'}(\boldsymbol{n}) (\boldsymbol{\sigma}_S)_{ij} (\tau_I)_{i'j'} c_{j,j'}(\boldsymbol{n}) \end{aligned} \tag{4.102}$$

4.9.3 pion nucleon term in momentum space

Let us consider derivative couping of pion and nucleon in momentum space for more exact calculation. As shown in free pion, by rescale pion field, we can get a very simple free pion action,

$$\begin{aligned} &\hat{\phi}(\boldsymbol{m}) = \sqrt{m_\pi^2 + \boldsymbol{q}_m^2}\hat{\pi}(\boldsymbol{m}), \quad \hat{\phi}(-\boldsymbol{m}) = \sqrt{m_\pi^2 + \boldsymbol{q}_m^2}\hat{\pi}(-\boldsymbol{m}), \\ &\phi(\boldsymbol{n}) = \frac{1}{N^3} \sum_{\boldsymbol{m}} \hat{\phi}(\boldsymbol{m}) e^{i\boldsymbol{q}_m \cdot \boldsymbol{n}} = \frac{1}{N^3} \sum_{\boldsymbol{m}} \hat{\phi}(-\boldsymbol{m}) e^{-i\boldsymbol{q}_m \cdot \boldsymbol{n}}, \\ &H_{\pi\pi} a_t \to a_t a^3 \sum_j \sum_{\boldsymbol{n}} \frac{1}{2} \phi_j(\boldsymbol{n}) \phi_j(\boldsymbol{n}). \end{aligned} \tag{4.103}$$

Then for πN coupling term, (mistake for a^4?)

$$H_{\pi NN} \alpha_t \to \frac{g_A}{2 f_\pi} \alpha_t a^4 \sum_{\boldsymbol{n}} \sum_{S,i,j} \sum_{I,i',j'} c^\dagger_{i,i'}(\boldsymbol{n}, n_t) (\boldsymbol{\sigma}_S)_{ij} (\tau_I)_{i'j'} c_{j,j'}(\boldsymbol{n}, n_t) \times \hat{\nabla}_S \pi_I(\boldsymbol{n}, n_t) \tag{4.104}$$

Because in the code, it would be easier to use path integral over scaled pion $\phi(\boldsymbol{n})$ (or $\pi'_I(\boldsymbol{n})$), to compute $\pi - N$ coupling, one have to convert π'_I into true pion field π_I. Considering DFT, (suppressing isospin and time index)

Thus, for given $\pi'_I(\boldsymbol{n})$ we can obtain $\pi_I(\boldsymbol{n})$ by the successive Fourier transformation and division. (I.e. convert $\pi'_I(\boldsymbol{n}) \to \hat{\pi}'_I(\boldsymbol{q}) \to \hat{\pi}_I(\boldsymbol{q}) \to \pi_I(\boldsymbol{n})$.)

$$\hat{\pi}(\boldsymbol{q}) = \sum_{\boldsymbol{n}'} e^{-i\boldsymbol{q}\cdot\boldsymbol{n}'} \pi(\boldsymbol{n}') = \sum_{\boldsymbol{n}'} e^{-i\boldsymbol{q}\cdot\boldsymbol{n}'} \left(\frac{1}{L^3} \sum_{\boldsymbol{p}} e^{i\boldsymbol{p}\cdot\boldsymbol{n}'} \frac{\pi'_I(\boldsymbol{p})}{\sqrt{\boldsymbol{p}^2 + m_\pi^2}} \right) \tag{4.105}$$

[10] For example, in 2-d, around $\boldsymbol{n}$,

$$\begin{aligned} \Delta_1 \pi(\boldsymbol{n}) &= \frac{1}{2}[\Delta_1 \pi(\boldsymbol{n}_{pion}) + \Delta_1 \pi(\boldsymbol{n}_{pion} + \hat{2})] \\ &= \frac{1}{2}[\frac{1}{2}(\pi(\boldsymbol{n}_{pion} + \hat{1}) - \pi(\boldsymbol{n}_{pion})) + \frac{1}{2}(\pi(\boldsymbol{n}_{pion} + \hat{2} + \hat{1}) - \pi(\boldsymbol{n}_{pion} + \hat{2}))] \end{aligned} \tag{4.100}$$

As already shown in the first chapter, one can introduce qhop function,

$$H_{\pi NN}\alpha_t \quad \rightarrow \quad \frac{g_A}{2f_\pi}\alpha_t a^4 \sum_{\boldsymbol{n}} \sum_{S,i,j} \sum_{I,i',j'} c^\dagger_{i,i'}(\boldsymbol{n},n_t)(\boldsymbol{\sigma}_S)_{ij}(\tau_I)_{i'j'}c_{j,j'}(\boldsymbol{n},n_t) \times \sum_{n'_S} \pi(\boldsymbol{n}+n'_S\hat{s})\Delta(n'_S).$$

4.10 nucleon-nucleon contact term in lattice

At leading order, the contact terms can be written as

$$S^E_{4N} = \frac{C\alpha_t}{2}\sum_{\boldsymbol{n}}[\rho(\boldsymbol{n})]^2 + \frac{C_I\alpha_t}{2}\sum_{\boldsymbol{n}}\sum_{I=1,2,3}[\rho_I(\boldsymbol{n})]^2, \tag{4.106}$$

$$\begin{aligned}\rho(\boldsymbol{n}) &= \sum_{i,j=0,1} c^*_{i,j}(\boldsymbol{n})c_{i,j}(\boldsymbol{n}),\\ \rho_I(\boldsymbol{n}) &= \sum_{i,j,j'=0,1} c^*_{i,j}(\boldsymbol{n})[\tau_I]_{jj'}c_{i,j'}(\boldsymbol{n})\end{aligned} \tag{4.107}$$

As shown in the first chapter, we may introduce auxiliary field s and s_I,

$$\exp\left(-\frac{C\alpha_t}{2}[\rho(\boldsymbol{n})]^2\right) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} ds \exp\left[-\frac{1}{2}s^2 + \sqrt{-C\alpha_t}\rho(\boldsymbol{n})\cdot s\right], \tag{4.108}$$

$$\exp\left(-\frac{C_I\alpha_t}{2}\sum_I[\rho_I(\boldsymbol{n})]^2\right) = \int\prod_I\frac{ds_I}{\sqrt{2\pi}}\exp\left[-\frac{1}{2}\sum_I s_I^2 + i\sqrt{C_I\alpha_t}\sum_I\rho_I(\boldsymbol{n})\cdot s_I\right], \tag{4.109}$$

where, $C<0$ and $C_I>0$. Define auxiliary action,

$$S_{ss}(s,s_I) = \frac{1}{2}\sum_{\boldsymbol{n}} s(\boldsymbol{n})^2 + \frac{1}{2}\sum_{\boldsymbol{n}}\sum_I s_I^2(\boldsymbol{n}) \tag{4.110}$$

$$\begin{aligned}\exp[-S^E_{4N}] &\propto \int DsDs_I \exp[-S_{ss}(s,s_I)]\exp\left[+\sum_{\boldsymbol{n}}\sqrt{-C\alpha_t}\rho(\boldsymbol{n})\cdot s + \sum_{\boldsymbol{n}} i\sqrt{C_I\alpha_t}\sum_I\rho_I(\boldsymbol{n})\cdot s_I\right]\\ &= \int DsDs_I \exp[-S_{ss}(s,s_I) - S_{sNN}(s,s_I,c,c^*)]\end{aligned} \tag{4.111}$$

because of measure, there are normalization factors in exact equation but we would not need to specify.

4.10.1 Equivalence of different expressions of LO contact interaction

Let us summarize different possible expressions of LO contact interaction.

- Original Weinberg contact interaction at leading order is

$$:-\frac{1}{2}C'_1\bar{N}N\bar{N}N - \frac{1}{2}C'_2\bar{N}\boldsymbol{\sigma}N\cdot\bar{N}\boldsymbol{\sigma}N: \tag{4.112}$$

  where, $C'_1<0$ and $C'_2<0$.

- It is preferred to have positive coefficients because of reducing sign problem, we may write it as

$$:-\frac{1}{2}C_1\bar{N}N\bar{N}N - \frac{1}{2}C_2\bar{N}\tau N\cdot\bar{N}\tau N: \tag{4.113}$$

The equivalence with original Weinberg's form can be shown by using identity

$$: \bar{N}N\bar{N}N := -\frac{1}{2} : \bar{N}\vec{\sigma}N \cdot \bar{N}\vec{\sigma}N : -\frac{1}{2} : \bar{N}\vec{\tau}N \cdot \bar{N}\vec{\tau}N : \tag{4.114}$$

and we got $C_2 = -C_2' > 0, C_1 = C_1' - 2C_2' < 0$.

- Another possible form is

$$C_{S=0,I=1}\left(\frac{1}{4} - \frac{1}{4}\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2\right)\left(\frac{3}{4} + \frac{1}{4}\tau_1 \cdot \tau_2\right) + C_{S=1,I=0}\left(\frac{3}{4} + \frac{1}{4}\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2\right)\left(\frac{1}{4} - \frac{1}{4}\tau_1 \cdot \tau_2\right) \tag{4.115}$$

The equivalence with other form can be shown by requiring anti-symmetric two nucleon states for S-wave $P_s = +1$

$$P_s P_\sigma P_\tau = -1, \quad P_\sigma = \frac{1 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2}{2}. \tag{4.116}$$

Thus, by using both identity, $\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2\tau_1\tau_2 = -3$, $\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 = -2 - \tau_1 \cdot \tau_2$, it can be written as

$$\frac{1}{4}(3C_{01} + C_{10}) + \frac{1}{4}(C_{01} - C_{10})\tau_1 \cdot \tau_2 \tag{4.117}$$

- By expanding above form we get

$$C_0 + C_S\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + C_I\tau_1 \cdot \tau_2 + C_{SI}\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2\tau_1 \cdot \tau_2 \tag{4.118}$$

such that

$$\begin{aligned} C_0 &= -3C_{SI} = -\frac{3}{2}(C_S + C_I), \\ C_0 &= \frac{3}{16}(C_{01} + C_{10}) = -3C_{SI}, \\ C_S &= \frac{1}{16}(-3C_{01} + C_{10}), \quad C_I = \frac{1}{16}(C_{01} - 3C_{10}). \end{aligned} \tag{4.119}$$

Though all of them are equivalent, for numerical calculation some form may be preferred.

If we smear the contact interaction, we may consider it as a kind of mixture of leading order and higher order interaction.

4.11 Chiral EFT action in lattice

Let us summarize the lattice action for chiral EFT.

However, the expressions given here use approximate free action and scaled pions. Thus, somewhat outdated.

4.11.1 Transfer matrix without pions and auxiliary fields

In case of approximate derivative form,

$$\mathcal{Z}_{LO} \propto \mathrm{Tr}\left[M_{LO}^{(N_t-1)} \cdots M_{LO}^{(0)}\right], \tag{4.120}$$

$$\begin{aligned} M^{(n_t)} &= : \exp\Big[- H_{free}\alpha_t - \frac{1}{2}C\alpha_t \sum_{\boldsymbol{n}_s}[\rho(\boldsymbol{n}_s)]^2 - \frac{1}{2}C\alpha_t \sum_{\boldsymbol{n}_s}\sum_{I}[\rho_I(\boldsymbol{n}_s)]^2 \\ &\quad + \frac{g_A^2\alpha_t^2}{8f_\pi^2 q_\pi} \sum_{S_1,S_2,I}\sum_{\boldsymbol{n}_{s1}\boldsymbol{n}_{s2}} G_{S_1S_2}(\boldsymbol{n}_{s1} - \boldsymbol{n}_{s2})\rho_{S_1,I}(\boldsymbol{n}_{s1})\rho_{S_2,I}(\boldsymbol{n}_{s2})\Big] : \end{aligned} \tag{4.121}$$

where[11]

$$G_{S_1S_2}(\boldsymbol{n}_s) = \frac{\int D\pi'_I \Delta_{S_1}\pi'_I(\boldsymbol{n}_s)\Delta_{S_2}\pi'_I(0)\exp[-S_{\pi\pi}]}{\int D\pi'_I \exp[-S_{\pi\pi}]}$$
$$= \frac{1}{16}\sum_{\nu_1,\nu_2,\nu_3=0,1}\sum_{\nu'_1,\nu'_2,\nu'_3=0,1}(-1)^{\nu_{S_1}}(-1)^{\nu'_{S_2}}\langle\pi'_I(\boldsymbol{n}_s+\nu-\nu')\pi'_I(0)\rangle \quad (4.123)$$

or using coefficient function in momentum space,

$$M_{LO} = :\exp\Big\{-H_{free}\alpha_t - \frac{\alpha_t}{L^3}\sum_{\boldsymbol{q}} f(\boldsymbol{q})[C_{S=0,I=1}V_{S=0,I=1}(\boldsymbol{q}) + C_{S=1,I=0}V_{S=1,I=0}(\boldsymbol{q})]$$
$$+\frac{g_A^2\alpha_t^2}{8f_\pi^2 q_\pi}\sum_{S_1,S_2,I}\sum_{\boldsymbol{n}_1,\boldsymbol{n}_2}G_{S_1S_2}(\boldsymbol{n}_1-\boldsymbol{n}_2)\rho_{S_1,I}(\boldsymbol{n}_1)\rho_{S_2,I}(\boldsymbol{n}_2)\Big\}: \quad (4.124)$$

Coefficient function

$$f(\boldsymbol{q}) = f_0^{-1}\exp[-b\sum_l(1-\cos q_l)], \quad f_0 = \frac{1}{L^3}\sum_{\boldsymbol{q}}\exp[-b\sum_l(1-\cos q_l)]. \quad (4.125)$$

In fact, better form may be using the expression given in the first chapter,

$$V_{OPE} = -\frac{g_A^2}{8f_\pi^2}\sum_{n'n,S',S,I}:\rho_{S',I}(n')f_{SS'}(n'-n)\rho_{S,I}(n): \quad (4.126)$$

4.11.2 Transfer matrix with pion but no auxiliary field

$$\mathcal{Z}_{LO} \propto \int \mathcal{D}\pi'_I \exp[-S_{\pi\pi}(\pi'_I)]\mathrm{Tr}\left[M_{LO}^{(N_t-1)}(\pi'_I)\cdots M_{LO}^{(0)}(\pi'_I)\right], \quad (4.127)$$

$$M_{LO}^{(n_t)}(\pi'_I) =: \exp[-H_{LO}^{(n_t)}(\pi'_I)\alpha_t]: \quad (4.128)$$

where, contact interaction for C and C_I are considered.

$$H_{LO}(\pi'_I) = H_{free} + \frac{C}{2}\sum_{\boldsymbol{n}_s}[\rho(\boldsymbol{n}_s)]^2 + \frac{C_I}{2}\sum_{\boldsymbol{n}_s}\sum_I[\rho_I(\boldsymbol{n}_s)]^2$$
$$+\frac{g_A}{2f_\pi}\sum_{S,I}\sum_{\boldsymbol{n}_s}\Delta_S\pi'_I(\boldsymbol{n}_s,n_t)\rho_{S,I}(\boldsymbol{n}_s) \quad (4.129)$$

4.11.3 Transfer matrix with pions and auxiliary fields

If we use auxiliary formalism, we get

$$\mathcal{Z}_{LO} \propto \int \mathcal{D}\pi'_I\mathcal{D}s\mathcal{D}s_I \exp[-S_{\pi\pi}(\pi'_I) - S_{ss}(s,s_I)]\mathrm{Tr}\left[M_{LO}^{(N_t-1)}(\pi'_I,s,s_I)\cdots M_{LO}^{(0)}(\pi'_I,s,s_I)\right], \quad (4.130)$$

[11] This can be related with continuum expression,(check?)

$$V^{OPE} = \sum_{S_1,S_2,I}\int d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2 G_{S_1S_2}(\boldsymbol{r}_1-\boldsymbol{r}_2):\rho_{S_1,I}(\boldsymbol{r}_1)\rho_{S_2,I}(\boldsymbol{r}_2):,$$
$$G_{S_1S_2}(\boldsymbol{r}_1-\boldsymbol{r}_2) = -(\frac{g_A}{2f_\pi})^2\int\frac{d^3q}{(2\pi)^3}\frac{q_{S_1}q_{S_2}e^{i\boldsymbol{q}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)}}{q^2+m_\pi^2} \quad (4.122)$$

We can write M_{LO} as normlaized integral

$$M_{LO} = \frac{\int D\pi'_I Dse^{-S_\pi - S_s} M^{(n_t)}(\pi'_I, s)}{\int D\pi'_I Dse^{-S_\pi - S_s}}, \tag{4.131}$$

with

$$\begin{aligned} M^{(n_t)}(\pi'_I, s, s_I) &= :\exp\Big\{ - H_{free}\alpha_t - \frac{g_A\alpha_t}{2f_\pi\sqrt{q_\pi}} \sum_{S,I} \Delta_S \pi'_I(\boldsymbol{n}_s, n_t)\rho_{S,I}(\boldsymbol{n}_s) \\ &\quad + \sqrt{-C\alpha_t}\sum_{\boldsymbol{n}_s} s(\boldsymbol{n}_s, n_t)\rho(\boldsymbol{n}_s) + i\sqrt{C_I\alpha_t}\sum_I \sum_{\boldsymbol{n}_s} s_I(\boldsymbol{\sigma}_s, n_t)\rho_I(\boldsymbol{n}_s)\Big\} \end{aligned} \tag{4.132}$$

and

$$\begin{aligned} S^{(n_t)}_{\pi\pi}(\pi'_I) &= \frac{1}{2}\sum_{\boldsymbol{n},I} \pi'_I(\boldsymbol{n}, n_t)\pi'_I(\boldsymbol{n}, n_t) - \frac{\alpha_t}{q_\pi}\sum_{\boldsymbol{n},I,l} \pi'_I(\boldsymbol{n}, n_t)\pi'_I(\boldsymbol{n}+\hat{l}, n_t) \\ S^{(n_t)}_{ss} &= \frac{1}{2}\sum_{\boldsymbol{n},\boldsymbol{n}'} s(\boldsymbol{n}, n_t) f^{-1}(\boldsymbol{n}-\boldsymbol{n}')s(\boldsymbol{n}', n_t) + (\text{other auxiliary fields}) \end{aligned} \tag{4.133}$$

with

$$f^{-1}(\boldsymbol{n}-\boldsymbol{n}') = \frac{1}{L^3}\sum_{\boldsymbol{q}} \frac{1}{f(\boldsymbol{q})} e^{-i\boldsymbol{q}\cdot(\boldsymbol{n}-\boldsymbol{n}')}. \tag{4.134}$$

If one use improved derivative operator, it can be generlaized with hopping coefficients.

$$\exp(-S^{OPEP}_{int}(c^*, c)) = \int \prod_I D\pi_I \exp(-S_{\pi_I\pi_I}(\pi_I) - S_{\pi_I}(c^*, c, \pi_I)). \tag{4.135}$$

with free pion action

$$\begin{aligned} S_{\pi_I\pi_I}(\pi_I) &= \frac{1}{2}\alpha_t m_\pi^2 \sum_{\boldsymbol{n},n_t,I} \pi_I^2(\boldsymbol{n}, n_t) \\ &\quad + \frac{1}{2}\alpha_t \sum_{k=0,1,2\ldots} (-1)^k w_k \sum_{\boldsymbol{n},n_t,I,\hat{l}} \pi_I(\boldsymbol{n}, n_t)\left[\pi_I(\boldsymbol{n}+k\hat{l}, n_t) + \pi_I(\boldsymbol{n}-k\hat{l}, n_t)\right] \end{aligned} \tag{4.136}$$

where w_k is the same hopping coefficients for free nucleons (because it is an approximation for Laplacian.) In above expression π'_I is scaled to absorb the m_π^2 and w_0 terms.

The pion coupling to the nucleon is

$$S_\pi(c^*, c, \pi_I) = \frac{g_A\alpha_t}{2f_\pi}\sum_{\boldsymbol{n},n_t,l,I} \Delta_l\pi_I(\boldsymbol{n}, n_t)c^*(\boldsymbol{n}, n_t)\sigma_l\tau_I c(\boldsymbol{n}, n_t), \tag{4.137}$$

where $l = 1, 2, 3$ and one can approximate the derivative

$$\Delta_l\pi_I(\boldsymbol{n}, n_t) = \frac{1}{2}\sum_{k=1,2,\ldots} (-1)^{k-1} o_k \left[\pi(\boldsymbol{n}+k\hat{l}, n_t) - \pi(\boldsymbol{n}-k\hat{l}, n_t)\right], \tag{4.138}$$

with coefficients o_k corresponding to a hopping parameter expansion of momentum,

$$P(p_l) = \sum_{k=1,2,\ldots} (-1)^{k-1} o_k \sin(kp_l) \tag{4.139}$$

The hopping coefficients are chosen to match the continuum result, $P(p_l) = p_l$.

For example, for $k = 1$, $o_1 = 1, o_2 = 0, o_3 = 0$, for $k \le 2$, $o_1 = \frac{4}{3}, o_2 = \frac{1}{6}, o_3 = 0$, and for $k \le 3$, $o_1 = \frac{3}{2}, o_2 = \frac{3}{10}, o_3 = \frac{1}{30}$.

4.12 New non-local contact interaction

Ref: PRL119,222505(2017)

To reduce the sign oscillation problem, one introduce new non-local SU(4) interaction.

$$H_B = H_{free} + V_0 + V_{OPE} \tag{4.140}$$

4.12.1 Free Hamiltonian

- $\sum_{\langle \boldsymbol{n}'\boldsymbol{n}\rangle}$: summation over nearest neighbor lattice sites of $\boldsymbol{n}$.
- $\sum_{\langle \boldsymbol{n}'\boldsymbol{n}\rangle_i}$: sum over nearest neighbor lattice sites of $\boldsymbol{n}$ along the i-th spatial axis.
- $\sum_{\langle\langle \boldsymbol{n}'\boldsymbol{n}\rangle\rangle_i}$: sum over next-to-nearest neighbor lattice sites of $\boldsymbol{n}$ along the i-th spatial axis.
- $\sum_{\langle\langle\langle \boldsymbol{n}'\boldsymbol{n}\rangle\rangle\rangle_i}$: sum over next-to-next-to-nearest neighbor lattice sites of $\boldsymbol{n}$ along the i-th spatial axis.

$$\begin{aligned} H_{free} &= \frac{49}{12m}\sum_{\boldsymbol{n}} a^\dagger(\boldsymbol{n})a(\boldsymbol{n}) - \frac{3}{4m}\sum_{\boldsymbol{n},i}\sum_{\langle \boldsymbol{n}'\boldsymbol{n}\rangle_i} a^\dagger(\boldsymbol{n}')a(\boldsymbol{n}) \\ &+\frac{3}{40m}\sum_{\boldsymbol{n},i}\sum_{\langle\langle \boldsymbol{n}'\boldsymbol{n}\rangle\rangle_i} a^\dagger(\boldsymbol{n}')a(\boldsymbol{n}) - \frac{1}{180m}\sum_{\boldsymbol{n},i}\sum_{\langle\langle\langle \boldsymbol{n}'\boldsymbol{n}\rangle\rangle\rangle_i} a^\dagger(\boldsymbol{n}')a(\boldsymbol{n}) \end{aligned} \tag{4.141}$$

This is an improved action. Note that the local term got additional factors from

$$\sum_{l=1,2,3} a^\dagger(\boldsymbol{n})(a(\boldsymbol{n}+0\hat{l}) + a(\boldsymbol{n}-0\hat{l})) = 6a^\dagger(\boldsymbol{n})a(\boldsymbol{n}).$$

4.12.2 nonlocal operators

Nonlocal annihilation and creation operators, s_{NL} is a free parameter to be fitted,

$$\begin{aligned} a_{NL}(\boldsymbol{n}) &= a(\boldsymbol{n}) + s_{NL}\sum_{\langle \boldsymbol{n}'\boldsymbol{n}\rangle} a(\boldsymbol{n}') \\ a^\dagger_{NL}(\boldsymbol{n}) &= a^\dagger(\boldsymbol{n}) + s_{NL}\sum_{\langle \boldsymbol{n}'\boldsymbol{n}\rangle} a^\dagger(\boldsymbol{n}'), \end{aligned} \tag{4.142}$$

Point-like densities

$$\begin{aligned} \rho(\boldsymbol{n}) &= a^\dagger(\boldsymbol{n})a(\boldsymbol{n}), \\ \rho_S(\boldsymbol{n}) &= a^\dagger(\boldsymbol{n})[\sigma_S]a(\boldsymbol{n}), \\ \rho_I(\boldsymbol{n}) &= a^\dagger(\boldsymbol{n})[\tau_I]a(\boldsymbol{n}), \\ \rho_{S,I}(\boldsymbol{n}) &= a^\dagger(\boldsymbol{n})[\sigma_S\tau_I]a(\boldsymbol{n}) \end{aligned} \tag{4.143}$$

Smeared nonlocal densities,

$$\begin{aligned} \rho_{NL}(\boldsymbol{n}) &= a^\dagger_{NL}(\boldsymbol{n})a_{NL}(\boldsymbol{n}), \\ \rho_{S,NL}(\boldsymbol{n}) &= a^\dagger_{NL}(\boldsymbol{n})[\sigma_S]a_{NL}(\boldsymbol{n}), \\ \rho_{I,NL}(\boldsymbol{n}) &= a^\dagger_{NL}(\boldsymbol{n})[\tau_I]a_{NL}(\boldsymbol{n}), \\ \rho_{S,I,NL}(\boldsymbol{n}) &= a^\dagger_{NL}(\boldsymbol{n})[\sigma_S\tau_I]a_{NL}(\boldsymbol{n}) \end{aligned} \tag{4.144}$$

The new nonlocal SU(4) interaction is defined as

$$V_0 = \frac{c_0}{2} \sum_{\boldsymbol{n}',\boldsymbol{n},\boldsymbol{n}''} : \rho_{NL}(\boldsymbol{n}') f_{s_L}(\boldsymbol{n}'-\boldsymbol{n}) f_{s_L}(\boldsymbol{n}-\boldsymbol{n}'') \rho_{NL}(\boldsymbol{n}'') : \tag{4.145}$$

where, with c_0, s_L are free parameters to be fitted,

$$\begin{aligned} f_{s_L}(\boldsymbol{n}) &= 1 \text{ for } |\boldsymbol{n}| = 0, \\ &= s_L \text{ for } |\boldsymbol{n}| = 1, \\ &= 0 \text{ otherwise .} \end{aligned} \tag{4.146}$$

The action can be changed with auxiliary field s as shown in the first chapter,

$$V_{ss}^{(n_t)} = \frac{1}{2} s^2(\boldsymbol{n}, n_t), \tag{4.147}$$

$$V_s^{(n_t)} = -\sqrt{-c_0} \sum_{\boldsymbol{n}\boldsymbol{n}'} \rho_{NL}(\boldsymbol{n}) f_{s_L}(\boldsymbol{n}-\boldsymbol{n}') s(\boldsymbol{n}', n_t). \tag{4.148}$$

Note that transfer matrix is $M \propto \exp(-V_s^{(n_t)} \sqrt{\alpha_t})$

4.12.3 one pion exchange term

$$V_{OPE} = -\frac{1}{2} \frac{g_A^2}{4 f_\pi^2} \sum_{\boldsymbol{n}',\boldsymbol{n},S',S,I} : \rho_{S',I}(\boldsymbol{n}') f_{S'S}(\boldsymbol{n}'-\boldsymbol{n}) \rho_{S,I}(\boldsymbol{n}) :, \tag{4.149}$$

where

$$f_{S'S}(\boldsymbol{n}'-\boldsymbol{n}) = \frac{1}{L^3} \sum_{\boldsymbol{q}} \frac{\exp(-i\boldsymbol{q}\cdot(\boldsymbol{n}'-\boldsymbol{n}) - b_\pi \boldsymbol{q}^2) q_{S'} q_S}{\boldsymbol{q}^2 + m_\pi^2}, \tag{4.150}$$

and each q_S is an integer multiplied by $2\pi/L$. $b_\pi = 0.7$ is chosen.

This OPE exchange can be rewritten as pion action

$$V_{\pi\pi}^{(n_t)} = \frac{1}{2} \sum_{\boldsymbol{n},\boldsymbol{n}',I} \pi_I(\boldsymbol{n}', n_t) f^{\pi\pi}(\boldsymbol{n}'-\boldsymbol{n}) \pi_I(\boldsymbol{n}, n_t), \tag{4.151}$$

$$\begin{aligned} V_\pi^{(n_t)} &= -\frac{g_A}{2 f_\pi} \sum_{\boldsymbol{n},\boldsymbol{n}',S,I} \rho_{S,I}(\boldsymbol{n}') f_S^\pi(\boldsymbol{n}'-\boldsymbol{n}) \pi_I(\boldsymbol{n}, n_t) \\ &= +\frac{g_A}{2 f_\pi} \sum_{\boldsymbol{n},\boldsymbol{n}',S,I} \pi_I(\boldsymbol{n}', n_t) f_S^\pi(\boldsymbol{n}'-\boldsymbol{n}) \rho_{S,I}(\boldsymbol{n}) \end{aligned} \tag{4.152}$$

with

$$f_S^\pi(\boldsymbol{n}'-\boldsymbol{n}) = \frac{1}{L^3} \sum_{\boldsymbol{q}} \exp(-i\boldsymbol{q}\cdot(\boldsymbol{n}'-\boldsymbol{n}))(i q_S), \tag{4.153}$$

$$f^{\pi\pi}(\boldsymbol{n}'-\boldsymbol{n}) = \frac{1}{L^3} \sum_{\boldsymbol{q}} \exp(-i\boldsymbol{q}\cdot(\boldsymbol{n}'-\boldsymbol{n}) + b_\pi \boldsymbol{q}^2)(\boldsymbol{q}^2 + m_\pi^2). \tag{4.154}$$

4.12.4 transfer matrix

$$M = \int Ds^{(n_t)} D\pi^{(n_t)} M^{(n_t)}, \tag{4.155}$$

$$M^{(n_t)} =: \exp\left(-H_{free}\alpha_t - V_s^{(n_t)}\sqrt{\alpha_t} - V_{ss}^{(n_t)} - V_\pi^{(n_t)}\alpha_t - V_{\pi\pi}^{(n_t)}\alpha_t\right): \tag{4.156}$$

Where one can use auxiliary pion field $\phi_I(\boldsymbol{n})$,

$$\begin{aligned} -V_{\pi\pi}^{(n_t)}\alpha_t &= -\frac{\alpha_t}{2}\sum_{\boldsymbol{n}\boldsymbol{n}'} \pi_I(\boldsymbol{n}) f^{\pi\pi}(\boldsymbol{n}'-\boldsymbol{n})\pi_I(\boldsymbol{n}) \\ &= -\frac{\alpha_t}{2}\frac{1}{L^3}\sum_{\boldsymbol{q}} \hat{\pi}_I(\boldsymbol{q})\hat{\pi}_I(-\boldsymbol{q})\exp(b_\pi \boldsymbol{q}^2)(\boldsymbol{q}^2+m_\pi^2) \\ &= -\frac{\alpha_t}{2}\frac{1}{L^3}\sum_{\boldsymbol{q}} \hat{\phi}_I(\boldsymbol{q})\hat{\phi}_I(-\boldsymbol{q}) = -\frac{\alpha_t}{2}\sum_{\boldsymbol{n}} \phi_I(\boldsymbol{n})\phi_I(\boldsymbol{n}) \end{aligned} \tag{4.157}$$

where

$$\hat{\phi}_I(\boldsymbol{q}) = \sqrt{\exp(b_\pi \boldsymbol{q}^2)(\boldsymbol{q}^2+m_\pi^2)}\hat{\pi}_I(\boldsymbol{q}) \tag{4.158}$$

One may refer the first chapter for more detailed derivation.

Chapter 5

Numerical Realization

If we denote all relevant bosonic fields as U, by using transfer matrix formulation, we would define

$$Z_\Psi(L_t) = \int \mathcal{D}[U] e^{-S[U]} \langle \Psi | [M(U)]^{L_t} | \Psi \rangle \tag{5.1}$$

Any observable can be written as

$$\langle O \rangle_{\Psi, L_t} = \frac{\int \mathcal{D}[U] e^{-S[U]} \langle \Psi | M \dots O M \dots M | \Psi \rangle}{\int \mathcal{D}[U] e^{-S[U]} \langle \Psi | [M(U)]^{L_t} | \Psi \rangle} \tag{5.2}$$

By sampling U according to given probability $P[U]$, we will have

$$\langle O \rangle_{\Psi, L_t} \simeq \frac{\frac{1}{N} \sum_{[U]} P[U] \frac{1}{P[U]} e^{-S[U]} \langle \Psi | M \dots O M \dots M | \Psi \rangle}{\frac{1}{N} \sum_{[U]} P[U] \frac{1}{P[U]} e^{-S[U]} \langle \Psi | [M(U)]^{L_t} | \Psi \rangle} = \frac{\frac{1}{N} \sum_{[U] \in P[U]} \frac{1}{P[U]} e^{-S[U]} \langle \Psi | M \dots O M \dots M | \Psi \rangle}{\frac{1}{N} \sum_{[U] \in P[U]} \frac{1}{P[U]} e^{-S[U]} \langle \Psi | [M(U)]^{L_t} | \Psi \rangle} \tag{5.3}$$

Usually, we define

$$P[U] = e^{-S[U]} |\det X[U, L_t]|, \quad \det X[U, L_t] = \langle \Psi | [M(U)]^{L_t} | \Psi \rangle = |\det X[U, L_t]| e^{i\theta(U, L_t)} \tag{5.4}$$

Then,

$$\langle O \rangle_{\Psi, L_t} \simeq \frac{\sum_{[U] \in P[U]} e^{i\theta(U, L_t)} \frac{\langle \Psi | M \dots O M \dots M | \Psi \rangle}{|\det X[U, L_t]|}}{\sum_{[U] \in P[U]} e^{i\theta(U, L_t)}} \tag{5.5}$$

However, in principle we can use any kind of probability distribution $P[U]$.

5.1 Rough Sketch

Basically the code structure will be such that

(1) Initialization, Declaration

- preparation for common arrays
- assign random values for auxiliary variables

(2) Main Monte Carlo

- make new configuration
- Compute Probability of old and new configuration

– check acceptance and update the configuration

(3) Computing observables

– Compute observables and averages

(4) Finalization

Of course, each steps are composed of many smaller steps.
The main object is to compute an expectation value of operator

5.2 Nuclear wave function

In the code, we define initial one body wave functions of np-th particle in spin-isospin state α at lattice point $\boldsymbol{n}$ as $v_{np}(\boldsymbol{n}, \alpha, n_t = 0)$. Then, the many body wave function will be a slater determinant of them. However, we only need to keep track of one-body wave function evolution in auxiliary field formulation. Any boson fields or auxiliary field configuration can be written as $s(\boldsymbol{n}, \beta, n_t)$ for all lattice points and time. The action of transfer matrix is calculated as series of single particle state vectors and dual vectors,

$$\begin{aligned} |\phi_i^{(n_t+1)}\rangle &= M^{(n_t)}(s)|\phi_i^{(n_t)}\rangle, \\ \langle\tilde{\phi}_i^{(n_t-1)}| &= \langle\tilde{\phi}_i^{(n_t)}|M^{(n_t)}(s) \end{aligned} \tag{5.6}$$

Then, final matrix element X can be computed by

$$\begin{aligned} X_{j'j}(s) &= \langle\phi_{j'}|M^{L_t}|\phi_j\rangle = \langle v_{j'}(n_t = 0)|v_j(n_t = L_t)\rangle \\ &= \langle vd_{j'}(n_t = L_t)|v_j(n_t = L_t)\rangle \end{aligned} \tag{5.7}$$

where we defined dual vectors,[1]

$$|vd_j(n_t - 1)\rangle = M(n_t)|vd(n_t)\rangle, \quad |vd_j(L_t)\rangle = |v_j(0)\rangle \tag{5.8}$$

[2]

In the same way, we can write

$$\begin{aligned} X_{j'j}(s) &= \langle\phi_{j'}|M^{L_t}|\phi_j\rangle \\ &= \langle\tilde{\phi}_{j'}^{(L_t)}|M^{L_t}|\phi_j^{(0)}\rangle \\ &= \langle\tilde{\phi}_{j'}^{(n_t)}|\phi_j^{(n_t)}\rangle \quad \text{for any } n_t \end{aligned} \tag{5.9}$$

If the initial state is not normalized such as $v_{np}(\boldsymbol{n}, ns, ni, n_t = 0) = 1$, whenever the scalar product of vectors appears, they must be re-normalized by multiplying $1/N^3$.

5.3 Transfer matrix calculation

We want to compute the transfer matrix elements for given auxiliary field $s(\boldsymbol{n}, n_t)$,

$$\langle\Psi|\{M_A(s, L_t - 1)\dots M_A(s, 0)\}|\Psi\rangle = \det X(s), \tag{5.10}$$

[1] Is $M(s)$ a hermitian, real?

[2] If we are interested in computing different time length t, we need to compute $X_{j'j}(s, t = L_t)$ and $X_{j'j}(s, t = L_t - 1) = \langle v_{np=j'}(n_t = 0)|v_{np=j}(n_t = L_t - 1)\rangle$.

with

$$M_A(s,n_t) =: \exp\left[-\alpha_t \hat{H}_{free} + \sum_{\boldsymbol{n}} A[s(\boldsymbol{n},n_t)]\rho(\boldsymbol{n})\right] : \tag{5.11}$$

and

$$X_{j'j}(s) = \langle \phi_{j'}|M(s,L_t-1)\dots M(s,0)|\phi_j\rangle. \tag{5.12}$$

Thus, in effect, even though we are considering multi-particle states, we only need to computes the action of transfer matrix on a single particle state.

Suppose we have defined a one particle wave vector $|\phi\rangle$ as [3]

$$\langle \boldsymbol{n}|\phi\rangle = \langle 0|a(\boldsymbol{n})|\phi\rangle = \phi(\boldsymbol{n}). \tag{5.15}$$

We get (since it is a single particle state complete set is $1 = |0\rangle\langle 0| + \sum_p |p\rangle\langle p|$),

$$\begin{aligned}
&\langle \boldsymbol{n}|a^\dagger(\boldsymbol{n}')a(\boldsymbol{n}'))|f\rangle = \langle \boldsymbol{n}|a^\dagger(\boldsymbol{n}')|0\rangle\langle 0|a(\boldsymbol{n}'))|f\rangle = \delta_{\boldsymbol{n},\boldsymbol{n}'}f(\boldsymbol{n}),\\
&\langle \boldsymbol{m}|a^\dagger(\boldsymbol{n}')a(\boldsymbol{n})s(\boldsymbol{n})|f\rangle = \delta_{\boldsymbol{n}',\boldsymbol{m}}s(\boldsymbol{n})f(\boldsymbol{n}),\\
&\langle \boldsymbol{m}|s(\boldsymbol{n}')a^\dagger(\boldsymbol{n}')a(\boldsymbol{n})|f\rangle = \delta_{\boldsymbol{n}',\boldsymbol{m}}s(\boldsymbol{n}')f(\boldsymbol{n}).
\end{aligned} \tag{5.16}$$

In general, one-body operators can be written as $\sum_{ij} A_{ij}a^\dagger(\boldsymbol{n}_i)a(\boldsymbol{n}_j)$ and as long as it acts on one-body state, we can write

$$:\exp(\sum_{ij} A_{ij}a^\dagger(\boldsymbol{n}_i)a(\boldsymbol{n}_j)) :=: 1 + \sum_{ij} A_{ij}a^\dagger(\boldsymbol{n}_i)a(\boldsymbol{n}_j) : \tag{5.17}$$

Then

$$\begin{aligned}
\langle \boldsymbol{n}| :\exp(\sum_{ij} A_{ij}a^\dagger(\boldsymbol{n}_i)a(\boldsymbol{n}_j)) : |\phi\rangle &= \langle \boldsymbol{n}| : 1 + \sum_{ij} A_{ij}a^\dagger(\boldsymbol{n}_i)a(\boldsymbol{n}_j) : |\phi\rangle = \langle \boldsymbol{n}|\phi\rangle + \sum_{ij} A_{ij}\delta_{\boldsymbol{n},\boldsymbol{n}_i}\langle \boldsymbol{n}_j|\phi\rangle\\
&= \langle \boldsymbol{n}|\phi\rangle + \sum_{\boldsymbol{n}_j} A_{\boldsymbol{n},\boldsymbol{n}_j}\langle \boldsymbol{n}_j|\phi\rangle
\end{aligned} \tag{5.18}$$

In other words,

$$\boxed{\langle n| : \left(1 + \sum_{ij} A_{ij}a^\dagger(\boldsymbol{n}_i)a(\boldsymbol{n}_j)\right) : |\phi\rangle = \langle n|\phi\rangle + \sum_j A_{\boldsymbol{n}_i\boldsymbol{n}_j}\langle \boldsymbol{n}_j|\phi\rangle} \tag{5.19}$$

For a simple cases,

$$\begin{aligned}
|\phi_1'\rangle &= \sum_{\boldsymbol{n}'} a^\dagger(\boldsymbol{n}')a(\boldsymbol{n}')|\phi\rangle,\\
|\phi_2'\rangle &= \sum_{\boldsymbol{n}'} a^\dagger(\boldsymbol{n}')a(\boldsymbol{n}'-\boldsymbol{l})|\phi\rangle = \sum_{\boldsymbol{n}'} a^\dagger(\boldsymbol{n}'+\boldsymbol{l})a(\boldsymbol{n}')|\phi\rangle,\\
|\phi_3'\rangle &= \sum_{\boldsymbol{n}'} a^\dagger(\boldsymbol{n}')a(\boldsymbol{n}'+\boldsymbol{l})|\phi\rangle = \sum_{\boldsymbol{n}'} a^\dagger(\boldsymbol{n}'-\boldsymbol{l})a(\boldsymbol{n}')|\phi\rangle
\end{aligned} \tag{5.20}$$

[3] For more explicit derivation, one can use single particle state is

$$\langle \boldsymbol{n}|\phi\rangle = \sum_{\boldsymbol{p}} c_{\boldsymbol{p}}\langle \boldsymbol{n}|a^\dagger_{\boldsymbol{p}}|0\rangle = \sum_{\boldsymbol{p}} c_{\boldsymbol{p}}\phi_p(\boldsymbol{n}), \quad a(\boldsymbol{n}) = \sum_{\boldsymbol{p}} \phi_{\boldsymbol{p}}(\boldsymbol{n})a_{\boldsymbol{p}} \tag{5.13}$$

Or one can express state as

$$a(\boldsymbol{n})|f\rangle = f(\boldsymbol{n})|0\rangle \tag{5.14}$$

we have respectively

$$\langle \boldsymbol{n}|\phi_1'\rangle = \langle \boldsymbol{n}|\phi\rangle, \quad \langle \boldsymbol{n}|\phi_2'\rangle = \langle \boldsymbol{n}-\boldsymbol{l}|\phi\rangle, \quad \langle \boldsymbol{n}|\phi_3'\rangle = \langle \boldsymbol{n}+\boldsymbol{l}|\phi\rangle \tag{5.21}$$

Thus, simply acts as hopping lattice values at lattice points. Also note that because of periodic boundary condition of in space. Actual hopping should be calculated as

$$\langle \boldsymbol{n}|\sum_{\boldsymbol{n}'} a^\dagger(\boldsymbol{n}')a(\boldsymbol{n}'-\boldsymbol{l})|\phi\rangle = \langle \mathrm{mod}(N+\boldsymbol{n}-\boldsymbol{l},N)|\phi\rangle \tag{5.22}$$

Let us consider one transfer matrix acting on one particle state vector, with implicit spin indices,

$$\langle \boldsymbol{n}|\phi(n_t+1)\rangle = \langle \boldsymbol{n}|M(s,n_t)|\phi(n_t)\rangle = \langle \boldsymbol{n}|\left(1-\alpha_t H_{free}+\sum_{\boldsymbol{n}'} A[s(\boldsymbol{n}',n_t)]\rho(\boldsymbol{n}')\right)|\phi(n_t)\rangle. \tag{5.23}$$

We can easily compute $\langle \boldsymbol{n}|\phi(n_t+1)\rangle$ by considering 'improved action' with hopping operators.

$$\begin{aligned}\langle \boldsymbol{n}|:1-H_{free}\alpha_t:|\phi\rangle &= \langle \boldsymbol{n}|\phi\rangle - \frac{\alpha_t}{2m}\sum_{j=0}^{j_{max}}\sum_{\boldsymbol{n}',l=1,2,3}(-1)^j\omega_j\langle \boldsymbol{n}[a^\dagger(\boldsymbol{n}')a(\boldsymbol{n}'+j\hat{l})+a^\dagger(\boldsymbol{n}')a(\boldsymbol{n}'-j\hat{l})]|\phi\rangle \\ &= \langle \boldsymbol{n}|\phi\rangle - \frac{\alpha_t}{2m}\sum_{j=0}^{j_{max}}\sum_{l=1,2,3}(-1)^j\omega_j\left(\langle \boldsymbol{n}+j\hat{l}|\phi\rangle+\langle \boldsymbol{n}-j\hat{l}|\phi\rangle\right)\end{aligned} \tag{5.24}$$

Interaction with auxiliary is simple except the derivative coupling

$$\phi_\alpha^{(n_t+1)}(\boldsymbol{n}) = \langle \boldsymbol{n};\alpha|:\sum_{\boldsymbol{n}'}A[s(\boldsymbol{n}',n_t)]\rho(\boldsymbol{n}'):|\phi\rangle = \sum_\beta A[s(\boldsymbol{n},n_t)]\rho_{\alpha\beta}\phi_\beta^{(n_t)}(\boldsymbol{n}) \tag{5.25}$$

where α,β represent spin and isospin and $\rho_{\alpha\beta}$ is an matrix in spin and isospin. For the last time-step of $\langle\phi|M|\phi^{(n_t-1)}\rangle$, one can use

$$\langle\phi'|a^\dagger(\boldsymbol{n})a(\boldsymbol{n})|\phi\rangle = \langle\phi'|\boldsymbol{n}\rangle\langle\boldsymbol{n}|\phi\rangle \tag{5.26}$$

More detail on spin and isospin is explained in next section.

5.4 More examples of operator action on states

Let us consider actions of operators on states with spin and isospins.

For one-body states, let us consider a general density operator,

$$\hat{\rho}_S(\boldsymbol{n}_s) = \sum_{ii'} a_i^\dagger(\boldsymbol{n}_s)[\boldsymbol{\sigma}_S]_{ii'}a_{i'}(\boldsymbol{n}_s), \tag{5.27}$$

where i represents general quantum numbers of one-body states.

Then, for one-body states $|\phi\rangle$ in $|\boldsymbol{n},\alpha\rangle$ basis,

$$\begin{aligned}\langle \boldsymbol{n},\alpha|\phi'\rangle &= \langle \boldsymbol{n},\alpha|\sum_{\boldsymbol{n}_s}\hat{\rho}_S(\boldsymbol{n}_s)|\phi\rangle = \sum_{\boldsymbol{n}_s}\sum_{\boldsymbol{n}',\beta}\langle \boldsymbol{n},\alpha|\hat{\rho}_S(\boldsymbol{n}_s)|\boldsymbol{n}',\beta\rangle\langle \boldsymbol{n}',\beta|\phi\rangle, \\ &= \sum_{\boldsymbol{n}_s,\beta}[\boldsymbol{\sigma}_S]_{\alpha\beta}\delta_{\boldsymbol{n},\boldsymbol{n}_s}\langle \boldsymbol{n}_s,\beta|\phi\rangle = \sum_\beta[\boldsymbol{\sigma}_S]_{\alpha\beta}\langle \boldsymbol{n},\beta|\phi\rangle.\end{aligned} \tag{5.28}$$

For two-body states, ϕ_{2B} in $|\boldsymbol{n}_1, \alpha_1, \boldsymbol{n}_2, \alpha_2\rangle$ basis,

$$\begin{aligned}
&\langle \boldsymbol{n}_1, \alpha_1, \boldsymbol{n}_2, \alpha_2| \sum_{\boldsymbol{n}_{s1}, \boldsymbol{n}_{s2}} : \hat{\rho}_{S_1}(\boldsymbol{n}_{s1}) \hat{\rho}_{S_2}(\boldsymbol{n}_{s2}) : |\phi\rangle \\
= &\sum_{\boldsymbol{n}_1' \boldsymbol{n}_2'} \sum_{\beta_1, \beta_2} \langle \boldsymbol{n}_1, \alpha_1, \boldsymbol{n}_2, \alpha_2| \sum_{\boldsymbol{n}_{s1}, \boldsymbol{n}_{s2}} : \hat{\rho}_{S_1}(\boldsymbol{n}_{s1}) \hat{\rho}_{S_2}(\boldsymbol{n}_{s2}) : |\boldsymbol{n}_1', \beta_1, \boldsymbol{n}_2', \beta_2\rangle \langle \boldsymbol{n}_1', \beta_1, \boldsymbol{n}_2', \beta_2|\phi\rangle \\
= &\sum_{\beta_1, \beta_2} \Big[[\boldsymbol{\sigma}_{S_1}]_{\alpha_2\beta_2} [\boldsymbol{\sigma}_{S_2}]_{\alpha_1\beta_1} \langle \boldsymbol{n}_1, \beta_1, \boldsymbol{n}_2, \beta_2|\phi\rangle - [\boldsymbol{\sigma}_{S_1}]_{\alpha_1\beta_2} [\boldsymbol{\sigma}_{S_2}]_{\alpha_2\beta_1} \langle \boldsymbol{n}_2, \beta_1, \boldsymbol{n}_1, \beta_2|\phi\rangle \\
&- [\boldsymbol{\sigma}_{S_1}]_{\alpha_2\beta_1} [\boldsymbol{\sigma}_{S_2}]_{\alpha_1\beta_2} \langle \boldsymbol{n}_2, \beta_1, \boldsymbol{n}_1, \beta_2|\phi\rangle + [\boldsymbol{\sigma}_{S_1}]_{\alpha_1\beta_1} [\boldsymbol{\sigma}_{S_2}]_{\alpha_2\beta_2} \langle \boldsymbol{n}_1, \beta_1, \boldsymbol{n}_2, \beta_2|\phi\rangle \Big]
\end{aligned} \tag{5.29}$$

5.4.1 Non-local operators

Let us consider the case of non-local interactions. As introduced, in previous chapter, new non-local contact term gives

$$V_s^{(n_t)} = -\sqrt{-c_0} \sum_{\boldsymbol{n}} \rho_{NL}(\boldsymbol{n}) s_{smear}(\boldsymbol{n}, n_t) \tag{5.30}$$

where I introduced a smeared auxiliary field

$$s_{smear}(\boldsymbol{n}) = s(\boldsymbol{n}) + s_L \sum_{\langle \boldsymbol{n}'\boldsymbol{n} \rangle} s(\boldsymbol{n}'), \tag{5.31}$$

and Smeared nonlocal densities,

$$\rho_{NL}(\boldsymbol{n}) \quad = \quad a_{NL}^\dagger(\boldsymbol{n}) a_{NL}(\boldsymbol{n}), \tag{5.32}$$

and non-local operators are

$$\begin{aligned}
a_{NL}(\boldsymbol{n}) &= a(\boldsymbol{n}) + s_{NL} \sum_{\langle \boldsymbol{n}'\boldsymbol{n} \rangle} a(\boldsymbol{n}') \\
a_{NL}^\dagger(\boldsymbol{n}) &= a^\dagger(\boldsymbol{n}) + s_{NL} \sum_{\langle \boldsymbol{n}'\boldsymbol{n} \rangle} a^\dagger(\boldsymbol{n}'),
\end{aligned} \tag{5.33}$$

In fact, we can introduce larger smearing with $\langle\langle \boldsymbol{n}'\boldsymbol{n} \rangle\rangle$ and so on, but it is a simple extension. To compute the action of

$$|\phi(n_t)\rangle = \hat{V}_s(n_t - 1)|\phi(n_t - 1)\rangle, \tag{5.34}$$

Compute smeared auxiliary field $s_{smear}(\boldsymbol{n}, n_t - 1)$ is straightforward. In a similar way, we may define $\phi_{smear}(\boldsymbol{n})$ such that

$$\phi_{smear}(\boldsymbol{n}) = \langle 0|a_{NL}(\boldsymbol{n})|\phi\rangle = \phi(\boldsymbol{n}) + s_{NL} \sum_{l=1,2,3} \left[\phi(\boldsymbol{n} + \hat{l}) + \phi(\boldsymbol{n} - \hat{l}) \right]. \tag{5.35}$$

Then, action of transfer matrix can be considered as (constant factor $\sqrt{-c_0 \alpha_t}$ is omitted.)

$$\begin{aligned}
M|\phi\rangle &= (1 - H_{free} - V_s)\,|\phi\rangle = |\phi_1\rangle - V_s|\phi\rangle = |\phi_{new}\rangle, \\
|\phi_1\rangle &= (1 - H_{free})|\phi\rangle, \\
-V_s|\phi\rangle &= +\sum_{\boldsymbol{n}} \rho_{NL}(\boldsymbol{n}) s_{smear}(\boldsymbol{n}, n_t - 1)|\phi\rangle \\
&= \sum_{\boldsymbol{n}} a_{NL}^\dagger(\boldsymbol{n})|0\rangle \times s_{smear}(\boldsymbol{n}, n_t - 1)\phi_{smear}(\boldsymbol{n}).
\end{aligned} \tag{5.36}$$

Thus, action on a s.p wave function is

$$\begin{aligned}\langle \boldsymbol{n}|\phi_{new}\rangle &= \langle \boldsymbol{n}|\phi_1\rangle \\ &+\sum_{\boldsymbol{n}'} z_{smear}(\boldsymbol{n}')\left\langle \boldsymbol{n}\left| a^\dagger(\boldsymbol{n}')+s_{NL}\sum_{l=1,2,3}(a^\dagger(\boldsymbol{n}'+\hat{l})+a^\dagger(\boldsymbol{n}'-\hat{l}))\right|0\right\rangle \end{aligned} \quad (5.37)$$

where $z_{smear}(\boldsymbol{n}) = s_{smear}(\boldsymbol{n}, n_t-1)\phi_{smear}(\boldsymbol{n})$.

Another explanation

$$\langle \boldsymbol{n}| : \sum_{\boldsymbol{n}',\boldsymbol{n}''} \rho_{NL}(\boldsymbol{n}') f_{s_L}(\boldsymbol{n}'-\boldsymbol{n}'')s(\boldsymbol{n}'') : |f\rangle \quad (5.38)$$

Define

$$\begin{aligned} s_{smeared}(\boldsymbol{n}) &= \sum_{\boldsymbol{n}'} f_{s_L}(\boldsymbol{n}-\boldsymbol{n}')s(\boldsymbol{n}') = s(\boldsymbol{n}) + \sum_{\langle \boldsymbol{n}',\boldsymbol{n}\rangle} s_L s(\boldsymbol{n}'), \\ f_{smeared}(\boldsymbol{n}) &= f(\boldsymbol{n}) + \sum_{\langle \boldsymbol{n}',\boldsymbol{n}\rangle} s_{NL} f(\boldsymbol{n}') \end{aligned} \quad (5.39)$$

Then,

$$\begin{aligned} &\langle \boldsymbol{n}| : \sum_{\boldsymbol{n}',\boldsymbol{n}''} \rho_{NL}(\boldsymbol{n}') f_{s_L}(\boldsymbol{n}'-\boldsymbol{n}'')s(\boldsymbol{n}'') : |f\rangle \\ = &\sum_{\boldsymbol{n}'}\left(\delta_{\boldsymbol{n}\boldsymbol{n}'} + s_{NL}\sum_{\langle \boldsymbol{n}'',\boldsymbol{n}'\rangle}\delta_{\boldsymbol{n},\boldsymbol{n}''}\right) s_{smeared}(\boldsymbol{n}')f_{smeared}(\boldsymbol{n}') \end{aligned} \quad (5.40)$$

pion coupling term

$$V_\pi^{(n_t)} = \frac{g_A}{2f_\pi}\sum_{\boldsymbol{n},\boldsymbol{n}',S,I}\rho_{S,I}(\boldsymbol{n}')f_S^\pi(\boldsymbol{n}'-\boldsymbol{n})\pi_I(\boldsymbol{n},n_t), \quad (5.41)$$

We may introduce

$$\phi_{SI}(\boldsymbol{n}) = \sum_{\boldsymbol{n}'} f_S^\pi(\boldsymbol{n}'-\boldsymbol{n})\pi_I(\boldsymbol{n},n_t) \quad (5.42)$$

Then

$$\begin{aligned} M|f\rangle &\rightarrow -V_\pi^{(n_t)}|f\rangle = -\frac{g_A}{2f_\pi}\sum_{\boldsymbol{n},S,I}\rho_{S,I}(\boldsymbol{n}')\phi_{SI}(\boldsymbol{n})|f\rangle \\ &= -\frac{g_A}{2f_\pi}\sum_{\boldsymbol{n},S,I} a^\dagger_{s1,i1}(\boldsymbol{n})[\tau_I]_{i1,i2}[\sigma_S]_{s1,s2}a_{s2,i2}(\boldsymbol{n})\phi_{SI}(\boldsymbol{n})|f\rangle \end{aligned} \quad (5.43)$$

5.5 Transfer matrix projection method

To make the M.T. calculation to get lowest energy states efficiently, transfer matrix projection method can be used. This method use simple approximate Hamiltonian to project out higher energy states from initial Slater determinant free particle standing waves, $|\Psi_{Z,N}^{free}\rangle$ and obtain trial wave function closer to ground state for faster convergence.

First get trial wave function by using

$$|\Psi(t')\rangle = \exp[-H_{SU(4)}t']|\Psi_{Z,N}^{free}\rangle, \quad (5.44)$$

with this trial wave function, define amplitude,

$$Z(t) = \langle \Psi(t')| \exp[-H_{LO}t]|\Psi(t')\rangle, \tag{5.45}$$

and transient energy

$$E(t) = -\frac{\partial}{\partial t}[\ln Z(t)]. \tag{5.46}$$

Then, at large t limits, we get ground state energy

$$\lim_{t\to\infty} E(t) = E_0. \tag{5.47}$$

Note that trial wave function $|\Psi(t')\rangle$ must be non-orthogonal to ground state $|\Psi_0\rangle$.

For some normal ordered operator,

$$Z_O(t) = \langle \Psi(t')| \exp[-H_{LO}t/2] O \exp[-H_{LO}t/2]|\Psi(t')\rangle, \tag{5.48}$$

$$\lim_{t\to\infty} \frac{Z_O(t)}{Z(t)} = \langle \Psi_0|O|\Psi_0\rangle. \tag{5.49}$$

5.6 Hybrid Monte Carlo

The hybrid Monte Carlo method is to make the importance sampling to be more efficient by using the Hamiltonian dynamics for Markov Chain updates. In other words, by constructing Hamiltonian $H(x,p)$ such that the Hamiltonian dynamics actually leads to the distribution of x satisfies some target distribution $p(x)$.

For any energy function $E(\theta)$ with variable θ, we can define cannonical distribution, $p(\theta)$ as

$$p(\theta) = \frac{1}{Z} e^{-E(\theta)}. \tag{5.50}$$

By setting energy function as Hamiltonian, canonical distribution becomes

$$p(\boldsymbol{x},\boldsymbol{p}) \propto e^{-H(\boldsymbol{x},\boldsymbol{p})} = e^{-[U(\boldsymbol{x})-K(\boldsymbol{p})]} = e^{-U(\boldsymbol{x})} e^{-K(\boldsymbol{p})} \propto p(\boldsymbol{x})p(\boldsymbol{p}) \tag{5.51}$$

Thus, the distribution disjoints and it means the cannonical distribution $p(\boldsymbol{x})$ of $\boldsymbol{x}$ is independent of conjugate momentum $\boldsymbol{p}$. Therefore, we can use Hamiltonian dynamics to sample from the joint canonical distribution over $\boldsymbol{p}$ and $\boldsymbol{x}$ and simply ignore the momentum contributions. Now, we can choose $K(\boldsymbol{p}) = \frac{1}{2}\boldsymbol{p}^T\boldsymbol{p}$ and $U(\boldsymbol{x}) = -\log p(\boldsymbol{x})$. If we can calculate $\frac{dU(\boldsymbol{x})}{d\boldsymbol{x}}$, the molecular dynamic can be used.

Once the fermion integral is done, we have auxiliary field integration,

$$Z_\Psi = \prod_{\boldsymbol{n},n_t} [\int d_A s(\boldsymbol{n},n_t)] \det X(s) = \prod_{\boldsymbol{n},n_t} [\int d_A s(\boldsymbol{n},n_t)] e^{\log[\det X(s)]}, \tag{5.52}$$

For a choice of auxiliary field,

$$\begin{aligned} \int d_A s(\boldsymbol{n},n_t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} ds(\boldsymbol{n},n_t) e^{-\frac{1}{2}s^2(\boldsymbol{n},n_t)}, \\ A[s(\boldsymbol{n},n_t)] &= \sqrt{-C\alpha_t}\, s(\boldsymbol{n},n_t), \end{aligned} \tag{5.53}$$

we have weights for $s(\boldsymbol{n},n_t)$,

$$Z_\Psi \propto \int \mathcal{D}s\; e^{-\sum_{\boldsymbol{n}} \frac{1}{2}s^2(\boldsymbol{n},n_t)} e^{\log[\det X(s)]} \tag{5.54}$$

Thus we might do importance sampling with weights, $e^{-\sum_{\boldsymbol{n}} \frac{1}{2}s^2(\boldsymbol{n},n_t)} e^{\log[\det X(s)]}$. But, there will be many rejected moves for sampling s. Instead, we may introduce adjoint field variable $p(\boldsymbol{n}, n_t)$ which is normal distributed and change

$$\begin{aligned} Z_\Psi &\propto \int \mathcal{D}p \int \mathcal{D}s \exp\left[-\left(\sum_{\boldsymbol{n}} \frac{1}{2}p^2(\boldsymbol{n},n_t) + \frac{1}{2}s^2(\boldsymbol{n},n_t)\right) + \log[\det X(s)]\right] \\ &= \int \mathcal{D}p \int \mathcal{D}s \exp\left[-H(s,p)\right], \\ H(s,p) &= \sum_{\boldsymbol{n}} \frac{1}{2}p^2(\boldsymbol{n},n_t) + V(s), \quad V(s) = \left(\sum_{\boldsymbol{n}} \frac{1}{2}s^2(\boldsymbol{n},n_t)\right) - \log[\det X(s)] \end{aligned} \tag{5.55}$$

Then, if we move s and p according to Molecular dynamic way, all such s will have the same H values and can be acceptable...(?). Because MD only choose sampling with same $H(s,p)$, we have to disrupt them after some samplings so that sample with different H.

Molecular Dynamics equation is [4]

Given an arbitrary initial configuration $s^0(\boldsymbol{n}, n_t)$, the conjugate momentum is chosen from a random Gaussian distribution,

$$P[p_s^0(\boldsymbol{n},n_t)] \propto \exp(-\frac{1}{2}[p_s^0(\boldsymbol{n},n_t)]^2). \tag{5.56}$$

Molecular dynamic calculation of equation of motion is done up to final step. But, at first, the method begins with a "half-step" forward in the conjugate momentum,

$$\tilde{p}_s^0(\boldsymbol{n},n_t) = p_s^0(\boldsymbol{n},n_t) - \frac{\epsilon_{step}}{2}\left[\frac{\partial V(s)}{\partial s(\boldsymbol{n},n_t)}\right]_{s=s^0}. \tag{5.57}$$

and then next steps are

$$\begin{aligned} s^{i+1}(\boldsymbol{n},n_t) &= s^i(\boldsymbol{n},n_t) + \epsilon_{step}\tilde{p}^i(\boldsymbol{n},n_t), \\ \tilde{p}^{i+1}(\boldsymbol{n},n_t) &= \tilde{p}^i(\boldsymbol{n},n_t) - \epsilon_{step}\left[\frac{\partial V(s)}{\partial s(\boldsymbol{n},n_t)}\right]_{s=s^{i+1}}. \end{aligned} \tag{5.58}$$

until the last half-step backward in $\tilde{p}_s$

$$p_s^{N_{step}}(\boldsymbol{n},n_t) = \tilde{p}_s^{N_{step}}(\boldsymbol{n},n_t) + \frac{\epsilon_{step}}{2}\left[\frac{\partial V(s)}{\partial s(\boldsymbol{n},n_t)}\right]_{s=s^0(?)} \tag{5.59}$$

Note that, $\tilde{p}^i$ and s^i are only intermediate steps and we need only to compare $s^0(\boldsymbol{n},n_t), p_s^0$ and $s^{N_{step}}(\boldsymbol{n},n_t), p_s^{N_{step}}$ and decide whether to accept it or not. The new configuration is accepted if

$$r < \exp[-H(s^{N_s step}, p_s^{N_s step}) + H(s^0, p_s^0)]. \tag{5.60}$$

with random number $r \in [0,1)$.

In case of several auxiliary configuration, we have

$$\exp(-V(s)) \to |Z(L_t)| \exp[-S_{ss}(s) - S_{s_I s_I}(s_I) - S_{\pi_I \pi_I}(\pi_I)], \tag{5.61}$$

where $|Z(L_t)| \propto \ln|\det X(s, s_I, \pi_I)|$.

[4]Note that there is no time advance for s and p. MD evolution is just for updating auxiliary field $s(\boldsymbol{n}, n_t)$. And also, to advance MD, initial momentum p can be half-step advance first and half-step back at last.

Another note: To do molecular dynamics, we use leap-frog method. Make first move conjugate momentum in half and use the value for the advance of postion and so on. Then move momentum half-step back.

The derivative of $V(s)$ can be computed by ,

$$\begin{aligned}\frac{\partial V(s)}{\partial s(\boldsymbol{n},n_t)} &= \frac{\partial S_{ss}(s)}{\partial s(\boldsymbol{n},n_t)} - \frac{\partial \mathrm{Re}\ln\det X}{\partial s(\boldsymbol{n},n_t)} \\ &= \frac{\partial S_{ss}(s)}{\partial s(\boldsymbol{n},n_t)} - \mathrm{Re}\left[\frac{1}{\det X}\sum_{k,l}\frac{\partial \det X}{\partial X_{kl}}\frac{\partial X_{kl}}{\partial s(\boldsymbol{n},n_t)}\right] \\ &= \frac{\partial S_{ss}(s)}{\partial s(\boldsymbol{n},n_t)} - \mathrm{Re}\left[\sum_{k,l}X^{-1}_{lk}(s)\frac{\partial X_{kl}(s)}{\partial s(\boldsymbol{n},n_t)}\right] \end{aligned} \tag{5.62}$$

and (the derivation of this is shown in next subsection)

$$\frac{\partial X_{j'j}(s)}{\partial s(\boldsymbol{n},n_t)} = \frac{\partial A(s)}{\partial s(\boldsymbol{n},n_t)}\langle vd_{j'}(n_t+1)|\boldsymbol{n}\rangle\langle\boldsymbol{n}|v_j(n_t)\rangle. \tag{5.63}$$

5.6.1 Derivative of single particle transfer matrix X

Hybrid Monte Carlo requires the calculation of functional derivative of matrix X. We can compute this by

$$\begin{aligned}\frac{\partial X_{j'j}(s)}{\partial s(\boldsymbol{n},n_t)} &= \frac{\partial}{\partial s(\boldsymbol{n},n_t)}\langle\phi_{j'}|M(s,L_t-1)\dots M(s,0)|\phi_j\rangle \\ &= \underbrace{\langle\phi_{j'}|M(s,L_t-1)\dots M(s,n_t+1)}_{=\langle vd_{j'}(n_t+1)|}\frac{\partial M(s,n_t)}{\partial s(\boldsymbol{n},n_t)}\underbrace{M(s,n_t-1)\dots M(s,0)|\phi_j\rangle}_{=|v_j(n_t)\rangle}\end{aligned} \tag{5.64}$$

and using the functional derivative form,[5]

$$\frac{\partial}{\partial s(\boldsymbol{n},n_t)} : \exp\left[-\alpha_t\hat{H}_{free} + \sum_{\boldsymbol{n}'}A[s(\boldsymbol{n}',n_t)]\rho(\boldsymbol{n}')\right] := \frac{\partial A(s)}{\partial s(\boldsymbol{n},n_t)}\rho(\boldsymbol{n}) \tag{5.66}$$

, thus,

$$\frac{\partial X_{j'j}(s)}{\partial s(\boldsymbol{n},n_t)} = \frac{\partial A(s)}{\partial s(\boldsymbol{n},n_t)}\langle vd_{j'}(n_t+1)|\boldsymbol{n}\rangle\langle\boldsymbol{n}|v_j(n_t)\rangle \tag{5.67}$$

5.7 Example: HMC update for non-local chiral action

Let us look at more detail on the HMC update with an example. In HMC, we can write

$$\begin{aligned}\mathcal{Z}(L_t) &= \int \mathcal{D}p\mathcal{D}p^I_\pi\mathcal{D}s\mathcal{D}\pi_I e^{-\sum_{\boldsymbol{n}}\left[\frac{1}{2}p(\boldsymbol{n})^2+\frac{1}{2}s(\boldsymbol{n})^2+\frac{1}{2}p^I_\pi(\boldsymbol{n})^2+\frac{1}{2}\phi^2_I(\boldsymbol{n})\right]} \\ &\quad\times\langle\Psi|M^{L_t}(s,\pi_I)|\Psi\rangle \\ &= \int \mathcal{D}p\mathcal{D}p^I_\pi\mathcal{D}s\mathcal{D}\pi_I\exp\left(-\sum_{\boldsymbol{n}}\left[\frac{1}{2}p(\boldsymbol{n})^2 + +\frac{1}{2}p^I_\pi(\boldsymbol{n})^2 + V(s,\pi_I)\right]\right)\end{aligned} \tag{5.68}$$

[5] Not quite sure about this

$$\begin{aligned}\frac{\partial M(s,n_t)}{\partial s(\boldsymbol{n},n_t)} &= \frac{\partial A(s)}{\partial s(\boldsymbol{n},n_t)}\rho(\boldsymbol{n})M(s,n_t)\ ?, \\ &\quad \text{or } \frac{\partial A(s)}{\partial s(\boldsymbol{n},n_t)}M(s,n_t)\rho(\boldsymbol{n})\ ?, \\ &\quad \text{or } \frac{\partial A(s)}{\partial s(\boldsymbol{n},n_t)}\rho(\boldsymbol{n})\ ?\end{aligned} \tag{5.65}$$

with

$$V(s,\pi_I)=\sum_{\boldsymbol{n}}\left[\frac{1}{2}s(\boldsymbol{n})^2+\frac{1}{2}\phi_I^2(\boldsymbol{n})\right]-\ln\det X(s,\pi_I,L_t) \tag{5.69}$$

In fact, the code use two different M matrix for probability calculation. Thus, actual HMC potential is

$$V(s,\pi_I)=\sum_{\boldsymbol{n}}\left[\frac{1}{2}s(\boldsymbol{n})^2+\frac{1}{2}\phi_I^2(\boldsymbol{n})\right]-a_0\ln\det X_0(s,\pi_I,L_t)-a_1\ln\det X_1(s,\pi_I,L_t) \tag{5.70}$$

The fermion transfer matrix gives HMC potential,

$$\langle\Psi|M^{Lt}|\Psi\rangle=\det X(s,\pi_I,L_t)=\exp(-(-\ln\det X(s,\pi_I,L_t))). \tag{5.71}$$

$$M^{(n_t)}=:\exp\left(-H_{free}\alpha_t-V_s^{(n_t)}\sqrt{\alpha_t}-V_\pi^{(n_t)}\alpha_t\right): \tag{5.72}$$

$$V_s^{(n_t)}=-\sqrt{-c_0}\sum_{\boldsymbol{n}\boldsymbol{n}'}\rho_{NL}(\boldsymbol{n})f_{s_L}(\boldsymbol{n}-\boldsymbol{n}')s(\boldsymbol{n}',n_t). \tag{5.73}$$

$$\begin{aligned}V_\pi^{(n_t)} &= -\frac{g_A}{2f_\pi}\sum_{\boldsymbol{n},\boldsymbol{n}',S,I}\rho_{S,I}(\boldsymbol{n}')f_S^\pi(\boldsymbol{n}'-\boldsymbol{n})\pi_I(\boldsymbol{n},n_t)\\ &= +\frac{g_A}{2f_\pi}\sum_{\boldsymbol{n},\boldsymbol{n}',S,I}\pi_I(\boldsymbol{n}',n_t)f_S^\pi(\boldsymbol{n}'-\boldsymbol{n})\rho_{S,I}(\boldsymbol{n})\end{aligned} \tag{5.74}$$

where, we can think $\sum_{\boldsymbol{n}}f_S^\pi(\boldsymbol{n}'-\boldsymbol{n})\pi_I(\boldsymbol{n})=\nabla_S\pi_I(\boldsymbol{n}')$. (Note that ,In the code, the second form $\sum_{\boldsymbol{n}'}\pi_I(\boldsymbol{n}')f_S^\pi(\boldsymbol{n}'-\boldsymbol{n})=-\nabla_S\pi_I(\boldsymbol{n}')$ is used Thus, be careful for the sign. Also, it is important to note that the derivative is done with auxiliary pion not true pion.)

Then,

$$\begin{aligned}\frac{\partial V(s,\pi_I)}{\partial s(\boldsymbol{n},n_t)} &= s(\boldsymbol{n},n_t)-a_0\mathrm{Re}\left[\sum_{kl}X_{lk}^{-1}\langle zd_k(n_t+1)|\frac{(-V_s^{(n_t)}\sqrt{\alpha_t})}{\partial s(\boldsymbol{n},n_t)}|zv_l(n_t)\rangle\right]-a_1\left[(X_0\to X_1))\right],\\ \frac{\partial V(s,\pi_I)}{\partial\phi_I(\boldsymbol{n},n_t)} &= \phi_I(\boldsymbol{n},n_t)-a_0\sum_S\sum_{\boldsymbol{n}'}\frac{\partial\nabla_S\pi_I(\boldsymbol{n}',n_t)}{\partial\phi_I(\boldsymbol{n},n_t)}\mathrm{Re}\left[\sum_{kl}X_{lk}^{-1}\langle zd_k(n_t+1)|\frac{\partial(-V_\pi^{(n_t)}\alpha_t)}{\partial\nabla_S\pi_I(\boldsymbol{n}',n_t)}|zv_l(n_t)\rangle\right]\\ &\quad -a_1\left[(X_0\to X_1))\right]\end{aligned} \tag{5.75}$$

And

$$\begin{aligned}\langle zd_k(n_t+1)|\frac{\partial(-V_s^{(n_t)}\sqrt{\alpha_t})}{\partial s(\boldsymbol{n},n_t)}|zv_l(n_t)\rangle &= \sqrt{-c_0\alpha_t}\langle zd_k(n_t+1)|\sum_{\boldsymbol{n}'}\hat{\rho}_{NL}(\boldsymbol{n}')f_{s_L}(\boldsymbol{n}'-\boldsymbol{n})|zv_l(n_t)\rangle\\ &= \sqrt{-c_0\alpha_t}\sum_{\boldsymbol{n}'}\langle zd_k(n_t+1)|\boldsymbol{n}'\rangle_{smear}f_{s_L}(\boldsymbol{n}'-\boldsymbol{n})\langle\boldsymbol{n}'|zv_l(n_t)\rangle_{smear},\\ \langle zd_k(n_t+1)|\frac{\partial(-V_\pi^{(n_t)}\alpha_t)}{\partial\nabla_S\pi_I(\boldsymbol{n},n_t)}|zv_l(n_t)\rangle &= -\frac{g_A}{2f_\pi}\langle zd_k(n_t+1)|\hat{\rho}_{SI}(\boldsymbol{n})|zv_l(n_t)\rangle\\ &= =-\frac{g_A}{2f_\pi}\Big(\langle zd_k(n_t+1)|\boldsymbol{n}\rangle\sigma_S\tau_I\langle\boldsymbol{n}|zv_l(n_t)\rangle\Big)\end{aligned} \tag{5.76}$$

We may define,

$$dV(\boldsymbol{n},n_t,S,I)=\mathrm{Re}\left[\sum_{kl}X_{lk}^{-1}\sum_{s_1,s_2,i_1,i_2}\langle zd_k(n_t+1)|\boldsymbol{n},s_1i_1\rangle(\sigma_S)_{s_1s_2}(\tau_I)_{i_1i_2}\langle\boldsymbol{n},s_2i_2|zv_l(n_t)\rangle\right] \tag{5.77}$$

Then,

$$\begin{aligned}\frac{\partial V(s,\pi_I)}{\partial\phi_I(\boldsymbol{n},n_t)} &= \phi_I(\boldsymbol{n},n_t)-\sum_S\sum_{\boldsymbol{n}'}\frac{\partial\nabla_S\pi_I(\boldsymbol{n}',n_t)}{\partial\phi_I(\boldsymbol{n},n_t)}(-\frac{g_A\alpha_t}{2f_\pi})dV(\boldsymbol{n},n_t,S,I)\\ &= \phi_I(\boldsymbol{n},n_t)+\frac{g_A\alpha_t}{2f_\pi}\sum_S\frac{1}{L^3}\sum_{\boldsymbol{q}}e^{i\boldsymbol{q}\cdot\boldsymbol{n}}(-i\boldsymbol{q})_S\frac{\widehat{dV}(\boldsymbol{q},n_t,S,I)}{\sqrt{\boldsymbol{q}^2+m_\pi^2}}.\end{aligned}\tag{5.78}$$

The second term can be computed either as

$$\begin{aligned}&\frac{g_A\alpha_t}{2f_\pi}\sum_S\frac{1}{L^3}\sum_{\boldsymbol{q}}e^{i\boldsymbol{q}\cdot\boldsymbol{n}}(-i\boldsymbol{q})_S\frac{\widehat{dV}(\boldsymbol{q},n_t,S,I)}{\sqrt{\boldsymbol{q}^2+m_\pi^2}}\\ =\;&\frac{g_A\alpha_t}{2f_\pi}\sum_S\sum_{\boldsymbol{n}'}\Delta_S(\boldsymbol{n}-\boldsymbol{n}')pdV(\boldsymbol{n}'),\quad \widehat{pdV}(\boldsymbol{q})=\frac{\widehat{dV}(\boldsymbol{q})}{\sqrt{\boldsymbol{q}^2+m_\pi^2}},\end{aligned}\tag{5.79}$$

or as

$$\frac{\partial V(s,\pi_I)}{\partial\phi_I(\boldsymbol{n},n_t)} = \phi_I(\boldsymbol{n},n_t)+\frac{g_A\alpha_t}{2f_\pi}\sum_S W(\boldsymbol{n},n_t,S,I),\quad \widehat{dW}(\boldsymbol{q},n_t,S,I)=(-i\boldsymbol{q})_S\frac{\widehat{dV}(\boldsymbol{q},n_t,S,I)}{\sqrt{\boldsymbol{q}^2+m_\pi^2}}$$

5.8 Example: Obervable in Unitary limit calculation

Until now the calculation concerned is

$$Z(L_t)=\langle\Psi|M^{L_t}|\Psi\rangle=\int d_As\;\langle\Psi|M^{L_t}(s)|\Psi\rangle\tag{5.80}$$

Thus, if the initial many particle wave is a linear combination of exact many-body eigen states,

$$\begin{aligned}|\Psi\rangle &= \sum_k c_k|\Psi_k\rangle,\quad H|\Psi_k\rangle=E_k\Psi_k\rangle,\\ Z(L_t) &= \sum_k|c_k|^2e^{-E_kL_t}\end{aligned}\tag{5.81}$$

Thus, we can compute ground state energy by

$$\begin{aligned}E(t) &= \frac{1}{\alpha_t}\log\frac{Z(t-\alpha_t)}{Z(t)},\\ \lim_{t\to\infty}E(t) &= E_0+\ldots\end{aligned}\tag{5.82}$$

Because the actual MC sampling should be done with positive definite weights, we separate

$$\det X(s,t)=|\det X(s,t)|e^{i\theta(s,t)}=e^{\log|\det X(s,t)|}e^{i\theta(s,t)}\tag{5.83}$$

and include $e^{\log|\det X(s,t)|}$ part into weights. Thus, actual MC average is done by calculating

$$Z(t)=\langle e^{i\theta(s,t)}\rangle_t\tag{5.84}$$

where $\langle\ldots\rangle_t$ means MC average using $e^{\log|\det X(s,t)|}$ as part of weights. Then, in the same way,

$$Z(t-\alpha_t)=\left\langle\frac{e^{\log|\det X(s,t-1)|}e^{i\theta(s,t-1)}}{e^{\log|\det X(s,t)|}}\right\rangle_t\tag{5.85}$$

On the other hand, we may define probability distribution as

$$P[s]\propto e^{-S_s}[a_0|\det X(s,t)|+a_1|\det X(s,t-\alpha_t)|]\tag{5.86}$$

with some constant a_0 and a_1. Let us introduce simplified notation, $V_0 = |\det X(s,t)|$ and $V_1 = |\det X(s,t-\alpha_t)|$. Then, we may write the probability action as

$$P[s] \propto e^{-act}, \quad act = S_s - \log(a_0 V_0 + a_1 V_1) \tag{5.87}$$

Note that because of the change in probability choice , one have to compensate the change in the $Z(L_t)$ calculation. However, in other observables which were inserted in the calculation

$$\langle\Psi|M^{L_t-n_t}O(n_t)M^{n_t}|\Psi\rangle = \int ds e^{-S_s}\langle\Psi|M^{L_t}(s)O(t)|\Psi\rangle = \int ds e^{-S_s+V(s)}e^{-V(s)}\det X(s,O) \to \frac{1}{N}\sum_i{}' e^{-V(s_i)}\det X(s_i,O) \tag{5.88}$$

The new correlator including observable is calculated and used to obtain the expectation value of the observable. Note that if the observable is inserted at n_t,

$$\langle\Psi|M^{L_t}(s)O(t)|\Psi\rangle = \langle vd(n_t, L_t-1)|M(n_t)O(n_t)|v(n_t,L_t-1)\rangle \tag{5.89}$$

Thus, one have to use zvecs and zdualvecs for $L_t - 1$.

5.9 Example: density operator evaluation

Let us consider a expectation value of $:\rho^3(\boldsymbol{n})/3!:$ summed over $\boldsymbol{n}$(actually the operator should be a summation over spin and iso-spin). For a given $\boldsymbol{n}$, one have to evaluate

$$\langle\Psi(s)|\frac{1}{3!}:\left(\sum_{s,i}\rho_{s,i}(\boldsymbol{n},n_t)\right)^3:|\Psi(s)\rangle \tag{5.90}$$

and then summed over $\boldsymbol{n}$ and averaged over s. To evaluate this matrix element, let us consider,

$$\langle\Psi_0|M\cdots:\exp\left(\sum_{\boldsymbol{n}'}\sum_{s,i}\epsilon(\boldsymbol{n}')\rho_{s,i}(\boldsymbol{n}',n_t)\right):\cdots M|\Psi_0\rangle = \det X([s],[\epsilon]),$$

$$X_{ij}([s],[\epsilon]) = \langle\phi_i|M\cdots:\exp\left(\sum_{\boldsymbol{n}'}\sum_{s,i}\epsilon(\boldsymbol{n}')\rho_{s,i}(\boldsymbol{n}',n_t)\right):\cdots M|\phi_j\rangle \tag{5.91}$$

Then for given $\epsilon(\boldsymbol{n})$ function, one can compute X_{ij} and thus $\det X$. Thus, the original expectation value may be considered as

$$\langle\Psi(s)|\frac{1}{3!}:\left(\sum_{s,i}\rho_{s,i}(\boldsymbol{n},n_t)\right)^3:|\Psi(s)\rangle = \frac{\partial^3}{\partial\epsilon(\boldsymbol{n})^3}\det X([s],[\epsilon]=0) \tag{5.92}$$

In fact, since we only need derivative of at a specific $\boldsymbol{n}$, we may set $\epsilon(\boldsymbol{n}') = \epsilon\delta_{\boldsymbol{n}',\boldsymbol{n}}$ and evaluate, $X_{ij}([s],\epsilon,\boldsymbol{n})$, [6]

$$X_{ij}([s],\epsilon,\boldsymbol{n}) = \epsilon\sum_{s,i}\langle zdvecs(n_t)|\boldsymbol{n},s,i\rangle\langle\boldsymbol{n},s,i|zvecs(n_t)\rangle \tag{5.93}$$

Then, one can obtain the derivative as numerical differences of $\det X([s],\epsilon,\boldsymbol{n})$ at various ϵ values,

$$\frac{\partial^3}{\partial\epsilon(\boldsymbol{n})^3}\det X([s],[\epsilon]=0) = \frac{\partial^3}{\partial\epsilon^3}|_{\epsilon=0}\det X([s],\epsilon,\boldsymbol{n}) \tag{5.94}$$

In a similar way, one can compute the expectation value of

$$\langle\Psi(s,L_t/2)|:\rho(\boldsymbol{n}_1)\rho(\boldsymbol{n}_2):|\Psi(s,L_t/2)\rangle = \frac{\partial^2}{\partial\epsilon(\boldsymbol{n}_1)\partial\epsilon(\boldsymbol{n}_2)}|_{\epsilon=0}\det X([s],\epsilon(\boldsymbol{n}_1),\epsilon(\boldsymbol{n}_2)),$$

$$X_{ij}([s],\epsilon(\boldsymbol{n}_1),\epsilon(\boldsymbol{n}_2)) = \langle\phi_i(L_t/2)|(1+\epsilon(\boldsymbol{n}_1)\rho(\boldsymbol{n}_1)+\epsilon(\boldsymbol{n}_2)\rho(\boldsymbol{n}_2))|\phi_j(L_t/2)\rangle. \tag{5.95}$$

[6] Need verification whether it should be n_t or n_t+1 for zdvecs.

Chapter 6

scattering in lattice

To fix LECs, we need to compute scattering phase shifts. Also we may want to obtain the scattering information

6.1 Lüscher's method

This section requires more clear explanation.

Lüscher's formula relates the two-particle energy levels in a periodic cube of length L to the S-wave phase shift,

$$p \cot \delta_0(p) = \frac{1}{\pi L} S(\eta), \quad \eta = (\frac{Lp}{2\pi})^2, \tag{6.1}$$

where L is the lattice size, p is related with energy level $E = \frac{p^2}{m} = \frac{\eta}{m}(\frac{2\pi}{L})^2$. $S(\eta)$ is the three dimensional zeta function,

$$S(\eta) = \lim_{\Lambda \to \infty} \left[\left(\sum_{\boldsymbol{n}} \frac{\theta(\Lambda^2 - \boldsymbol{n}^2)}{\boldsymbol{n}^2 - \eta} \right) - 4\pi\Lambda \right] \tag{6.2}$$

If we draw graph $S(\eta)$ with some large value of Λ, $S(\eta) = 0$ have several roots and closest to zero root is $\eta = -0.095901$. This corresponds to infinite scattering length, or unitary limits. ($\eta < 0$ means it is a bound state??)

In lattice simulation, one computes the energy level E and equivalently p or η in finite volume. (However, actually it is not trivial to obtain p from finite volume energy $E(L)$.) Thus, one can compute $S(\eta)$ and p. From this information , one can obtain $\cot \delta_0(p) = \frac{1}{p}\frac{S(\eta)}{\pi L}$. In other words, phase shift for energy E can be obtained. If L is varied, one can obtain the phase shifts at different energies. In this way, one can computes the scattering phase shifts from finite volume calculation.

If we only consider low energy scattering, we may expand $S(\eta)$ for $|\eta| < 1$,

$$S(\eta) = -\frac{1}{\eta} + \lim_{\Lambda \to \infty} \left[\left(\sum_{\boldsymbol{n} \neq 0} \frac{\theta(\Lambda^2 - \boldsymbol{n}^2)}{\boldsymbol{n}^2 - \eta} \right) - 4\pi\Lambda \right] = -\frac{1}{\eta} + S_0 + S_1\eta + S_2\eta^2 + S_3\eta^3 + \dots \tag{6.3}$$

where,

$$\begin{aligned} S_0 &= \left[\left(\sum_{\boldsymbol{n} \neq 0} \frac{\theta(\Lambda^2 - \boldsymbol{n}^2)}{\boldsymbol{n}^2} \right) - 4\pi\Lambda \right], \\ S_j &= \sum_{\boldsymbol{n} \neq 0} \frac{1}{(\boldsymbol{n}^2)^{j+1}}, \quad j \geq 1. \end{aligned} \tag{6.4}$$

where $\boldsymbol{n} = (n_1, n_2, n_3)$ are integers.[1] In other words, regardless the details of the interaction or system, the low energy limit is universal.(Be careful that one can not simply send $p \to 0$ for finite L values because spectrum p is related with lattice size.)

6.1.1 Fermion-Dimer S-wave phase shift

REF: Eur. Phys. J. A(2013) 49:151 How to obtain the phase shift $\delta_0(p)$ from finite volume energy $E(L)$ for the fermion-dimer system.

Fermion-dimer energy in the periodic box of size Lb for s-wave scattering:

$$E^{fd}(p, L) = E^{fd}(p, \infty) + \tau^d(\eta)\Delta E_0^d(L). \tag{6.6}$$

We want to extract p satisfying above equation from a direct finite volume energy computed in the lattice, $E^{fd}(L)$ and dimer binding energy $B(L)$.

The first term,

$$E^{fd}(p, \infty) = \frac{p^2}{2m_d} + \frac{p^2}{2m} - B(\infty), \tag{6.7}$$

shows the relation between momentum and the energy from infinite volume limit. Here dimer mass m_d and $B(\infty)$ have to be extracted from the lattice result $B(L)$. Approximately, they can be obtained from $B(L)$ with very large L values.

The second term is a finite volume corrections to the fermion-dimer energy due to the dimer wave function wrapping around the periodic boundary, where $\Delta E_{\vec{0}}^d(L) = B(\infty) - B(L)$ is the finite volume energy shift for the bound dimer state in the two-body center of mass frame. (Thus, $\Delta E_{\vec{0}}^d(L)$ can be obtained easily from $B(L)$.)

$$\tau^d(\eta) = \frac{1}{\mathcal{N}} \sum_{\boldsymbol{k}} \frac{\tau(\boldsymbol{k}, 1/2)}{(\boldsymbol{k}^2 - \eta^2)^2}, \tag{6.8}$$

where

$$\mathcal{N} = \sum_{\boldsymbol{k}} \frac{1}{(\boldsymbol{k}^2 - \eta^2)^2}, \quad \tau(\boldsymbol{k}, 1/2) = \frac{1}{3} \sum_{i=1}^{3} \cos(k_i L/2) \tag{6.9}$$

$\boldsymbol{k}$ is all possible center of mass momentum $\boldsymbol{k}$ of dimer(? I am not sure what is the actual summation of $\boldsymbol{k}$.). (Because of η, this is a function of p. Thus the equation for $E^{fd}(p, L)$ is a non-linear function of p and can be solved by iteration starting from initial guess $\tau^d(\eta) = 1$.)

6.2 Spherical Wall method

This section requires more clear explanation.

[1] Including negative integer, 0, positive integer. By setting large Λ values, we can calculate coefficients regardless of lattice size,

$$\begin{aligned} S_0 &= -8.913631, & S_1 &= 16.532288, \\ S_2 &= 8.401924, & S_3 &= 6.945808, \\ S_4 &= 6.426119, & S_5 &= 6.202149, \\ S_6 &= 6.098184, & S_7 &= 6.048263. \end{aligned} \tag{6.5}$$

6.3 Adiabatic projection method

The Euclidean time evolution is called 'projection method' because it projects the initial state into a ground state or excitation spectrum of the system by Euclidean time evolution.

Adiabatic projection method exploits that there are two time scales in the projection. The first one is a faster time scale to form a alpha clusters. The second one is a slow time scale to form a superpositions of clusters. Thus, at a properly chosen time [2] , One can obtain the continuum state information.

For an example, let us consider 3-nucleons system which forms a nucleon-dimer two-body scattering state.

Choose a C.M. frame and set the origin at the one nucleon. [3] We may prepare several initial states corresponding to a nucleon-dimer with separation $\vec{R}$, $|\vec{R}\rangle$ and get a dressed cluster states

$$\begin{aligned} |\vec{R}\rangle &= a_\uparrow^\dagger(\vec{R})a_\uparrow^\dagger(\vec{0})a_\downarrow^\dagger(\vec{0})|0\rangle, \\ |\vec{R}\rangle_\tau &= \exp(-H\tau)|\vec{R}\rangle. \end{aligned} \tag{6.10}$$

In fact, since we need to have total momentum zero state of clusters. One can make such state as factorized in long separation ,

$$|\vec{R}\rangle = \sum_{\boldsymbol{r}} |\boldsymbol{r}+\vec{R}\rangle \otimes |\boldsymbol{r}\rangle \tag{6.11}$$

where $\boldsymbol{r}$ represent a position of one cluster. The sum of all possible $\boldsymbol{r}$ makes the state translation invariant and thus provide total momentum zero state.

For the case of L number of lattice points in one direction, we may have L^3-1 number of possible $\vec{R}$ values. In the limit of large τ, dressed cluster states $|\vec{R}\rangle_\tau$ will span the low energy spectrum of the original Hamiltonian.

The dressed cluster states will not be orthogonal in general. Thus, we will have norm matrix

$$[N_\tau]_{\vec{R},\vec{R}'} = {}_\tau\langle\vec{R}|\vec{R}'\rangle_\tau \tag{6.12}$$

We may define inverse of norm matrix and

$$\begin{aligned} \delta_{\vec{R},\vec{R}'} &= \sum_{\vec{R}''}[N_\tau^{-1}]_{\vec{R},\vec{R}''}[N_\tau]_{\vec{R}'',\vec{R}'} = \sum_{\vec{R}''}[N_\tau^{-1}]_{\vec{R},\vec{R}''\tau}\langle\vec{R}''|\vec{R}'\rangle_\tau \\ &= {}_\tau(\vec{R}|\vec{R}'\rangle_\tau. \end{aligned} \tag{6.13}$$

where, dual vector is defined as

$${}_\tau(\vec{R}|v\rangle = \sum_{\vec{R}''}[N_\tau^{-1}]_{\vec{R},\vec{R}''\tau}\langle\vec{R}''|v\rangle. \tag{6.14}$$

The dual vector will annihilate any vector which is orthogonal to all dressed cluster states,

$${}_\tau\langle\vec{R}|v\rangle = 0 \text{ for all } \vec{R} \quad \Rightarrow \quad {}_\tau(\vec{R}|v\rangle = 0 \text{ for all } \vec{R}. \tag{6.15}$$

Also, as shown before

$${}_\tau(\vec{R}|\vec{R}\rangle_\tau = \delta_{\vec{R},\vec{R}'}. \tag{6.16}$$

[2] But how to get the proper time scale for given system?

[3] C.M. frame means the total momentum of the system is zero. Suppose we choose a spin up proton is at the origin. However, since there is a wave function for a proton spin up, the origin corresponds to the average central position of a spin up proton and there will be a distribution of probability to find spin up proton around the origin.

By computing the matrix elements of Hamiltonian, we can write the adiabatic Hamiltonian as

$$\begin{aligned}[H^a_\tau]_{\vec{R},\vec{R}'} &= {}_\tau(\vec{R}|H|\vec{R}')_\tau, \\ &= \sum_{\vec{R}''}[N^{-1}_\tau]_{\vec{R},\vec{R}''\,\tau}\langle\vec{R}''|H|\vec{R}'\rangle_\tau. \end{aligned} \tag{6.17}$$

With similarity transform, One can obtain adiabatice Hamilronian which is Hermitian,

$$[H^{a'}_\tau]_{\vec{R},\vec{R}'} = \sum_{\vec{R}'',\vec{R}'''}\left[N^{-1/2}_\tau\right]_{\vec{R},\vec{R}''\,\tau}\langle\vec{R}''|H|\vec{R}'''\rangle_\tau\left[N^{-1/2}_\tau\right]_{\vec{R}''',\vec{R}'} \tag{6.18}$$

what exactly is the definition of $\left[N^{-1/2}_\tau\right]_{\vec{R}''',\vec{R}'}$? Defined as $N^{-1}_\tau = N^{-1/2}_\tau \cdot N^{-1/2}_\tau$?

In other words, (1) Prepare many $|\vec{R}\rangle$ states (2) compute dressed states $|\vec{R}\rangle_\tau$ (3) compute the norm matrix $[N_\tau]_{\vec{R},\vec{R}'}$ and also compute expectation value ${}_\tau\langle\vec{R}''|H|\vec{R}'''\rangle_\tau$ (4) compute $\left[N^{-1/2}_\tau\right]_{\vec{R}''',\vec{R}'}$ (5) One can obtain $[H^{a'}_\tau]_{\vec{R},\vec{R}'}$ and also $[H^a_\tau]_{\vec{R},\vec{R}'}$. (6) One can compute the phase shifts between clusters by solving $[H^a_\tau]_{\vec{R},\vec{R}'}$ eigen-value equation.

In the code, the computation of matrix element can be done

$$\begin{aligned}{}_\tau\langle\vec{R}|H|\vec{R}'\rangle_\tau &= \left(\sum_{\boldsymbol{r}}\langle\boldsymbol{r}+\vec{R}|\otimes\langle\boldsymbol{r}|\right)e^{-H\tau}He^{-H\tau}\left(\sum_{\boldsymbol{r}'}|\boldsymbol{r}'+\vec{R}'\rangle\otimes|\boldsymbol{r}'\rangle\right) \\ &\simeq \sum_{\boldsymbol{r}}\left(\langle\boldsymbol{r}+\vec{R}|\otimes\langle\boldsymbol{r}|\right)e^{-H\tau}He^{-H\tau}\left(|\vec{R}'\rangle\otimes|\vec{0}\rangle\right) \end{aligned} \tag{6.19}$$

where the position of one cluster is fixed at the origin in the initial state and the sum over possible shifts $\boldsymbol{r}$ is done as a part of MC simulation. Since the sum over $\boldsymbol{r}$ makes the total momentum of final state as zero, only the part of the initial state which have zero total momentum can contribute the matrix element. Also, the sum over $\boldsymbol{r}$ can use some probability distribution so that

$$\sum_{\boldsymbol{r}} f(\boldsymbol{r}) = \sum_{\boldsymbol{r}} P(\boldsymbol{r})\frac{f(\boldsymbol{r})}{P(\boldsymbol{r})} \simeq \frac{1}{N}\sum_i{}' \frac{f_i}{P_i}, \tag{6.20}$$

where $\sum'_i$ is a sum over sampling via probability distribution P.

Chapter 7

Sign Problem

When we compute the Monte Carlo calculation, we needs some weight function which have to be positive definite because it should be interpreted as probability. However, in some cases, the weight becomes complex or negative which makes it difficult to get reliable numerical results. In example case with complex weight $\det X(s,t)$, we have to compute expectation value of $Z(t) = \langle e^{i\theta(s,t)} \rangle_t$ in limit of large t. However, this expectation value rapidly decreases to zero because of the sign ocillation for large t, there is a cancellation between positive weight and negative weights. Thus, it is very difficult to compute observable reliably because we needs

$$\langle O \rangle = \frac{\langle O e^{i\theta} \rangle_{pq}}{\langle e^{i\theta} \rangle_{pq}}, \quad \langle O \rangle_{pq} \equiv \frac{\int ds |\det X(s)| O}{\int ds |\det X(s)|} \tag{7.1}$$

And, if the lattice volume is Ω and number of fermions Δf,

$$\langle e^{i\theta} \rangle_{pq} = \frac{Z_{full}}{Z_{pq}} = e^{-\Omega \Delta f} \to 0. \tag{7.2}$$

In case of lattice QCD, the complex action appears with chemical potential μ,

$$[\det X(\mu)]^* = \det X(-\mu^*) \tag{7.3}$$

7.1 Origin of sign problem?

Let us consider a general matrix M which have eigen states ϕ such that $M\phi = \lambda\phi$. Here, we want to prove that if there exists some anti-symmetric unitary matrix U, $U^T = -U$, such that $U^\dagger M U = M^*$, then $\det M$ is semi-positive definite.

Let us define a vector $\tilde{\phi} = U\phi^*$. Then,

$$\begin{aligned} M\tilde{\phi} &= M(U\phi^*) = U(U^\dagger M U)\phi^* = UM^*\phi^* = U(M\phi)^* = U(\lambda\phi)^* = \lambda^*(U\phi^*) \\ &= \lambda^* \tilde{\phi}. \end{aligned} \tag{7.4}$$

Thus, $\tilde{\phi}$ is also eigen-vector of M with eigen-value λ^*. On the other hand,

$$\begin{aligned} \phi^\dagger \tilde{\phi} &= \phi^\dagger U \phi^* = (\phi^\dagger U \phi^*)^T = \phi^\dagger U^T \phi^* \\ &= -\phi^\dagger U \phi^* = 0. \end{aligned} \tag{7.5}$$

[1] Thus, ϕ and $\tilde{\phi}$ is always orthogonal as long as such U exists. Thus, implies the eigenvalues of M is

[1] In a similar way, using $U^* = -U^\dagger$,

$$\begin{aligned} \tilde{\phi}^\dagger \phi &= \phi^T U^\dagger \phi = (\phi^T U^\dagger \phi)^T = \phi^T U^* \phi \\ &= -\phi^T U^\dagger \phi = 0. \end{aligned} \tag{7.6}$$

always paired and determinant would be $\det M \propto \lambda^*\lambda \propto |\lambda|^2 \geq 0$. When λ is real, it implies there exists degenerate eigen states and also $\det M \geq 0$.

For example, simplest case is operator $M = I$ and $M = iI$. Any antisymmetric unitary matrix will satisfy the condition for $M = I$ if $M = I$ is even dimensional. On the other hand, there is no such matrix for $M = iI$ in any dimension.

Another example is , in (iso)spin space[2] , $i\sigma_{S=1,2,3}$ would not show any sign problem because

$$\sigma_2^\dagger(i\sigma_{1,3})\sigma_2 = -i\sigma_{1,3} = [i\sigma_{1,3}]^*, \quad \sigma_2^\dagger(i\sigma_2)\sigma_2 = i\sigma_2 = [i\sigma_2]^*. \tag{7.8}$$

On the other hand, operator σ_S (without i) would show sign problem.

In spin-isospin space, $\sigma_2 I_\tau$, $\sigma_2\tau_{1,3}$ or $\tau_2 I_\sigma$, $\tau_2\sigma_{1,3}$ can acts as a antisymmetric operators. However, there would be some constraints on the operators.

Actual amplitude oe transfer matrix have dependence on space, spin and iso-spin. But, we can use different gauge(unitary matrix) at different position so that most problem would occur in spin and isospin part. In terms of spin and iso-spin, possible operator forms are

$$I, iI, \sigma_S, i\sigma_S, \tau_I, i\tau_I, \sigma_S\tau_I, i\sigma_S\tau_I \tag{7.9}$$

and their combinations.

Consequence: Let us consider the two consecutive unitary transformation, $V^\dagger M V = M'$ and $U^\dagger M' U = (M')^*$ and $U^T = -U$. The overall transformation is, $(VU)^\dagger M(VU) = (V^\dagger M V)^* = V^T M^* V^*$ and (VU) is not anti-symmetric. However, $\det M = \det M' \geq 0$.

Because ${}^4He$, which is spin and isospin singlet, does not have preferred spin and iso-spin direction, we can rotate them separately. Thus, $H = C_S i\boldsymbol{\sigma}_S + C_I i\tau_I$ case. If we use transformation by τ_2, $\tau_2 H \tau_2 = C_S i\boldsymbol{\sigma}_S + C_I(i\tau_I)^*$ and then transform by σ_2, $(\sigma_2^\dagger\tau_2^\dagger)H(\tau_2\sigma_2) = H^*$. Thus, in case of isospin singlet channel, c_S and c_I term does not gives sign problem from interference.

modified action

Instead of using strict leading order action, it is possible to modify the action such that (1) smearing contact interactions and (2) additional contact terms which are effectively accounting for higher order interactions. One reason for introducing smearing contact interaction is to avoid clustering instability of LO interaction.

However, in terms of physics there are only two low energy constants C_{1S0}, C_{3S1} or C, C_I to be fixed from phase shifts at leading order, and also additional contact interactions, C_S, C_{SI} , may leads to non-physical S-wave symmetric spin-isospin states. To avoids such incidents, we will set relations C_S, C_{SI} such that they are not independent. For two-body states, contact terms acts as operators,

$$\frac{1}{2}\bar{N}A_i N\bar{N}B_j N|\alpha\rangle_{2B} \to \frac{1}{2}(\hat{A}_1^i\hat{B}_2^j + \hat{A}_2^i\hat{B}_1^j)|\alpha\rangle_{2B} \tag{7.10}$$

Then, contact interactions corresponds to following operators

$$\hat{O} = C\ I + C_{S^2}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 + C_{I^2}\tau_1\cdot\tau_2 + C_{S^2I^2}\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\tau_1\cdot\tau_2. \tag{7.11}$$

Thus, to make symmetric spin-isospin states does not contribute,

$$\begin{aligned}\hat{O}|S=0,I=0\rangle &= (C - 3C_{S^2} - 3C_{I^2} + 9C_{S^2I^2})|S=0,I=0\rangle = 0,\\ \hat{O}|S=1,I=1\rangle &= (C + C_{S^2} + C_{I^2} + C_{S^2I^2})|S=1,I=1\rangle = 0,\end{aligned} \tag{7.12}$$

[2]Because,

$$\sigma_2^\dagger\sigma_{1,3}\sigma_2 = \sigma_2\sigma_{1,3}\sigma_2 = -\sigma_{1,3} \quad \sigma_2^\dagger\sigma_2\sigma_2 = \sigma_2. \tag{7.7}$$

we set

$$C = -3C_{S^2,I^2} = -\frac{3}{2}(C_{S^2} + C_{I^2}), \tag{7.13}$$

and the smeared contact interactions are non-zero only for even parity channels where we have anti-symmetry in spin-siospin. (Note that if there was no C_{SI}, the relation implies the equivalence between C_S and C_I. We will have relation between C_{1S0}, C_{3S1} with C, C_I or C, C_S.) **Question:** But, if there is actually only two independent LECs, what is exactly the additional contact interactions do? Does it actually reflect some part of higher order correction?

Now, in momentum space,

$$\begin{aligned} \rho(\boldsymbol{q}_s) &= \sum_{\boldsymbol{n}_s} \rho(\boldsymbol{n}_s) e^{i\boldsymbol{q}_s\cdot\boldsymbol{n}_s}, \\ \rho_I(\boldsymbol{q}_s) &= \sum_{\boldsymbol{n}_s} \rho_I(\boldsymbol{n}_s) e^{i\boldsymbol{q}_s\cdot\boldsymbol{n}_s}, \end{aligned} \tag{7.14}$$

$$\boldsymbol{q}_s = \frac{2\pi}{L}\boldsymbol{k}_s, \quad \boldsymbol{k}_s \text{ are integers from 0 to L-1.} \tag{7.15}$$

Then leading order form, by introducing smearing in momentum space,

$$\begin{aligned} & -\frac{1}{2}C\alpha_t \sum_{\boldsymbol{n}_s}[\rho(\boldsymbol{n}_s)]^2 - \frac{1}{2}C_I\alpha_t \sum_{I=1,2,3}\sum_{\boldsymbol{n}_s}[\rho_I(\boldsymbol{n}_s)]^2 \\ = \quad & \frac{1}{L^3}\sum_{\boldsymbol{q}_s}\left[-\frac{1}{2}C\alpha_t\rho(\boldsymbol{q}_s)\rho(-\boldsymbol{q}_s) - \frac{1}{2}C_I\alpha_t \sum_{I=1,2,3}\rho_I(\boldsymbol{q}_s)\rho_I(-\boldsymbol{q}_s)\right] \\ \Rightarrow \quad & \frac{1}{L^3}\sum_{\boldsymbol{q}_s} f(\boldsymbol{q}_s^2)\left[-\frac{1}{2}C\alpha_t\rho(\boldsymbol{q}_s)\rho(-\boldsymbol{q}_s) - \frac{1}{2}C_I\alpha_t \sum_{I=1,2,3}\rho_I(\boldsymbol{q}_s)\rho_I(-\boldsymbol{q}_s)\right] \end{aligned} \tag{7.16}$$

where, modification was done in the form of

$$f(\boldsymbol{q}_s^2) = f_0^{-1}\exp\left[-b\sum_{l_s=1,2,3}(1-\cos q_{l_s})\right], \tag{7.17}$$

with normalization,

$$f_0 = \frac{1}{L^3}\sum_{\boldsymbol{q}_s}\exp\left[-b\sum_{l_s=1,2,3}(1-\cos q_{l_s})\right], \tag{7.18}$$

and coefficient b is fixed to reproduce the effective range. This form of correction gives at small $\boldsymbol{q}$ limits,

$$f(\boldsymbol{q}_s^2) \simeq f_0^{-1}\exp\left(-\frac{b}{2}\boldsymbol{q}_s^2\right) \tag{7.19}$$

Then modified action with higher derivative corrections are

$$\begin{aligned} H^{(n_t)}_{LO_2}(\pi'_I) &= H_{free} + \frac{1}{2}C\sum_{\boldsymbol{q}} f(\boldsymbol{q}) : \rho(\boldsymbol{q})\rho(-\boldsymbol{q}) : \\ &+\frac{1}{2}C_{S^2}\sum_{\boldsymbol{q}} f(\boldsymbol{q}) : \rho_S(\boldsymbol{q})\rho_S(-\boldsymbol{q}) : \\ &+\frac{1}{2}C_{I^2}\sum_{\boldsymbol{q}} f(\boldsymbol{q}) : \rho_I(\boldsymbol{q})\rho_I(-\boldsymbol{q}) : \\ &+\frac{1}{2}C_{S^2I^2}\sum_{\boldsymbol{q}} f(\boldsymbol{q}) : \rho_{S,I}(\boldsymbol{q})\rho_{S,I}(-\boldsymbol{q}) : \\ &+\frac{g_A}{2f_\pi\sqrt{q_\pi}}\sum_{\boldsymbol{n},S,I}\Delta_S\pi'_I(\boldsymbol{n},n_t)\rho_{S,I}(\boldsymbol{n}) \end{aligned} \tag{7.20}$$

We can change the expression into position space form by F.T.,

$$\frac{1}{L^3}\sum_{\boldsymbol{q}} f(\boldsymbol{q}^2)\rho(\boldsymbol{q})\rho(-\boldsymbol{q}) = \sum_{\boldsymbol{n}}\sum_{\boldsymbol{n}'} f(\boldsymbol{n}-\boldsymbol{n}')\rho(\boldsymbol{n})\rho(\boldsymbol{n}'). \tag{7.21}$$

From the Gaussian integration formula,

$$\exp\left(-\frac{1}{2}\sum_{\boldsymbol{n}\boldsymbol{n}'} f(\boldsymbol{n}-\boldsymbol{n}')\rho(\boldsymbol{n})\rho(\boldsymbol{n}')\right) \propto \int \mathcal{D}s \exp\left(\frac{1}{2}\sum_{\boldsymbol{n},\boldsymbol{n}'} s(\boldsymbol{n})f^{-1}(\boldsymbol{n}-\boldsymbol{n}')s(\boldsymbol{n}') + \sum_{\boldsymbol{n}}\rho(\boldsymbol{n})s(\boldsymbol{n})\right) \tag{7.22}$$

Then, auxiliary lattice action can be written as

$$\mathcal{Z}_{LO} \propto \int D\pi'_I DsDs_I \exp[-S_{\pi\pi} - S_{ss}]\mathrm{Tr}[M^{(L_t-1)}(\pi'_I, s, s_I)\times\ldots M^{(0)}(\pi'_I, s, s_I)]. \tag{7.23}$$

With auxiliary action,

$$\begin{aligned} S_{ss} &= \frac{1}{2}\sum_{\boldsymbol{n}} s^2(\boldsymbol{n}) + \frac{1}{2}\sum_I\sum_s [s_I(\boldsymbol{n})]^2 \\ &\Rightarrow \frac{1}{2}\sum_{\boldsymbol{n}_s,\boldsymbol{n}'_s,n_t} s(\boldsymbol{n}_s,n_t)f^{-1}(\boldsymbol{n}_s-\boldsymbol{n}'_s)s(\boldsymbol{n}'_s,n_t) + \frac{1}{2}\sum_I\sum_{\boldsymbol{n}_s,\boldsymbol{n}'_s,n_t} s_I(\boldsymbol{n}_s,n_t)f^{-1}(\boldsymbol{n}_s-\boldsymbol{n}'_s)s_I(\boldsymbol{n}'_s,n_t) \end{aligned} \tag{7.24}$$

and the function f^{-1} is defined as

$$f^{-1}(\boldsymbol{n}_s-\boldsymbol{n}'_s) = \frac{1}{L^3}\sum_{\boldsymbol{q}_s}\frac{1}{f(\boldsymbol{q}_s^2)}e^{-i\boldsymbol{q}_s\cdot(\boldsymbol{n}_s-\boldsymbol{n}'_s)} \tag{7.25}$$

In auxiliary formulation

$$\begin{aligned} M^{(n_t)}_{LO,aux}(s,s_S,s_I,s_{S,I},\pi'_I) &= :\exp\left\{-H_{free}\alpha_t - \frac{g_A\alpha_t}{2f_\pi\sqrt{q_\pi}}\sum_{\boldsymbol{n},S,I}\Delta_S\pi'_I(\boldsymbol{n},n_t)\rho_{S,I}(\boldsymbol{n})\right. \\ &+\sqrt{-C\alpha_t}\sum_{\boldsymbol{n}} s(\boldsymbol{n},n_t)\rho(\boldsymbol{n}) + i\sqrt{C_{S^2}\alpha_t}\sum_{\boldsymbol{n},S} s_S(\boldsymbol{n},n_t)\rho_S(\boldsymbol{n}) \\ &\left.+i\sqrt{C_{I^2}\alpha_t}\sum_{\boldsymbol{n},I} s_I(\boldsymbol{n},n_t)\rho_I(\boldsymbol{n}) + i\sqrt{C_{S^2,I^2}\alpha_t}\sum_{\boldsymbol{n},S,I} s_{SI}(\boldsymbol{n},n_t)\rho_{SI}(\boldsymbol{n})\right\} : \end{aligned} \tag{7.26}$$

Also we add $SU(4)$ symmetric transfer matrix

$$\begin{aligned} M_4^{(n_t)} &= :\exp[-H_4\alpha_t]:, \quad H_4 = H_{free} + \frac{1}{2}C_4\sum_{\boldsymbol{q}} f(\boldsymbol{q}) : \rho(\boldsymbol{q})\rho(-\boldsymbol{q}):, \quad C_4 < 0, \\ M_{4,aux}^{(n_t)}(s) &= :\exp\left\{-H_{free}\alpha_t + \sqrt{-C_4\alpha_t}\sum_{\boldsymbol{n}} s(\boldsymbol{n}, n_t)\rho(\boldsymbol{n})\right\}: \end{aligned} \tag{7.27}$$

Because the $SU(4)$ Hamiltonian corresponds to I structure in spin-isospin, there would be no sign problem for even number of nucleons.

Sign problem in modified action

In case of chiral EFT, the Hamiltonian have operator structures of

$$I, i\sigma_S, i\tau_I, i\sigma_S\tau_I, \sigma_S\tau_I$$

Among these, some can have antisymmetric unitary matrix such that satisfy previous conditions. [3]

	I	iI	$\boldsymbol{\sigma}_S$	$i\boldsymbol{\sigma}_S$	τ_I	$i\tau_I$	$\boldsymbol{\sigma}_S\tau_I$	$i\boldsymbol{\sigma}_S\tau_I$
$\boldsymbol{\sigma}_2$	O	X	X	O	τ_1, τ_3	$i\tau_2$	$\boldsymbol{\sigma}_1\tau_2, \boldsymbol{\sigma}_3\tau_2$	$i\boldsymbol{\sigma}_S\tau_1, i\boldsymbol{\sigma}_S\tau_3$
τ_2	O	X	$\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_3$	$i\boldsymbol{\sigma}_2$	X	O	$\boldsymbol{\sigma}_2\tau_1, \boldsymbol{\sigma}_2\tau_3$	$i\boldsymbol{\sigma}_1\tau_I, i\boldsymbol{\sigma}_3\tau_I$
$\boldsymbol{\sigma}_2\tau_3$	O	X	X	O	τ_2, τ_3	$i\tau_1$	$\boldsymbol{\sigma}_S\tau_1$	$i\boldsymbol{\sigma}_S\tau_2, i\boldsymbol{\sigma}_S\tau_3$

The possibility of unitary transformation which satisfies the condition depends on the operator structure and also the initial wave function. If the state is spin singlet or isospin singlet, we can use any σ_S or τ_I and may find some combination which satisfies the condition. However, if the states are not singlet, we cannot arbitrary transform states using σ_S and τ_I. Only available matrix which does not change the configuration would be σ_3 for non-zero spin, τ_3 for non-zero isospin state.

In some special case of initial state, which is even number of neutrons paired to spin-singlet and even number of protons paired to spin-singlet, it is possible to find an antisymmetric representation of both σ_2 and $\sigma_2\tau_3$. In such cases, all operators in the above expression would not pose sign problem. However, the exception is $i\tau_3$ and $\sigma_S\tau_3$ operators. This implies that ,in case of ^4He, $i\tau_3$ and $\sigma_S\tau_3$ operators will be the only source of sign problem. Of course, it depends on the initial states.

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[3]

$$\begin{aligned} &\boldsymbol{\sigma}_2^\dagger\boldsymbol{\sigma}_1\boldsymbol{\sigma}_2 = -\boldsymbol{\sigma}_1, \quad \boldsymbol{\sigma}_2^\dagger\boldsymbol{\sigma}_2\boldsymbol{\sigma}_2 = \boldsymbol{\sigma}_2, \quad \boldsymbol{\sigma}_2^\dagger\boldsymbol{\sigma}_3\boldsymbol{\sigma}_2 = -\boldsymbol{\sigma}_3 \\ &\boldsymbol{\sigma}_2^\dagger(\sigma_S\tau_2)\boldsymbol{\sigma}_2 = (\boldsymbol{\sigma}_S\tau_2)^*, \quad \boldsymbol{\sigma}_2^\dagger(i\boldsymbol{\sigma}_S)\boldsymbol{\sigma}_2 = (i\boldsymbol{\sigma}_S)^*, \\ &\quad \boldsymbol{\sigma}_2^\dagger(i\tau_2)\boldsymbol{\sigma}_2 = (i\tau_2)^*, \quad \boldsymbol{\sigma}_2^\dagger(i\boldsymbol{\sigma}_S\tau_1)\boldsymbol{\sigma}_2 = (i\boldsymbol{\sigma}_S\tau_1)^*, \quad \boldsymbol{\sigma}_2^\dagger(i\boldsymbol{\sigma}_S\tau_3)\boldsymbol{\sigma}_2 = (i\boldsymbol{\sigma}_S\tau_3)^* \end{aligned} \tag{7.28}$$

Chapter 8

Sign problem analysis

To check the properties of operators and their effects in sign problem, let us compute the phase factor of $\det X(s)$ for various combination of interactions.

$$\begin{aligned} M^{(n_t)}_{LP,aux}(s, s_S, s_I, s_{S,I}, \pi'_I) &= :\exp\left\{ -H_{free}\alpha_t - \frac{g_A\alpha_t}{2f_\pi\sqrt{q_\pi}} \sum_{\boldsymbol{n},S,I} \Delta_S \pi'_I(\boldsymbol{n}, n_t)\rho_{S,I}(\boldsymbol{n}) \right. \\ &\quad + \sqrt{-C\alpha_t} \sum_{\boldsymbol{n}} s(\boldsymbol{n}, n_t)\rho(\boldsymbol{n}) + i\sqrt{C_{S^2}\alpha_t} \sum_{\boldsymbol{n},S} s_S(\boldsymbol{n}, n_t)\rho_S(\boldsymbol{n}) \\ &\quad \left. + i\sqrt{C_{I^2}\alpha_t} \sum_{\boldsymbol{n},I} s_I(\boldsymbol{n}, n_t)\rho_I(\boldsymbol{n}) + i\sqrt{C_{S^2,I^2}\alpha_t} \sum_{\boldsymbol{n},S,I} s_{SI}(\boldsymbol{n}, n_t)\rho_{SI}(\boldsymbol{n}) \right\} : \end{aligned} \tag{8.1}$$

Also we add $SU(4)$ symmetric transfer matrix

$$\begin{aligned} M^{(n_t)}_4 &= :\exp[-H_4\alpha_t]:, \quad H_4 = H_{free} + \frac{1}{2}C_4 \sum_{\boldsymbol{q}} f(\boldsymbol{q}) : \rho(\boldsymbol{q})\rho(-\boldsymbol{q}) :, \quad C_4 < 0, \\ M^{(n_t)}_{4,aux}(s) &= :\exp\left\{ -H_{free}\alpha_t + \sqrt{-C_4\alpha_t} \sum_{\boldsymbol{n}} s(\boldsymbol{n}, n_t)\rho(\boldsymbol{n}) \right\} : \end{aligned} \tag{8.2}$$

Though the interpolating Hamiltonian was defined as

$$H = d_h H_{LO} + (1 - d_h)H_4, \tag{8.3}$$

all following results are for $d_h = 1$.

- all calculations are done for ^4He.
- $L = 6$, $L_t = 2 * L_{t,out} + L_{t,in}$, $L_{t,out} = 10$, $L_{t,in} = 4$, $1/a = 100$ MeV, $1/a_t = 150$ MeV.
- Only some of interactions are turned on/off by changing overall coupling strength. However, not all combinations are considered.
- we set $d_h = 1.0$.
- Here, $SU(4)$ represents the $SU(4)$ symmetric transfer matrix acting as a filter at the beginning and ending time steps. This is different from the above C_4 in interpolating Hamiltonian.

- c_0 represents the coupling $C(d_h) = d_h C + (1 - d_h)C_4$. In similar way, c_S, c_I,c_{SI} and g_A corresponds to $C_{S^2}(d_h)$, $C_{I^2}(d_h)$, $C_{S^2,I^2}(d_h)$ and $g_A(d_h)$.

$$
\begin{aligned}
&C_0 = -0.192 \times 10^{-4}, C_S = 0.4 \times 10^{-5}, C_I = 0.87 \times 10^{-5}, \\
&C_{SI} = 0.64 \times 10^{-5}, C_4 = -0.7 \times 10^{-4}, \text{ in MeV}^{-2}, \\
&g_A = 1.29
\end{aligned} \tag{8.4}
$$

Comments on results in Table.8.1 are

- When SU(4) interaction is off, the initial and final time steps would not projects to the ground state. Thus, the interaction is not strong enough and the system remains as dilute gas and binding energy does not change much from zero. Thus, the results without SU(4) interaction may not represent ground state well.
- In a similar reason, the complex phase becomes smaller without SU(4) interaction. Thus, from now on, let us consider the cases with $SU(4)$ interactions.
- To check sign problem better, it might be better to use larger $L_{t,in}$ values.
- Looking at the case with (or without) only one interaction, it seems to be the C_{SI} interaction have most important contribution to the phase.
- Looking at the case with two interactions, the main origin of phase seems to be the interference between c_{SI} and g_A. Without both c_{SI} and g_A, phase are usually small.
- The phase is very small(or zero) even when c_0, c_S, c_I, g_A interactions are on.
- The smallest value(or largest phase) occurs when only c_0 is off. It may be because c_0 interaction provides attractive $SU(4)$ interaction to the system to lessen the sign problem.

Table 8.1: Results of various couplings combinations. Index is for quick look up the result files and $L_{t,in}$ is the length of time step used in the calculation. The numbers represents the numbers multiplied to the default coupling values. Characters x, y, z represents the included isospin components in the calculation.

index	$SU(4)$	c_0	c_S	c_I	c_{SI}	g_A	$Re\langle e^{i\theta}\rangle$	B.E.	raw amplitude
full	O	O	O	O	O	O	0.922	-27.3(3)	0.641(3)
1	O	X	X	X	X	X	1.0	28.2(2)	1.46(3)
13	O	X	O	X	X	X	1.0	25.8(2)	1.41
14	O	X	X	O	X	X	1.0	21.5(2)	1.33
15	O	X	X	X	O	X	0.992	13.1(1)	1.18
16	O	X	X	X	X	O	1.0	29.8(1)	1.48
2	O	O	X	X	X	X	1.0	13.5(3)	1.20(5)
3	O	O	O	X	X	X	1.0	7.74(2)	1.11(3)
4	O	O	X	O	X	X	1.0	-0.4(3)	0.999(5)
5	O	O	X	X	O	X	0.991	-14.5(3)	0.817(4)
6	O	O	X	X	X	O	1.0	18.1(2)	1.27
29	O	X	X	X	O	O	0.951	18.6(1)	1.22
30	O	X	O	O	X	X	1.0	19.2(1)	1.29
31	O	X	O	X	O	X	0.991	7.77(9)	1.09
32	O	X	O	X	X	O	1.0	28.1(1)	1.45
33	O	X	X	O	O	X	0.989	0.1(1)	0.99
34	O	X	X	O	X	O	1.0	24.8(1)	1.39
17	O	O	O	O	X	X	1.0	-4.5(3)	0.942(5)
18	O	O	O	X	O	X	0.991	-21.6(3)	0.742(3)
19	O	O	O	X	X	O	1.0	13.6(2)	1.19
20	O	O	X	O	O	X	0.990	-31.9(3)	0.647(3)
21	O	O	X	O	X	O	0.998(1)	8.5(6)	1.12(1)
22	O	O	X	X	O	O	0.945	-5.2(3)	0.881(3)
23	O	O	O	O	O	X	0.9799	-37.7(3)	0.592(3)
24	O	O	O	O	X	O	0.998(1)	2.6(6)	1.04(1)
25	O	O	O	X	O	O	0.942	-12.2(3)	0.801(4)
26	O	O	X	O	O	O	0.938	-21.5(3)	0.704(2)
27	O	X	O	O	O	O	0.917	3.6(1)	0.96
0	X	X	X	X	X	X	1.0	0.	1.0
7	X	O	X	X	X	X	1.0	-1.58(6)	0.979(1)
8	X	X	O	X	X	X	1.0	-0.339(9)	0.955(1)
11	X	X	X	O	X	X	1.0	-0.88(1)	0.988
12	X	X	X	X	O	X	0.999	-1.65(2)	0.977
9	X	X	X	X	X	O	1.0	-0.10(1)	0.998
28	X	X	X	X	O	O	0.997	-1.63(2)	0.975
10	X	O	O	O	O	O	0.995	-5.07(7)	0.929

Table 8.2: Variation in coupling strength for ^4He

index	SU(4)	C_0	C_S	C_I	C_{SI}	g_A	$Re\langle e^{i\theta}\rangle$	B.E.
	1					3	0.586	
	1				3		0.871	
	1		3		3		0.997	
	1	3					1	
	1	1	3				1	
	1	1				3	0.369	
	1	1	3	3			0.997	
	1	1	1	1	1	$\sqrt{3}$,y	0.929	-28.3(2)
	1	1	1	1	1	$\sqrt{3}$,z	0.929	
	1	1	1	1		1	0.998	
	1	1	1	1	0.25	1	0.977	-3.8(3)
	1	1	1	1	0.5	1	0.959	-10.8(2)
	1	1	1	1	0.75	1	0.941	-18.9(2)
	1	1	1	1	1	1	0.922	-27.3(3)
	1	1	1	1	y	y	0.981	-12.3
	1	1	1	1	x	y	0.993	-13.3
	1	1	1	1	y	x	0.993	-13.5

Table 8.3: Variation in coupling strength for ^6He

index	SU(4)	C_0	C_S	C_I	C_{SI}	g_A	$Re\langle e^{i\theta}\rangle$	B.E.
	1	1					1	
	1	1	1				1	
	1	1		1,x			1	
	1	1		1,y			1	
	1	1		1,z			0.887	
	1	1	1	1,z			0.898	
	1	1	1	1,x,y			0.986	

Let us consider the cases with default interaction which gives no sign problem for ^6He. The default combination are

$$\begin{aligned} &SU(4), \quad C_0, \quad C_S i\sigma_S, \quad C_I i\tau_x, \\ &C_{SI} i\sigma_S\tau_y,\ C_{SI} i\sigma_S\tau_z, \quad g_A\sigma_S\tau_x. \end{aligned} \tag{8.5}$$

All these interactions can be simultaneously transformed to it's complex conjugate by $\sigma_2\tau_z$. Thus, these interactions does not give rise to any sign problem. Remaining interactions are

$$C_I i\tau_y,\ C_I i\tau_z,\ C_{SI} i\sigma_S\tau_x,\ g_A\sigma_S\tau_y,\ g_A\sigma_S\tau_z \tag{8.6}$$

Following table shows the effects of each terms to the complex phase of fermion determinant and binding energy for ^6He.

Table 8.4: Variation in coupling strength for ^6He

index	$C_I i\tau_y$	$C_I i\tau_z$	$C_{SI} i\sigma_S\tau_x$	$g_A\sigma_S\tau_y$	$g_A\sigma_S\tau_z$	Re$\langle e^{i\theta}\rangle$	B.E.
default						1.0	-21.2(3)
26	1					0.972	-22.2(4)
27		1				0.905	-22.0(3)
29			1			0.927	-24.3(3)
30				1		0.969	-16.2(3)
31					1	0.966	-14.9(3)
28	1	1				0.875	-24.1(3)
33	1		1			0.897	-28.3(3)
34	1			1		0.939	-17.7(3)
35	1				1	0.933	-17.0(2)
36		1	1			0.831	-27.2(4)
37		1		1		0.871	-16.7(4)
38		1			1	0.868	-16.3(3)
39			1	1		0.891	-20.0(4)
40			1		1	0.882	-18.9(3)
32				1	1	0.929	-9.8(2)
41	1	1	1			0.802	-31.6(4)
42	1	1		1		0.840	-19.3(3)
43	1	1			1	0.834	-18.8(3)
44	1		1	1		0.862	-24.5(3)
45	1		1		1	0.849	-22.6(4)
46	1			1	1	0.893	-11.5(4)
47		1	1	1		0.793	-22.9(4)
48		1	1		1	0.787	-21.9(4)
		1		1	1		
49			1	1	1	0.841	-14.7(4)
50	1	1	1	1		0.768	-27.9(5)
51	1	1	1		1	0.755	-26.5(5)
52	1	1		1	1	0.794	-13.7(4)
53	1		1	1	1	0.808	-19.5(4)
54		1	1	1	1	0.743	-17.4(5)
full	1	1	1	1	1	0.714	-23.0(4)

Chapter 9

Extrapolation

There are two extrapolation we are considering. One is the Euclidean time extrapolation, $T \to \infty$ and the other is the sign extrapolation with some parameter $d \to 1$. Let us consider sign extrapolation as

$$H(d) = H_0 + dH_1 + (1-d)H' \tag{9.1}$$

where H' is additional auxiliary interaction which may help the convergence and have some parameter C_4 and $H_0 + H_1$ is the original full Hamiltonian. Thus, at a finite time interval, the resulting energy will depends on N_t, C_4, d and we will take a limit to extract physical values

$$E_0 = \lim_{N_t \to \infty, d \to 1} E(N_t, C_4, d) \tag{9.2}$$

For the time extrapolation we will use following equation, (T. A. Lahde et.al. J. Phys. G: Nucl. Part. Phys.42(2015)034012)

$$E_A^j(N_t) = E_{A,0} + \sum_{k=1}^{k_{max}} |c_{A,j,k}| \exp\left(-\frac{\Delta_{A,k} N_t}{\Lambda_t}\right) \tag{9.3}$$

where, $t = N_t/\Lambda_t$, $\Delta_{A,k} = E_{A,k} - E_{A,0}$ and the index j denotes all different choices of environments(For example, the introduction of additional interaction $e^{H_4 t'}$ for faster ground state projection introduces dependence on t' and H_4). We require $E_{A,0}$ and $\Delta_{A,k}$ does not depends on the N_t or j.

On the other hand, sign extrapolation was done with

$$X(d_h, C_4) = X_0 + X_0^{SU(4)}(1-d_h) + \sum_{j=1}^{n} X_j^{SU(4)} \sin(j\pi d_h). \tag{9.4}$$

where $X_{0,j}^{SU(4)}$ are dependent on $SU(4)$ interaction. The form allows oscillation. And it satisfies the property at $d_h \to 1$ limit and $d_h \to 0$ limits.

Then, how we should use extrapolation? One possibility is to fit globally using all data with different N_t, d_h values but while keeping one fixed auxiliary interactions,

$$E(N_t, d_h) = E_0 + \tag{9.5}$$

Chapter 10

Explicit example?

Let us consider two nucleon system in 1-D lattice size $L = 3$ with external delta function potential at 0(this is not inter particle interaction)

$$M =: \exp\left[-H_{free}\alpha_t - C\alpha_t\rho_\uparrow(0)\right] : \tag{10.1}$$

for two nucleon state, $|k,\uparrow;k',\downarrow\rangle$,

$$M_{free}|k,\uparrow;k',\downarrow\rangle = e^{-E(k)\alpha_t}e^{-E(k')\alpha_t}|k,\uparrow;k',\downarrow\rangle \tag{10.2}$$

There are three lattice points $0,1,2$ and three momentum eigen states $|p_0\rangle, |p_1\rangle, |p_2\rangle$. Let us use single particle wave function as column vectors

$$\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = a^\dagger(0)|0\rangle, \quad \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = a^\dagger(1)|0\rangle, \quad \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = a^\dagger(2)|0\rangle. \tag{10.3}$$

This implies that we can express a momentum eigenstate as

$$|p\rangle = a_p^\dagger|0\rangle \propto \sum_{x_n} a^\dagger(x_n)e^{-ip\cdot x_n}|0\rangle = \begin{pmatrix} e^{-ip\cdot x_0} \\ e^{-ip\cdot x_1} \\ e^{-ip\cdot x_2} \end{pmatrix} \tag{10.4}$$

(For example, zero momentum state becomes $(1,1,1)^T$)

For a single particle state, one only needs linear expansion of transfer matrix, (note that this expression is only correct for single particle state)

$$\begin{aligned} M \quad \simeq \quad & 1 + \frac{\alpha_t}{2m}[a_\uparrow^\dagger(1)a_\uparrow(0) + a_\uparrow^\dagger(0)a_\uparrow(1) - 2a_\uparrow^\dagger(0)a_\uparrow(0)] \\ & + \frac{\alpha_t}{2m}[a_\uparrow^\dagger(2)a_\uparrow(1) + a_\uparrow^\dagger(1)a_\uparrow(2) - 2a_\uparrow^\dagger(1)a_\uparrow(1)] \\ & + \frac{\alpha_t}{2m}[a_\uparrow^\dagger(0)a_\uparrow(2) + a_\uparrow^\dagger(2)a_\uparrow(0) - 2a_\uparrow^\dagger(2)a_\uparrow(2)] \\ & - C\alpha_t a_\uparrow^\dagger(0)a_\uparrow(0) \end{aligned} \tag{10.5}$$

Then, we can express M as

$$M = \begin{pmatrix} 1 - \frac{\alpha_t}{m} - C\alpha_t & \frac{\alpha_t}{2m} & \frac{\alpha_t}{2m} \\ \frac{\alpha_t}{2m} & 1 - \frac{\alpha_t}{m} & \frac{\alpha_t}{2m} \\ \frac{\alpha_t}{2m} & \frac{\alpha_t}{2m} & 1 - \frac{\alpha_t}{m} \end{pmatrix} \tag{10.6}$$

For example, for the eigen-state of $p_1 = \frac{2\pi}{3}$

$$\begin{aligned} |p_1\rangle &= \begin{pmatrix} 1 \\ e^{-i\frac{2\pi}{3}} \\ e^{-i\frac{4\pi}{3}} \end{pmatrix} = \begin{pmatrix} 1 \\ -\frac{1}{2} - i\frac{\sqrt{3}}{2} \\ -\frac{1}{2} + i\frac{\sqrt{3}}{2} \end{pmatrix} \\ M_{free}|p_1\rangle &\sim e^{-E(p_1)\alpha_t}|p_1\rangle \end{aligned} \tag{10.7}$$

Let us consider two-nucleon states with zero center of mass momentum and consider zero-range two-nucleon interaction.

$$M =: \exp\left[-H_{free}\alpha_t - C\alpha_t \sum_{n=0}^{L-1} \rho_\uparrow(n)\rho_\downarrow(n)\right] : \tag{10.8}$$

For a zero-center of mass momentum state, with $L = 3$, we may have three different relative momentum states, (Note this represent different states from above example)

$$\begin{aligned} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} &= \frac{1}{\sqrt{3}}\left[a_\uparrow^\dagger(0)a_\downarrow^\dagger(0) + a_\uparrow^\dagger(1)a_\downarrow^\dagger(1) + a_\uparrow^\dagger(2)a_\downarrow^\dagger(2)\right]|0\rangle, \\ \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} &= \frac{1}{\sqrt{3}}\left[a_\uparrow^\dagger(1)a_\downarrow^\dagger(0) + a_\uparrow^\dagger(2)a_\downarrow^\dagger(1) + a_\uparrow^\dagger(3)a_\downarrow^\dagger(2)\right]|0\rangle, \\ \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} &= \frac{1}{\sqrt{3}}\left[a_\uparrow^\dagger(2)a_\downarrow^\dagger(0) + a_\uparrow^\dagger(0)a_\downarrow^\dagger(1) + a_\uparrow^\dagger(1)a_\downarrow^\dagger(2)\right]|0\rangle. \end{aligned} \tag{10.9}$$

expansion of M

$$\begin{aligned} M &= [1 + \frac{\alpha_t}{2m}\sum_{n=0}^{2}[a_\uparrow^\dagger(n+1)a_\uparrow(n) + a_\uparrow^\dagger(n)a_\uparrow(n+1) - 2a_\uparrow^\dagger(n)a_\uparrow(n)]] \times [\uparrow\leftrightarrow\downarrow] \\ &\quad -C\alpha_t \sum_{n=0}^{2} a_\uparrow^\dagger(n)a_\uparrow(n)a_\downarrow^\dagger(n)a_\downarrow(n) + (\text{ terms that vanish in this space }) \end{aligned} \tag{10.10}$$

Considering action of each operators on two nucleon states, we get

$$\begin{aligned} M &\to \begin{pmatrix} 1 - \frac{\alpha_t}{m} - C\alpha_t & \frac{\alpha_t}{2m} & \frac{\alpha_t}{2m} \\ \frac{\alpha_t}{2m} & 1 - \frac{\alpha_t}{m} & \frac{\alpha_t}{2m} \\ \frac{\alpha_t}{2m} & \frac{\alpha_t}{2m} & 1 - \frac{\alpha_t}{m} \end{pmatrix} \begin{pmatrix} 1 - \frac{\alpha_t}{m} - C\alpha_t & \frac{\alpha_t}{2m} & \frac{\alpha_t}{2m} \\ \frac{\alpha_t}{2m} & 1 - \frac{\alpha_t}{m} & \frac{\alpha_t}{2m} \\ \frac{\alpha_t}{2m} & \frac{\alpha_t}{2m} & 1 - \frac{\alpha_t}{m} \end{pmatrix} + \begin{pmatrix} -C\alpha_t & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} A - C\alpha_t & B & B \\ B & A & B \\ B & B & A \end{pmatrix} \end{aligned} \tag{10.11}$$

where

$$A = 1 - 2\frac{\alpha_t}{m} + \frac{3\alpha_t^2}{2m^2}, \quad B = \frac{\alpha_t}{m} - \frac{3\alpha_t}{4m^2}. \tag{10.12}$$

Then, one can obtain exact solution by solving the eigenvalue equation of M. (eigen-solution will be a linear combination of two-nucleon free states).

Note that above three states are not eigen-state of M_{free}. For example, one of the eigen-state is $(1,1,1)^T$ which corresponds to $|p_0,\uparrow\rangle \times |p_0,\downarrow\rangle$ which have zero relative momentum,

$$|p_0,\uparrow\rangle \times |p_0,\downarrow\rangle = \left(a^\dagger(0) + a^\dagger(1) + a^\dagger(2)\right)_\uparrow \left(a^\dagger(0) + a^\dagger(1) + a^\dagger(2)\right)_\downarrow |0\rangle \tag{10.13}$$

In fact, relative energy without interaction can be obtained as

$$E_{rel} = A + 2B\cos(\frac{2\pi}{N}k) \tag{10.14}$$

In fact, one can determine the phase-shift with finite range interaction from energy level.

In case of 1-D continuum with periodic boundary condition, in center of mass frame of two nucleon. Suppose interaction is parity symmetric. If there is no interaction, even parity wave function will be in the form of $\cos(px)$. If interaction is introduced, the wave function at long distance will change into $\cos(px+\delta_0(p))$. From the periodic condition, $\psi(L/2) = \psi(-L/2)$ and $\psi'(L/2) = \psi'(-L/2) = 0$, we get $\sin(p\frac{L}{2} + \delta_0(p)) = 0$. In other words, the phase shift can be a function of momentum as $\delta_0(p) = -p\frac{L}{2} + n\pi$.

In odd parity case, free wave function is $\sin(px)$ and will be shifted by interaction as $\sin(px+\delta_1(p))$. Periodic boundary condition, $\psi(L/2) = \psi(-L/2) = -\psi(-L/2) = 0$. Thus, $\sin(p\frac{L}{2} + \delta_1(p)) = 0$ and $\delta_1(p) = -p\frac{L}{2} + n\pi$. Thus, if one obtain energy eigenvalue, one can obtain phase shifts.

In a similar way, if one introduce wall interaction between two nucleons such that $\psi(R_{wall}) = 0$ (L must be larger than wall radius, $L > 2R_{wall}$). we can obtain relation with phase shift as

$$\begin{aligned} \cos(pR_{wall} + \delta_0(p)) = 0 \rightarrow \delta_0(p) = -pR_{wall} + (n + \frac{1}{2})\pi, \quad \text{even parity,} \\ \sin(pR_{wall} + \delta_1(p)) = 0 \rightarrow \delta_1(p) = -pR_{wall} + n\pi, \quad \text{odd parity.} \end{aligned} \tag{10.15}$$

Note that p will be a function of L or R_{wall}.

This is the basic of Lusher's method and wall boundary method.

Chapter 11

Pinhole algorithm