Lattice Methods for Nuclear Physics

Lecture 3: Auxiliary Fields and Projection Monte Carlo

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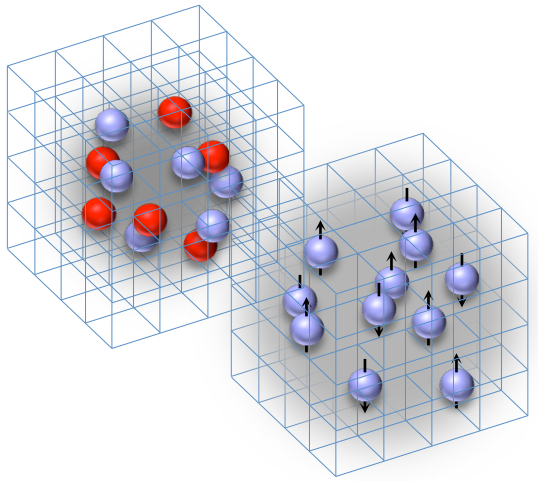
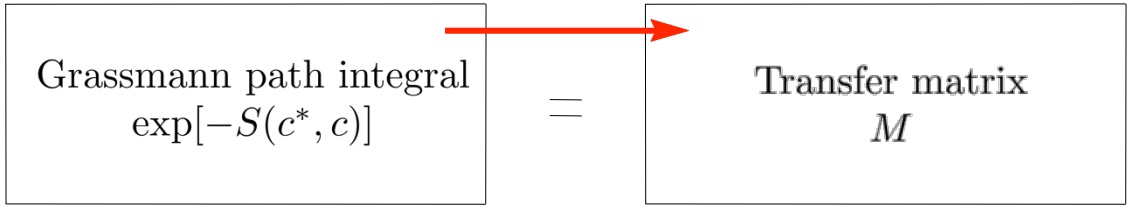


Auxiliary fields

In the first lecture we proved the exact equivalence between the Grassmann path integral and transfer matrix operator formalisms.



For our example of two-component fermions with zero-range interactions, we had found that

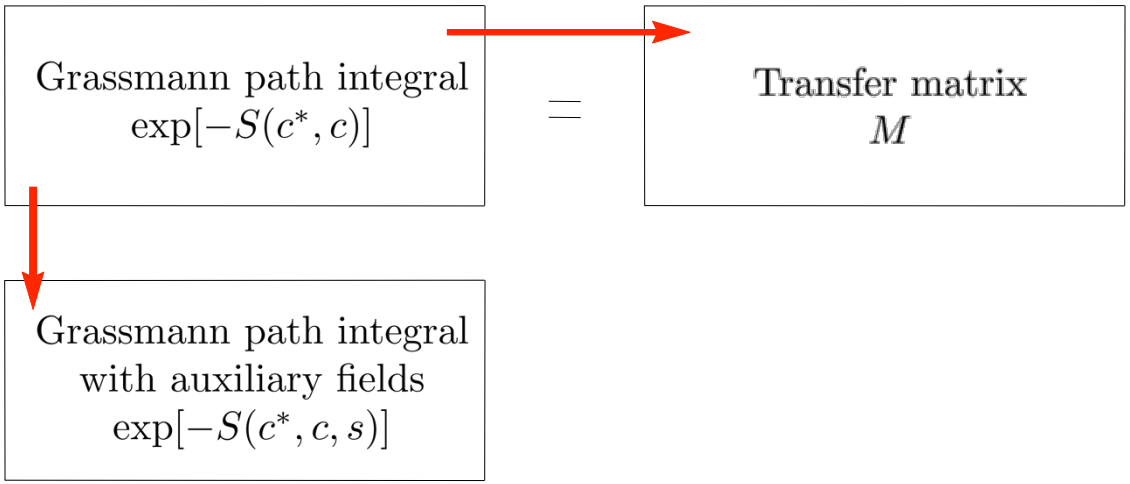
$$\mathcal{Z} = \int DcDc^* \exp\left[-S\left(c^*, c\right)\right] = Tr\left(M^{L_t}\right)$$

where

$$S(c^*, c) = S_{\text{free}}(c^*, c) + C\alpha_t \sum_{\vec{n}, n_t} \rho_{\uparrow}^{c^*,c}(\vec{n}, n_t)\rho_{\downarrow}^{c^*,c}(\vec{n}, n_t).$$

$$M =: \exp\left[-H_{\text{free}}\alpha_t - C\alpha_t \sum_{\vec{n}} \rho_{\uparrow}(\vec{n})\rho_{\downarrow}(\vec{n})\right] :$$

We now show the exact equivalence between the Grassmann path integral and the Grassmann path integral with auxiliary fields



Grassmann path integral with auxiliary fields

We can rewrite the same lattice Grassmann path integral using an auxiliary field

$$\mathcal{Z} = \prod_{\vec{n},n_t} \left[\int d_A s(\vec{n},n_t)\right] \int DcDc^* \exp\left[-S_A\left(c^*,c,s\right)\right]$$

$$S_A\left(c^*,c,s\right) = S_{\text{free}}(c^*,c) - \sum\nolimits_{\vec{n},n_t} A\left[s(\vec{n},n_t)\right] \rho^{c^*,c}(\vec{n},n_t)$$

There are many ways to introduce the auxiliary-field integral measure and coupling. The simplest is a Gaussian measure and linear coupling corresponding with the original Hubbard-Stratonovich transformation

$$\int d_A s(\vec{n},n_t) \to \tfrac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} ds(\vec{n},n_t) e^{-\frac{1}{2}s^2(\vec{n},n_t)}$$

$$A\left[s(\vec{n},n_t)\right] \to \sqrt{-C\alpha_t}\, s(\vec{n},n_t).$$

But there are many choices. The only requirements for exact equivalence are that

$$\int d_A s(\vec{n}, n_t) 1 = 1$$

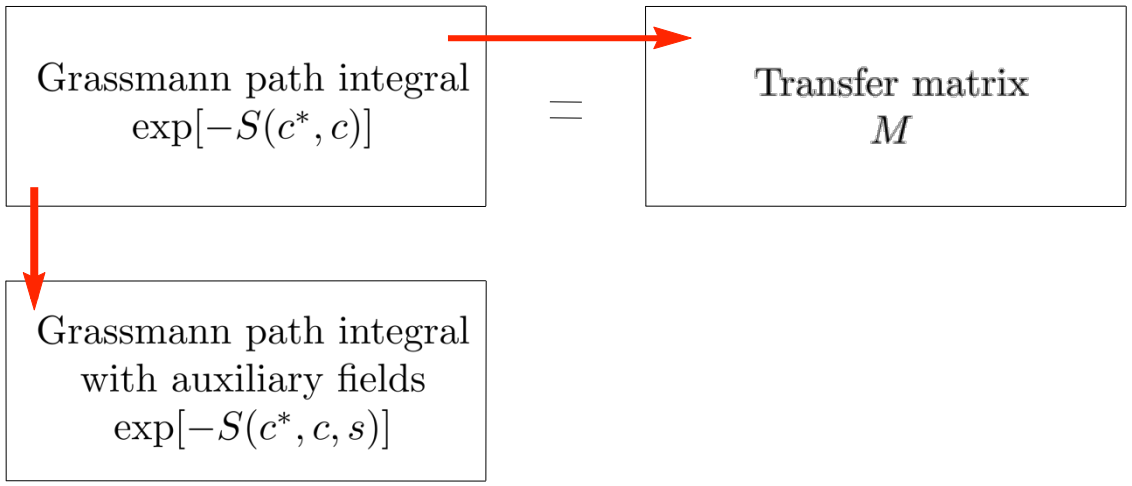
$$\int d_A s(\vec{n}, n_t)\, A\left[s(\vec{n}, n_t)\right] = 0$$

$$\int d_A s(\vec{n}, n_t)\, A^2\left[s(\vec{n}, n_t)\right] = -C\alpha_t$$

This can be used to derive several varieties of the discrete Hubbard-Stratonovich transformation as well as compact continuous auxiliary field transformations.

D.L., PRC 78 (2008) 024001;
Drut, Lähde, Ten, PRL 106 (2011) 205302

This demonstrates the exact equivalence of the following three lattice formulations for arbitrary lattice spacings:



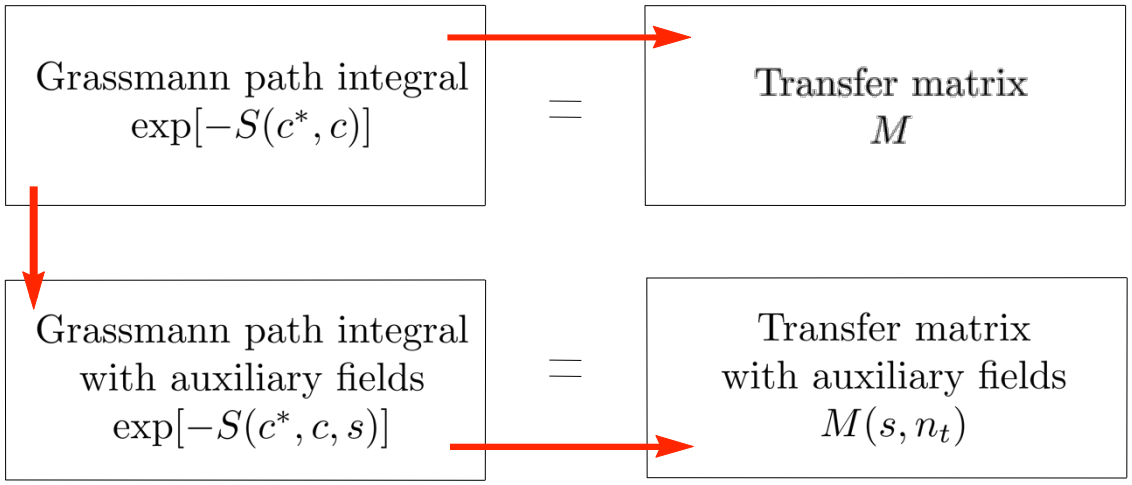
Transfer matrix operator with auxiliary fields

We use the equivalence of the Grassmann path integral and normal-ordered transfer matrix and apply it to the case of the auxiliary-field Grassmann path integral. We find

$$\mathcal{Z} = \prod_{\vec{n},n_t} \left[\int d_A s(\vec{n},n_t)\right] Tr\left\{M_A(s,L_t-1)\cdot\cdots\cdot M_A(s,0)\right\}$$

$$M_A(s,n_t) =: \exp\left\{-H_{\text{free}}\alpha_t + \textstyle\sum_{\vec{n}} A\left[s(\vec{n},n_t)\right]\rho(\vec{n})\right\}:$$

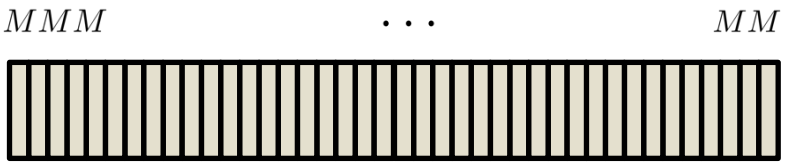
This shows the exact equivalence of the following four lattice formulations for arbitrary lattice spacings:



Projection Monte Carlo with auxiliary fields

Let us consider a system with A particles. The idea of projection Monte Carlo is to choose a given initial and final state. Very often they are chosen to be the same state. The initial and final state will sandwich a product of a string of transfer matrices. Pictorially the amplitude looks like this:

$$Z(L_t) = \langle \psi_{\rm init} |$$



$$| \psi_{\rm init} \rangle$$

Using auxiliary fields, we have

$$Z(L_t) = \prod_{\vec{n},n_t} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} ds(\vec{n},n_t) e^{-\frac{1}{2}s^2(\vec{n},n_t)} \right] Z(s,L_t)$$

where the auxiliary field amplitude is

$$Z(s, L_t) = \langle \psi_{\text{init}} | \underbrace{\qquad\qquad}_{M(s,L_t-1)M(s,L_t-2) \quad \cdots \quad M(s,1)M(s,0)} | \psi_{\text{init}} \rangle$$

For sufficiently large L_t the amplitude $Z(L_t)$ will be dominated by the ground state of our quantum system in the sector which is not orthogonal to our initial state. We will see the largest eigenvalue of the transfer matrix M, which we use to extract the corresponding ground state energy E_0

$$\lim_{L_t \to +\infty} Z(L_t)/Z(L_t - 1) = \lambda_{\max} = e^{-E_0 \alpha_t}$$

To make the discussion concrete, we continue on with our example of two-component fermions with zero-range interactions.

We can create a general single-particle state on the lattice with a creation operator multiplying a coefficient function f that depends on the spatial lattice sites and spin component i.

$$|f\rangle = \sum_{\vec{n},i} a_i^\dagger(\vec{n}) f(\vec{n},i)\,|0\rangle$$

For our projection Monte Carlo calculation we take our A-body initial state as an operator product

$$|\psi_{\rm init}\rangle = |f_1,\cdots,f_A\rangle = \left[\sum_{\vec{n},i} a_i^\dagger(\vec{n}) f_1(\vec{n},i)\right]\cdots\left[\sum_{\vec{n},i} a_i^\dagger(\vec{n}) f_A(\vec{n},i)\right]|0\rangle$$

For the purposes of coding the projection Monte Carlo calculation, it is convenient to view the identical nucleons as carrying a fictitious label $[j] = [1], \cdots, [A]$ that makes all of the particles distinguishable.

$$a_i(\vec{n}), a_i^\dagger(\vec{n}) \rightarrow a_{i,[j]}(\vec{n}), a_{i,[j]}^\dagger(\vec{n})$$

We will sum over all possible assignments of these operator labels and the anticommuting algebra of the operators will give the proper antisymmetry as required.

With these hidden labels our A-body initial state is

$$|\psi_{\rm init}\rangle = |f_1, \cdots, f_A\rangle$$
$$\rightarrow \tfrac{1}{\sqrt{A!}} \sum_P \left[\sum_{\vec{n},i} a^\dagger_{i,[P(1)]}(\vec{n}) f_1(\vec{n},i)\right] \cdots \left[\sum_{\vec{n},i} a^\dagger_{i,[P(A)]}(\vec{n}) f_A(\vec{n},i)\right] |0\rangle$$
$$= \tfrac{1}{\sqrt{A!}} \sum_{P'} {\rm sgn}(P') \left[\sum_{\vec{n},i} a^\dagger_{i,[1]}(\vec{n}) f_{P'(1)}(\vec{n},i)\right] \cdots \left[\sum_{\vec{n},i} a^\dagger_{i,[A]}(\vec{n}) f_{P'(A)}(\vec{n},i)\right] |0\rangle$$

where the summations are over all permutations, and sgn is the sign of the permutation. In the last line we get the usual Slater determinant wave function.

With these hidden indices our normal-ordered auxiliary-field transfer matrix at time step n_t can be written as

$$M(s,n_t) \rightarrow \left[1 - H_{\rm free,[1]}\alpha_t + \sum_{\vec{n}} \sqrt{-C\alpha_t} s(\vec{n},n_t)\rho_{[1]}(\vec{n})\right] \cdots$$
$$\cdots \left[1 - H_{\rm free,[A]}\alpha_t + \sum_{\vec{n}} \sqrt{-C\alpha_t} s(\vec{n},n_t)\rho_{[A]}(\vec{n})\right]$$

All other terms coming from higher powers coming from the exponential will vanish due to the normal ordering. This is because we have only one particle carrying each fictitious label $[j] = [1], \cdots, [A]$.

In the projection Monte Carlo calculation we compute the amplitude

$$Z(s, L_t) = \langle f_1, \cdots, f_A | \, M(s, L_t - 1) \cdots M(s, 0) \, | f_1, \cdots, f_A \rangle$$

for each configuration of the auxiliary field s. We note that this A-body amplitude is just the determinant of the matrix of single nucleon amplitudes

$$Z(s, L_t) = \det \mathbf{Z}(s, L_t)$$

$$\mathbf{Z}_{i,j}(s, L_t) = \langle f_i | \, M(s, L_t - 1) \cdots M(s, 0) \, | f_j \rangle$$

In summary, we want to compute the following ratio for large L_t:

$$\lim_{L_t \to +\infty} Z(L_t)/Z(L_t - 1) = \lambda_{\max} = e^{-E_0 \alpha_t}$$

Since we usually write the observable for our Markov chain in the numerator rather than the denominator, we will work with reciprocal of this ratio and calculate using auxiliary fields

$$\frac{Z(L_t - 1)}{Z(Lt)} = \frac{\prod_{\vec{n}, n_t} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} ds(\vec{n}, n_t) e^{-\frac{1}{2} s^2(\vec{n}, n_t)} \right] Z(s, L_t - 1)}{\prod_{\vec{n}, n_t} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} ds(\vec{n}, n_t) e^{-\frac{1}{2} s^2(\vec{n}, n_t)} \right] Z(s, L_t)}$$

where the auxiliary field amplitudes are

$$Z(s, L_t - 1) = \det \mathbf{Z}(s, L_t - 1)$$

$$Z(s, L_t) = \det \mathbf{Z}(s, L_t)$$

$$\mathbf{Z}_{i,j}(s, L_t - 1) = \langle f_i | \, M(s, L_t - 2) \cdots M(s, 0) \, | f_j \rangle$$

$$\mathbf{Z}_{i,j}(s, L_t) = \langle f_i | \, M(s, L_t - 1) \cdots M(s, 0) \, | f_j \rangle$$

In order to compute this using a Markov chain process, the updating of the auxiliary field is done most efficiently if you store the set of vectors for each single-particle initial state at each time step

$$|v_j(s, n_t)\rangle = M(s, n_t - 1) \cdots M(s, 0) | f_j \rangle$$

as well as the dual vectors at each time step propagating in the reverse temporal direction

$$\langle v_j(s, n_t)| = \langle f_i | M(s, L_t - 1) \cdots M(s, n_t)$$

So now if we need to compute the update to an auxiliary field value at time step n_t, we have an easy way to compute the change in the amplitude

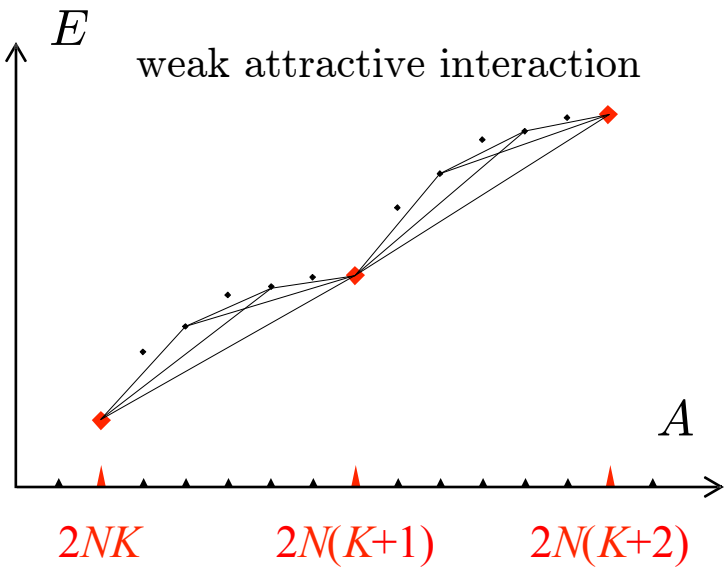
$$\mathbf{Z}_{i,j}(L_t) = \langle v_i(s, n_t + 1)|M(s, n_t)|v_j(s, n_t)\rangle$$

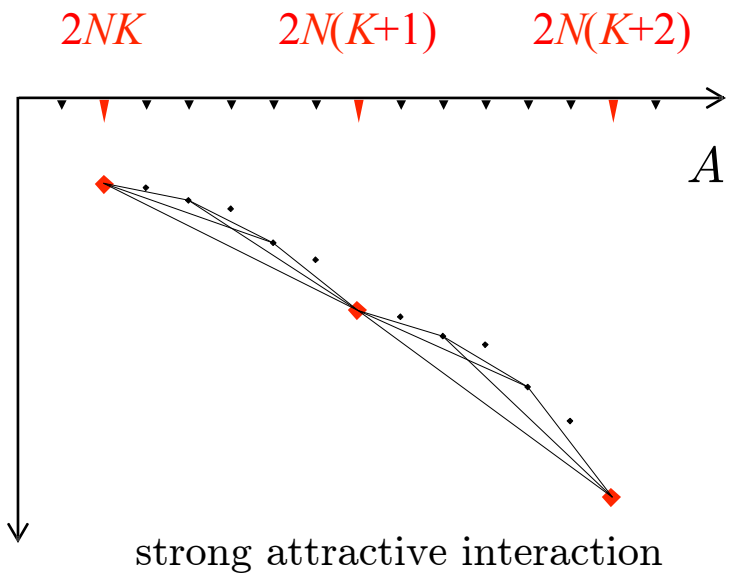
change here and re-evaluate

Theorem: Any fermionic theory with SU($2N$) symmetry and two-body potential energy that has a negative semi-definite Fourier transform obeys SU($2N$) convexity bounds.

Corollary: The system can be simulated without sign oscillations

Chen, D.L. Schäfer, PRL 93 (2004) 242302;
D.L., PRL 98 (2007) 182501





There are $2N$ species of fermions. Let the interaction have the form

$$\frac{1}{2}\sum_{\vec{n},\vec{m}} \rho(\vec{n})V(\vec{n}-\vec{m})\rho(\vec{m})$$

Where ρ is total density of particles summed over all $2N$ species. We compute the amplitude by coupling an auxiliary field s to the total density

$$M(s,n_t) =: \exp\left\{-H_{\text{free}}\alpha_t + \sum_{\vec{n}} s(\vec{n},n_t)\rho(\vec{n})\right\}:$$

in our auxiliary field transfer matrix. More details on the next slide.

The amplitude we calculate is

$$Z(L_t) = \langle f_1, \cdots, f_A | \, M^{L_t} \, | f_1, \cdots, f_A \rangle$$

Using the auxiliary field formalism, we compute the following path integral over auxiliary fields

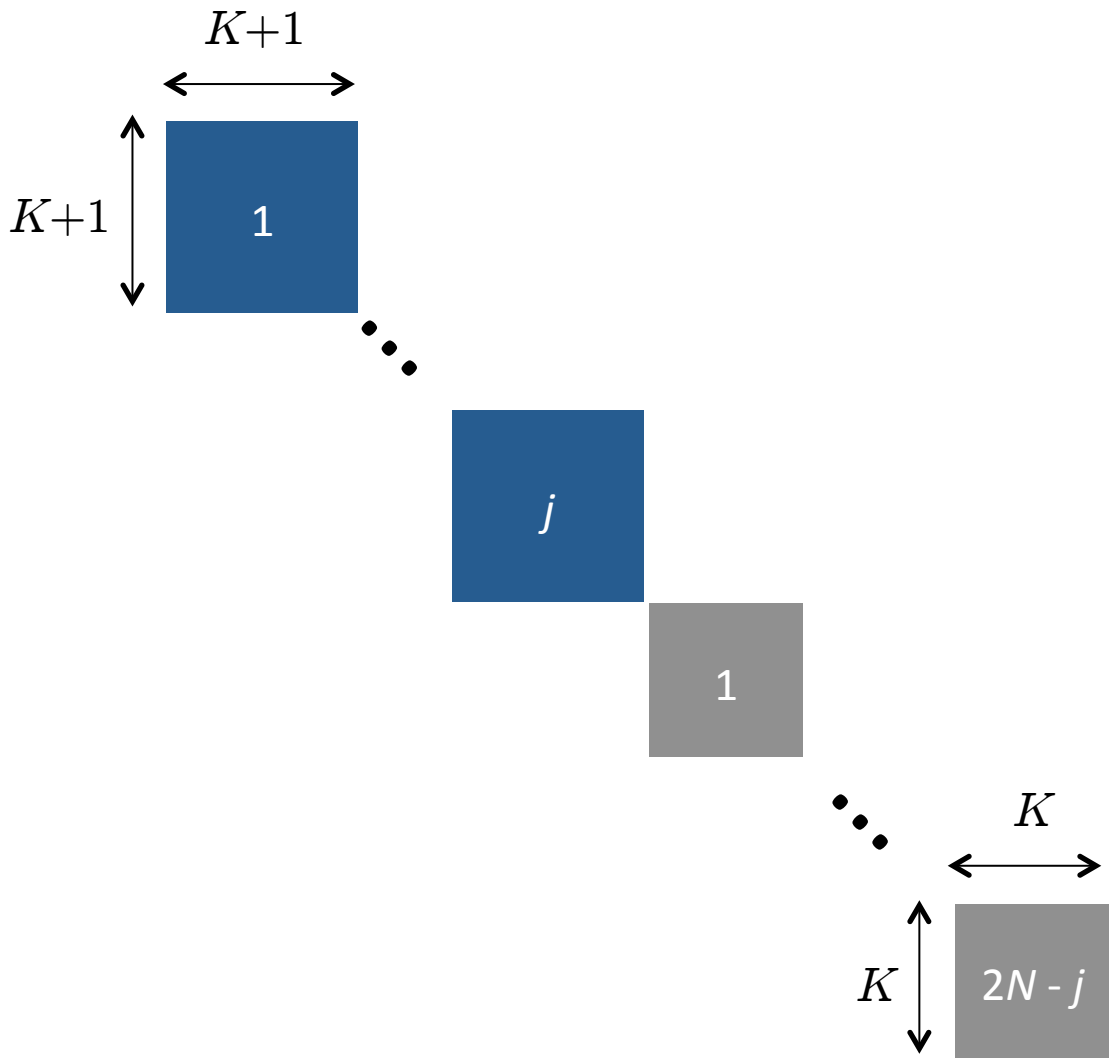
$$\int Ds \; e^{-S(s)} \; \det \mathbf{Z}(s, L_t)$$

$$S(s) = \frac{\alpha_t}{2} \sum_{n_t} \sum_{\vec{n}, \vec{n}'} s(\vec{n}, n_t) V^{-1}(\vec{n} - \vec{n}') s(\vec{n}', n_t)$$

$$\mathbf{Z}_{i,j}(s, L_t) = \langle f_i | \, M(s, L_t - 1) \cdots M(s, 0) \, | f_j \rangle$$

where V^{-1} is the inverse of the potential, computed by Fourier transformation to momentum space, taking the reciprocal in momentum space, and the reverse Fourier transformation back to coordinate space.

We choose an initial state with j species each with $K+1$ particles and $2N-j$ species each with K particles. The matrix has the following block diagonal structure



The path integral over auxiliary fields is then

$$Z_{j,K+1;2N-j,K} = \int Ds\; e^{-S(s)}\; \left[\det \mathbf{Z}_{(K+1)\times(K+1)}(s)\right]^{j} \left[\det \mathbf{Z}_{K\times K}(s)\right]^{2N-j}$$

The Hölder inequality states that for any positive p, q satisfying

$$1/p + 1/q = 1$$

we must have

$$\int dx\; |f(x)g(x)| \leq \left[\int dx\; |f(x)|^{p}\right]^{1/p} \times \left[\int dx\; |g(x)|^{q}\right]^{1/q}$$

Let n_1 and n_2 be integers such that $0 \leq 2n_1 < j < 2n_2$. We now apply the Hölder inequality with

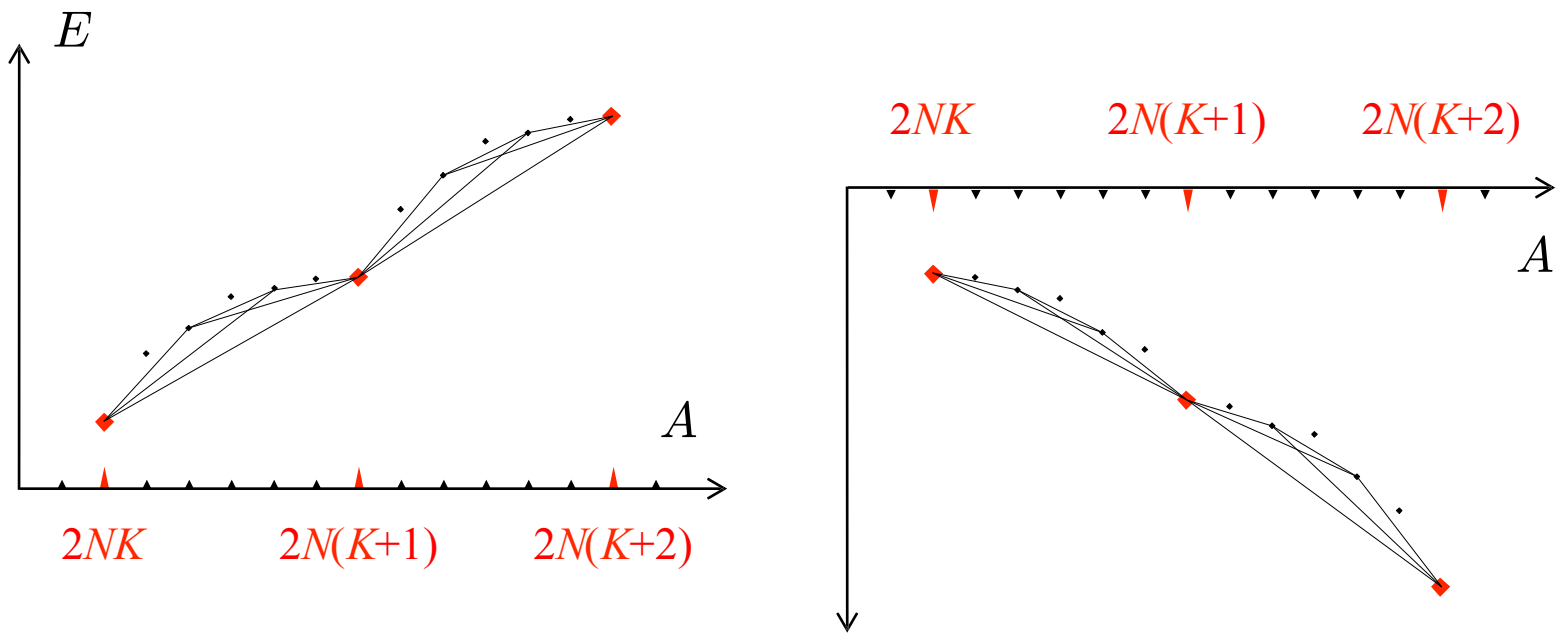
$$p = \frac{2n_2 - 2n_1}{j - 2n_1}, \quad q = \frac{2n_2 - 2n_1}{2n_2 - j}$$

This leads to an inequality for the path integrals for systems with different numbers of particles

$$Z_{j,K+1;2N-j,K} \leq \left[Z_{2n_2,K+1;2N-n_2,K}\right]^{\frac{j-2n_1}{2n_2-2n_1}} \times \left[Z_{2n_1,K+1;2N-n_1,K}\right]^{\frac{2n_2-j}{2n_2-2n_1}}$$

We now take the limit of large Euclidean time and derive convexity bounds for the ground state energies of the various systems with different numbers of particles.

$$E^0_{j,K+1;2N-j,K} \geq \frac{j-2n_1}{2n_2-2n_1} E^0_{2n_2,K+1;2N-n_2,K} + \frac{2n_2-j}{2n_2-2n_1} E^0_{2n_1,K+1;2N-n_1,K}$$



For similar convexity bounds applied to entanglement entropy bounds:

Drut, Porter, PRL 114, 050402 (2015)