UNIVERSITÄT BONN

JÜLICH FORSCHUNGSZENTRUM

From Quarks and Gluons to Nuclear Forces and Structure

Lecture 4: Fermions & Computers

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Fermions and Computers–why can't they get along?

- Fermions obey anti-commutation relations:

$$\{a_\lambda, a_\mu^\dagger\} = \delta_{\lambda,\mu} \ .$$

- Bosons, on the other hand, *commute*:

$$[a_\lambda, a_\mu^\dagger] = \delta_{\lambda,\mu} \ .$$

  - Fortunately, regular c-numbers also commute!
  - So we can represent bosonic fields with c-numbers.
- But we can calculate slater determinants, or explicitly anti-symmetrize fermionic wavefuntions, etc . . . But this hits the "Curse of Dimensionality"
- Calculations in a thermal bath: Grand-Canonical ensemble: Particle number not conserved (in principle infinite)

Let's first talk about bosonic states

Bosonic case:

$$[a_\lambda, a^\dagger_\mu] = \delta_{\lambda,\mu}, \quad [a_\lambda, a_\mu] = [a^\dagger_\lambda, a^\dagger_\mu] = 0 \,.$$

$$a^\dagger_j|0\rangle = |j\rangle \qquad (j \text{ is combined index for all degrees of freedom})$$

$$a_j|j\rangle = |0\rangle \qquad (|0\rangle \text{ is the "vacuum state"})$$

$$(a^\dagger_j)^n|0\rangle = |n_j\rangle \qquad (n\text{- particles each w/ } j \text{ quantum number(s)})$$

Application of $a^\dagger$ or a moves you throughout the *Fock* space:

$$\mathcal{F} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \cdots \mathcal{H}_{\Lambda_{max}}$$

$a^\dagger$ or a provide a basis for all operators in the Fock space

$\Longrightarrow$ can define states that span entire Fock space!

Bosonic coherent state

$$|\phi\rangle \equiv e^{\sum_i \phi_i a_i^\dagger}|0\rangle \quad \forall\ \phi_i \in \mathbb{C}$$

$$\begin{aligned}
&= \sum_{n_1, n_2, \ldots} \frac{(\phi_1 a_1^\dagger)^{n_1}}{n_1!} \frac{(\phi_2 a_2^\dagger)^{n_2}}{n_2!} \cdots |0\rangle \\
a_1|\phi\rangle &= \sum_{n_1, n_2, \ldots} \frac{a_1(\phi_1 a_1^\dagger)^{n_1}}{n_1!} \frac{(\phi_2 a_2^\dagger)^{n_2}}{n_2!} \cdots |0\rangle \\
&= \phi_1 \sum_{n_1', n_2, \ldots} \frac{(\phi_1 a_1^\dagger)^{n_1'}}{n_1'!} \frac{(\phi_2 a_2^\dagger)^{n_2}}{n_2!} \cdots |0\rangle \\
&= \phi_1|\phi\rangle \qquad \text{(similarly for } \langle\phi|a_k^\dagger = \langle\phi|\phi_k^*)
\end{aligned}$$

In general, $a_i|\phi\rangle = \phi_i|\phi\rangle \implies |\phi\rangle$ is an eigenstate of a_i w/ eigenvalue ϕ_i.

Note: $[a_i, a_j]|\phi\rangle = 0 \implies [\phi_i, \phi_j] = 0$. No problem since $\phi_{i,j} \in \mathbb{C}$!

Other properties of the Bosonic coherent state

- $|\phi\rangle$ clearly spans the enitire Fock space
- Has closure relation

$$1 = \int_{-\infty}^{\infty}\left[\prod_j \frac{d\phi_j^* d\phi_j}{2\pi i}\right] e^{\sum_k \phi_k^* \phi_k} |\phi\rangle\langle\phi|$$

$$= 1_0 \otimes 1_1 \otimes 1_2 \otimes \cdots \otimes 1_{\Lambda_{max}} \qquad \text{(overcomplete)}$$

- Overlap of two coherent states:

$$\langle\psi|\phi\rangle = e^{\sum_i \psi_i^* \phi_i} \neq 0$$

- Matrix element of *normal-ordered* operator

$$\langle\psi|a_k^\dagger a_j|\phi\rangle = \psi_k^*\phi_j\langle\psi|\phi\rangle = \psi_k^*\phi_j e^{\sum_i \psi_i^* \phi_i}$$

$$\langle\psi| : f(a_k^\dagger, a_j) : |\phi\rangle = f(\psi_k^*, \phi_j) e^{\sum_i \psi_i^* \phi_i}$$

Trace of an operator A

$$
\begin{aligned}
\mathrm{tr}A \equiv \sum_n \langle n|A|n\rangle &= \sum_n \int_{-\infty}^{\infty} \left[\prod_j \frac{d\phi_j^* d\phi_j}{2\pi i}\right] e^{\sum_k \phi_k^* \phi_k} \langle n|\phi\rangle\langle\phi|A|n\rangle \\
&= \int_{-\infty}^{\infty} \left[\prod_j \frac{d\phi_j^* d\phi_j}{2\pi i}\right] e^{\sum_k \phi_k^* \phi_k} \sum_n \langle\phi|A|n\rangle\langle n|\phi\rangle \\
&= \int_{-\infty}^{\infty} \left[\prod_j \frac{d\phi_j^* d\phi_j}{2\pi i}\right] e^{\sum_k \phi_k^* \phi_k} \langle\phi|A|\phi\rangle
\end{aligned}
$$

Some comments on bosonic coherent states

- Our case is called the "Canonical Coherent State"–other types of coherent states are relevant for signal processing, image processing, etc. . .
- "Classical Electric Field"–coherent state of photons in the classical limit
- "Gaussian wave packets" $\langle x|\phi\rangle$ minimize the uncertainty principle (see Schiff, QM, 1955)

Can we do the same for fermionic states?

We want $|\xi\rangle$ s.t. $a_i|\xi\rangle = \xi_i|\xi\rangle$, where ξ_i is an eigenvalue of operator a_i. If we have this, then we also have

$$\{a_i, a_j\}|\xi\rangle = 0 \implies \{\xi_i, \xi_j\} = 0.$$

So ξ_i CANNOT be a c-number!

Enter Grassmann numbers

Grassmann numbers

Define set of Grassmann numbers

$$\eta_1, \eta_2, \ldots, \eta_n, \eta_1^*, \eta_2^*, \ldots, \eta_n^*$$

such that $\{\eta_i, \eta_j\} = \{\eta_i^*, \eta_j^*\} = \{\eta_i^*, \eta_j\} = 0 \implies \eta_i^2 = 0$ (nilpotent).

Grassmann functions

Define set of Grassmann numbers

$$\left.\begin{aligned} f(\eta_i) &= f_0 + f_1\eta_i \\ g(\eta_i) &= g_0 + g_1\eta_i \end{aligned}\right\} \implies f(\eta_i) + g(\eta_i) = (f_0 + g_0) + (f_1 + g_1)\eta_i$$

We have a *Grassmann Algebra*!

Also! $\{\eta_i, a\} = \{\eta_j, a^\dagger\} = 0$

Integration and Differentiation, Grassmann style!

Rules for integrating and differentiating

$$\frac{\partial}{\partial \eta_i} \eta_j = \delta_{ij}$$

$$\int d\eta_i \, \eta_j = \delta_{ij}$$

$$\int d\eta_i = 0$$

Note: no limits on the integration! Purely formal manipulations.

Weird, huh?

Fermionic coherent state

$$|\xi\rangle \equiv e^{-\sum_i \xi_i a_i^\dagger}|0\rangle \quad \forall\ \xi_i \text{ Grassmann}$$

$$\begin{aligned}
&= \prod_i (1 - \xi_i a_i^\dagger)|0\rangle \\
a_1|\xi\rangle &= a_1(1 - \xi_1 a_1^\dagger)\prod_{i=2}(1 - \xi_i a_i^\dagger)|0\rangle \\
&= \xi_1 a_1 a_1^\dagger \prod_{i=2}(1 - \xi_i a_i^\dagger)|0\rangle \\
&= \xi_1(1 - a_1^\dagger a_1)\prod_{i=2}(1 - \xi_i a_i^\dagger)|0\rangle \\
&= \xi_1 \prod_{i=2}(1 - \xi_i a_i^\dagger)|0\rangle \\
&= \xi_1(1 - \xi_1 a_1^\dagger)\prod_{i=2}(1 - \xi_i a_i^\dagger)|0\rangle \\
&= \xi_1 \prod_i (1 - \xi_i a_i^\dagger)|0\rangle \\
&= \xi_1|\xi\rangle\ .
\end{aligned}$$

Properties of fermionic coherent states

- Define $\langle\xi| = \langle 0|e^{-\sum_i a_i \xi_i^*}$ and have that $\langle\xi|a_k^\dagger = \langle\xi|\xi_k^*$.
- Overlap $\langle\eta|\xi\rangle = e^{-\sum_i \eta_i^* \xi_i}$
- Matrix element of normal ordered operator

$$\langle\eta| : f(a_j^\dagger, a_i) : |\xi\rangle = f(\eta_j^*, \xi_i) e^{-\sum_i \eta_i^* \xi_i}$$

- Completeness relation:

$$1 = \int \left[\prod_i d\xi_i^* d\xi_i\right] e^{-\sum_i \xi_k^* \xi_k} |\xi\rangle\langle\xi|$$

Trace of operator A

$$\begin{aligned}
\mathrm{tr}A &= \sum_n \langle n|A|n\rangle \\
&= \int \left[\prod_j d\xi_j^* d\xi_j\right] e^{-\sum_k \xi_k^* \xi_k} \sum_n \langle n|\xi\rangle\langle\xi|A|n\rangle \\
&= \int \left[\prod_j d\xi_j^* d\xi_j\right] e^{-\sum_k \xi_k^* \xi_k} \langle -\xi|A \sum_n |n\rangle\langle n||\xi\rangle \\
&= \int \left[\prod_j d\xi_j^* d\xi_j\right] e^{-\sum_k \xi_k^* \xi_k} \langle -\xi|A|\xi\rangle \ .
\end{aligned}$$

Is there a physical interpretation of fermionic coherent states?

None that I know of.

Gaussian integration

Assume we have matrix A that is real and symmetric and invertible:

$$\int_{-\infty}^{\infty}\left[\prod_i \frac{d\phi_i}{\sqrt{2\pi}}\right] e^{-\frac{1}{2}\sum_{k,l}\phi_k A_{k,l}\phi_l}$$
$$=\int_{-\infty}^{\infty}\frac{d\vec{\phi}}{(2\pi)^{n/2}}e^{-\frac{1}{2}\vec{\phi}\cdot A\cdot\vec{\phi}}\ .$$

One can show that this is equal to

$$\frac{1}{\sqrt{\det A}}$$

For a complex (charged) scalar field and A Hermitian, have

$$\int_{-\infty}^{\infty}\left[\prod_i \frac{d\phi_i^* d\phi_i}{2\pi i}\right] e^{-\frac{1}{2}\sum_{k,l}\phi_k^* A_{k,l}\phi_l}$$
$$=\frac{1}{\det A}\ .$$

Now consider integration with Grassmann numbers on matrix M, where M has no constraints,

$$\int\left[\prod_i d\xi_i^* d\xi_i\right] e^{-\sum_{k,l}\xi_k^* M_{k,l}\xi_l}$$
$$=\det M\ .$$

Path-Integral formalism w/ fermions

We are interested in calculating

$$\langle O\rangle = \frac{1}{\mathcal{Z}}\mathrm{Tr}\left(O\, e^{-\beta H}\right)\ ,$$

where $\mathcal{Z} = \mathrm{Tr} e^{-\beta H}$.

We can express $\mathcal{Z}$ with fermionic coherent state $|\psi_0\rangle$:

$$\mathcal{Z} = \int \left[\prod_j d\psi^*_{j,0} d\psi_{j,0}\right] e^{-\sum_k \psi^*_{k,0}\psi_{k,0}} \langle -\psi_0 | e^{-\beta H} | \psi_0\rangle\ .$$

PI continued. . .

We now split the exponential up into N_t timesteps of width $\delta = \beta/N_t$,

$$e^{-\beta H} \equiv e^{-\delta H} e^{-\delta H} \cdots e^{-\delta H} \ .$$

We insert the complete set of fermionic coherent states,

$$1 = \int \left[\prod_\alpha d\psi^\dagger_\alpha d\psi_\alpha \right] e^{-\sum_\beta \psi^\dagger_\beta \psi_\beta} |\psi\rangle\langle\psi| \ ,$$

between each factor of the exponential, giving for the partition function $\mathcal{Z}$,

$$\mathcal{Z} = \lim_{N_t \to \infty} \int \prod_{t=0}^{N_t - 1} \left\{ \left[\prod_\alpha d\psi^\dagger_{\alpha,t} d\psi_{\alpha,t} \right] \langle \psi_{t+1} | e^{-\delta H} | \psi_t \rangle e^{-\sum_\beta \psi^\dagger_{\beta,t} \psi_{\beta,t}} \right\} \ .$$

Note: To account for the (red) minus sign in the partition function on the previous page, must have $\psi_{N_t} = -\psi_0 \implies$ anti-periodic boundary conditions in time!

The form of H

To go any further, must assume some form for H:

$$= H_0 + V_2 = \sum_{i,j} k_{ij} a_i^\dagger a_j + \frac{1}{2}\sum_{i,j} v_{ij} a_i^\dagger a_i a_j^\dagger a_j$$

$$= H_0 + V_2 = \sum_{i,j} k_{ij} a_i^\dagger a_j + \frac{1}{2}\sum_{i,j} v_{ij} n_i n_j \ ,$$

where $n_i \equiv a_i^\dagger a_i$ (number density operator). Here k is a "connectivity" matrix (think kinetic operator), and v represents 2-body matrix elements. Both are represented by c-numbers. Now consider the matrix element

$$\langle \psi_{t+1} | e^{-\delta(H_0+V_2)} | \psi_t \rangle$$

What's the problem?

H_0 will be quadratic in Grassmann fields – Great!
V_2 will be *quartic* in Grassman fields – Oh oh!

The Hubbard-Stratonovich Transformation

At its foundation, the HS transformation relies on the following relations,

$$
\begin{aligned}
e^{-\frac{1}{2}Un^2} &= \frac{1}{\sqrt{2\pi U}}\int_{-\infty}^{\infty} d\phi\, e^{-\frac{1}{2U}\phi^2 \pm i\phi n} \\
e^{\frac{1}{2}Un^2} &= \frac{1}{\sqrt{2\pi U}}\int_{-\infty}^{\infty} d\phi\, e^{-\frac{1}{2U}\phi^2 \pm \phi n}\,.
\end{aligned}
$$

Assumed $U \geq 0$ and the $\pm$ signs are equivalent. The real variable ϕ (that is integrated over) is an *auxiliary* field that allows us to ‘linearize-in-n’ the arguments of the exponential.

Applying HS trans. to our problem

Define $\tilde{\kappa} \equiv \delta\kappa$ and $\tilde{v} \equiv \delta v$, and we assume that eigenvalues of $\tilde{v}$ are real and > 0 (why??). If this holds, then

$$\langle\psi_{t+1}|e^{-\sum_{ij}\tilde{\kappa}_{ij}a_i^\dagger a_j - \frac{1}{2}\sum_{ij}\tilde{v}_{ij}n_i n_j}|\psi_t\rangle =$$

$$\int_{-\infty}^{\infty}\left[(\det\tilde{v})^{-\frac{1}{2}}\prod_k \frac{d\phi_k}{\sqrt{2\pi}}\right] e^{-\frac{1}{2}\sum_{ij}\phi_i[\tilde{v}^{-1}]_{ij}\phi_j}\langle\psi_{t+1}|e^{-\sum_{ji}\tilde{\kappa}_{jk}a_j^\dagger a_k \pm i\sum_j \phi_j n_j}|\psi_t\rangle\ .$$

Now we can evaluate the coherent state matrix elements:

$$\langle\psi_{t+1}|e^{-\sum_{ji}\tilde{\kappa}_{jk}a_j^\dagger a_k \pm i\sum_j \phi_j n_j}|\psi_t\rangle =$$

$$e^{-\sum_{ji}\tilde{\kappa}_{jk}\psi^\dagger_{j,t+1}\psi_{k,t} \pm i\sum_j \phi_j \psi^\dagger_{j,t+1}\psi_{j,t}}e^{\sum_i \psi^\dagger_{i,t+1}\psi_{i,t}} + \mathcal{O}(\delta^2)$$

$$= e^{-\sum_{ji}\tilde{\kappa}_{jk}\psi^\dagger_{j,t+1}\psi_{k,t} + \sum_j(1\pm i\phi_j)\psi^\dagger_{j,t+1}\psi_{j,t}} + \mathcal{O}(\delta^2)$$

The Partition function with auxiliary fields

Combining everything gives

$$\mathcal{Z} = \lim_{N_t \to \infty} \int_{-\infty}^{\infty} \mathcal{D}[\phi]\, e^{-\frac{1}{2}\sum_{ij,t} \phi_{i,t}[\tilde{v}^{-1}]_{ij}\phi_{j,t}}$$

$$\int \mathcal{D}\left[\psi^\dagger, \psi\right] \exp\left\{-\sum_{j,t}\left(\psi^\dagger_{j,t}\psi_{j,t} - (1 \pm i\phi_{j,t})\,\psi^\dagger_{j,t+1}\psi_{j,t}\right) - \sum_{ij,t}\tilde{\kappa}_{ij}\psi^\dagger_{i,t+1}\psi_{j,t}\right\} ,$$

where

$$\begin{aligned} \mathcal{D}[\phi] &= (\det \tilde{v})^{-N_t/2} \prod_i \prod_{t=0}^{N_t-1} \frac{1}{\sqrt{2\pi}} d\phi_{i,t} \\ \mathcal{D}\left[\psi^\dagger, \psi\right] &= \prod_x \prod_t^{N_t-1} d\psi^\dagger_{x,t} d\psi_{x,t} \, . \end{aligned}$$

Note the temporal index to the HS field for bookkeeping purposes ($\phi_i \to \phi_{i,t}$).

Finally integrating out the fermions!

Now I express the argument of the exponential in matrix form,

$$\mathcal{Z} = \lim_{N_t\to\infty} \int_{-\infty}^{\infty} \mathcal{D}[\phi]\, e^{-\frac{1}{2}\sum_{ij,t}\phi_{i,t}[\tilde{v}^{-1}]_{ij}\phi_{j,t}} \int \mathcal{D}\left[\psi^\dagger,\psi\right] \exp\left\{-\sum_{it',jt}\psi^\dagger_{it'} M[\phi]_{it',jt}\psi_{jt}\right\} ,$$

where the *fermion* matrix $M[\phi]$ is a *functional* of the field ϕ with c-number matrix elements:

$$\begin{aligned} M[\phi]_{it',jt} &= \delta_{ij}\delta_{t't} - (1 \pm i\phi_{j,t})\delta_{ij}\delta_{t',t+1} - \tilde{\kappa}_{ij}\delta_{t',t+1} \\ &\approx \delta_{ij}\delta_{t't} - e^{\pm i\phi_{j,t}}\delta_{ij}\delta_{t',t+1} - \tilde{\kappa}_{ij}\delta_{t',t+1} \ . \end{aligned}$$

We have a matrix and we have quadratic Grassmann terms. We must integrate!

$$\mathcal{Z} = \lim_{N_t\to\infty} \int_{-\infty}^{\infty} \mathcal{D}[\phi]\ e^{-\frac{1}{2}\sum_{ij,t}\phi_{i,t}[\tilde{v}^{-1}]_{ij}\phi_{j,t}} \det M[\phi] \ .$$

Observables $\hat{O}$ with the PI

One can also show, using the same steps as above, that

$$\langle \hat{O} \rangle = \lim_{N_t \to \infty} \frac{1}{\mathcal{Z}} \int_{-\infty}^{\infty} \mathcal{D}\left[\phi\right] \; O[\phi] \; e^{-\frac{1}{2} \sum_{ij,t} \phi_{i,t} [\tilde{v}^{-1}]_{ij} \phi_{j,t}} \, \det M[\phi] \; ,$$

where in principle, the operator O can also be functional of ϕ.
Note:

- Every term in M is a c-number
- Auxiliary field ϕ is a c-number, not dynamical in this case!
- Dynamics of fermions encoded in $M[\phi]$

Example for $\hat{O}$: the fermion correlator

We are interested in calculating

$$\langle a_\alpha(\tau)a^\dagger_\beta(0)\rangle = \lim_{N_t\to\infty}\frac{1}{\mathcal{Z}}\int_{-\infty}^{\infty}\mathcal{D}\left[\phi\right]\psi_{\alpha,\tau}\psi^\dagger_{\beta,0}\; e^{-\frac{1}{2}\sum_{ij,t}\phi_{i,t}[\tilde{v}^{-1}]_{ij}\phi_{j,t}}\det M[\phi]$$

But the RHS has Grassmann variables! So how do we calculate this term?

The generating functional

We introduce the generating functional (repeated indices summed):

$$Z_0[\eta^\dagger,\eta]=\int\mathcal{D}\left[\psi^\dagger,\psi\right]\,e^{-\psi_k^\dagger M_{kl}[\phi]\psi_l+\eta_k^\dagger\psi_k+\psi_k^\dagger\eta_k}$$

The original partition function is

$$\mathcal{Z}=\lim_{N_t\to\infty}\int_{-\infty}^{\infty}\mathcal{D}\left[\phi\right]\;\;e^{-\frac{1}{2}\sum_{ij,t}\phi_{i,t}[\tilde{v}^{-1}]_{ij}\phi_{j,t}}Z_0[\bar{\eta},\eta]\Big|_{\bar{\eta}=\eta=0}$$

I can pull down products of ψ_n and $\psi_m^\dagger$ by simply performing Grassman differentiation,

$$\begin{aligned}\int_{-\infty}^{\infty}\mathcal{D}\left[\phi\right]\;\;e^{-\frac{1}{2}\sum_{ij,t}\phi_{i,t}[\tilde{v}^{-1}]_{ij}\phi_{j,t}}\psi_n\psi_m^\dagger\;Z_0[\bar{\eta},\eta]\Big|_{\bar{\eta}=\eta=0}\\ =\int_{-\infty}^{\infty}\mathcal{D}\left[\phi\right]\;\;e^{-\frac{1}{2}\sum_{ij,t}\phi_{i,t}[\tilde{v}^{-1}]_{ij}\phi_{j,t}}\left(\overrightarrow{\frac{\partial}{\partial\eta_n^\dagger}}Z_0[\eta^\dagger,\eta]\overleftarrow{\frac{\partial}{\partial\eta_m}}\right)\Bigg|_{\eta^\dagger=\eta=0}\end{aligned}$$

We can formally integrate the generating functional

After completing the square in the argument and performing Grassmann gaussian integration

$$Z_0[\bar{\eta},\eta] = \det(M[\phi])e^{\bar{\eta}_k[M[\phi]^{-1}]_{kl}\eta_l}$$

This means that

$$\left.\left(\frac{\overrightarrow{\partial}}{\partial\eta_n^\dagger}Z_0[\eta^\dagger,\eta]\frac{\overleftarrow{\partial}}{\partial\eta_m}\right)\right|_{\eta^\dagger=\eta=0} = M[\phi]^{-1}_{n,m}\det M[\phi]$$

Therefore our fermion correlator is

$$\langle a_\alpha(\tau)a_\beta^\dagger(0)\rangle = \lim_{N_t\to\infty}\frac{1}{\mathcal{Z}}\int_{-\infty}^{\infty}\mathcal{D}\left[\phi\right]\psi_{\alpha,\tau}\psi_{\beta,0}^\dagger\; e^{-\frac{1}{2}\sum_{ij,t}\phi_{i,t}[\tilde{v}^{-1}]_{ij}\phi_{j,t}}\det M[\phi]$$

$$= \lim_{N_t\to\infty}\frac{1}{\mathcal{Z}}\int_{-\infty}^{\infty}\mathcal{D}\left[\phi\right]\; e^{-\frac{1}{2}\sum_{ij,t}\phi_{i,t}[\tilde{v}^{-1}]_{ij}\phi_{j,t}}\; M^{-1}[\phi]_{\alpha\tau,\beta 0}\det M[\phi]$$

A theory with fermions: the Hubbard Model

The Hubbard Hamiltonian :

$$
\begin{aligned}
H &\equiv H_{tb} + H_U \\
&\equiv -\kappa \sum_{\langle x,y\rangle,s} a^{\dagger}_{x,s} a_{y,s} - \frac{U}{2} \sum_{x} \left(n_{x,\uparrow} - n_{x,\downarrow}\right)^2 \ ,
\end{aligned}
$$

- κ is the nearest-neighbor hopping amplitude for electrons on the lattice
- U is the onsite interaction ($U \geq 0$)
- $\langle x, y\rangle$ denotes summation over nearest neighbors,
- s assumes the values $\uparrow$ (“spin up”) or $\downarrow$ (“spin down”).
- $n_{x,s} \equiv a^{\dagger}_{x,s} a_{x,s}$ is the number operator for spin s at position x

This particular form of the Hubbard Hamiltonian corresponds to a system at “half-filling”, where the average number of electrons per site is 1.

Case study: 1-site Hubbard model

We can solve this problem exactly

- No hopping (nowhere to hop to!) $\implies \kappa = 0$
- Fock space:

$$|0\rangle \oplus |\uparrow\rangle \oplus |\downarrow\rangle \oplus |\uparrow\downarrow\rangle$$

- Partition function:

$$\mathcal{Z} = 2(1 + e^{\beta U/2}) \; .$$

- Correlator:

$$C(\tau) = \begin{bmatrix} C_{\uparrow\uparrow}(\tau) & C_{\uparrow\downarrow}(\tau) \\ C_{\downarrow\uparrow}(\tau) & C_{\downarrow\downarrow}(\tau) \end{bmatrix} = \frac{1}{2\cosh\left(U\beta/4\right)} \begin{bmatrix} \cosh\left(\frac{U}{2}\left(\tau - \frac{\beta}{2}\right)\right) & 0 \\ 0 & \cosh\left(\frac{U}{2}\left(\tau - \frac{\beta}{2}\right)\right) \end{bmatrix} \; .$$

Our task: Use PI to calculate $C(\tau)$

- We must work with coherent states for each spin d.o.f.: $|\psi\rangle \to |\psi_\uparrow \psi_\downarrow\rangle$
- Utilize HS transformation to remove quartic terms in creation/annihilation operators

$$\langle \psi_{t+1,\uparrow}; \psi_{t+1,\downarrow} | e^{\frac{\tilde{U}}{2}(n_{x\uparrow} - n_{x\downarrow})^2} | \psi_{t,\uparrow}; \psi_{t,\downarrow} \rangle = \int_{-\infty}^{\infty} \frac{d\phi_t}{\sqrt{2\pi\tilde{U}}}\, e^{-\frac{1}{2\tilde{U}}\phi_t^2} \langle \psi_{t+1,\uparrow}; \psi_{t+1,\downarrow} | e^{\pm\phi_t(n_{x\uparrow} - n_{x\downarrow})} | \psi_{t,\uparrow}; \psi_{t,\downarrow} \rangle\,.$$

where $\tilde{U} = \delta U$.

Partition function $\mathcal{Z}$

$$\mathcal{Z} = \lim_{N_t\to\infty} \int_{-\infty}^{\infty} \left[\prod_{t=0}^{N_t-1} \frac{d\phi_t}{\sqrt{2\pi\tilde{U}}}\right] e^{-\frac{1}{2\tilde{U}}\sum_t \phi_t^2}$$

$$\int \left[\prod_t^{N_t-1} d\psi^\dagger_{t\uparrow} d\psi_{t\uparrow}\right] e^{-\sum_{t',t} \psi^\dagger_{t'\uparrow} M[\phi]_{t',t}\psi_{t\uparrow}} \int \left[\prod_t^{N_t-1} d\psi^\dagger_{t\downarrow} d\psi_{t\downarrow}\right] e^{-\sum_{t',t} \psi^\dagger_{t'\downarrow} M[-\phi]_{t',t}\psi_{t\downarrow}}$$

where

$$M[\phi]_{t',t} = \delta_{t't} - e^{-\phi_t}\delta_{t',t+1} \ ,$$

Integrate out fermionic fields:

$$\mathcal{Z} = \lim_{N_t\to\infty} \int_{-\infty}^{\infty} \left[\prod_{t=0}^{N_t-1} \frac{d\phi_t}{\sqrt{2\pi\tilde{U}}}\right] e^{-\frac{1}{2\tilde{U}}\sum_t \phi_t^2} \det M[\phi] \det M[-\phi] = \int_{-\infty}^{\infty} \left[\prod_{t=0}^{N_t-1} \frac{d\phi_t}{\sqrt{2\pi\tilde{U}}} e^{-\frac{1}{2\tilde{U}}\phi_t^2}\right] \det\left(M[\phi]M[-\phi]\right) \ .$$

Finally the correlator $C(\tau)$

$$C_{\uparrow\uparrow}(\tau) = \frac{1}{\mathcal{Z}} \int_{-\infty}^{\infty} \left[\prod_{t=0}^{N_t-1} \frac{d\phi_t}{\sqrt{2\pi\tilde{U}}} \right] M^{-1}_{\tau,0}[\phi]\, e^{-\frac{1}{2\tilde{U}}\sum_t \phi_t^2} \det\left(M[\phi]M[-\phi]\right)$$

$$= \frac{1}{\mathcal{Z}} \int_{-\infty}^{\infty} \left[\prod_{t=0}^{N_t-1} \frac{d\phi_t}{\sqrt{2\pi\tilde{U}}} e^{-\frac{1}{2\tilde{U}}\phi_t^2} \right] M^{-1}_{\tau,0}[\phi] \det\left(M[\phi]M[-\phi]\right) \; .$$

$$C_{\downarrow\downarrow}(\tau) = \frac{1}{\mathcal{Z}} \int_{-\infty}^{\infty} \left[\prod_{t=0}^{N_t-1} \frac{d\phi_t}{\sqrt{2\pi\tilde{U}}} \right] M^{-1}_{\tau,0}[-\phi]\, e^{-\frac{1}{2\tilde{U}}\sum_t \phi_t^2} \det\left(M[\phi]M[-\phi]\right)$$

$$= \frac{1}{\mathcal{Z}} \int_{-\infty}^{\infty} \left[\prod_{t=0}^{N_t-1} \frac{d\phi_t}{\sqrt{2\pi\tilde{U}}} e^{-\frac{1}{2\tilde{U}}\phi_t^2} \right] M^{-1}_{\tau,0}[-\phi] \det\left(M[\phi]M[-\phi]\right) \; .$$

Monte Carlo Integration

- Define $\vec{\phi} = (\phi_0\ ,\ \phi_1\ ,\ \ldots,\ \phi_{N_t-1})$
- Sample each component from a Gaussian distribution $\mathcal{N}_{0,\sqrt{\tilde{U}}}$
- Do this N times, each time performing the following calculations,

$$
\begin{aligned}
\mathcal{Z} &\approx \frac{1}{N} \sum_{\vec{\phi}\in\mathcal{N}_{0,\sqrt{\tilde{U}}}}^{N} \det\left(M[\phi]M[-\phi]\right) \\
C_{\uparrow\uparrow}(\tau) &\approx \frac{1}{N}\frac{1}{\mathcal{Z}} \sum_{\vec{\phi}\in\mathcal{N}_{0,\sqrt{\tilde{U}}}}^{N} M^{-1}_{\tau,0}[\phi]\det\left(M[\phi]M[-\phi]\right)\ .
\end{aligned}
$$

Let's do this!

Necessary ingredients to numerically do this problem

- Choose U, β, and N_t. This gives you $\delta = \beta/N_t$ and $\tilde{U} = U\delta$.
- Construct $M[\phi]_{t',t} = \delta_{t't} - e^{-\phi_t}\delta_{t',t+1}$

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & e^{-\phi 7} \\ -e^{-\phi 0} & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -e^{-\phi 1} & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -e^{-\phi 2} & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -e^{-\phi 3} & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -e^{-\phi 4} & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -e^{-\phi 5} & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -e^{-\phi 6} & 1 \end{pmatrix}$$

- Sampling normal distribution with `python3`: *numpy.random.normal*($\mu = 0, \sqrt{\tilde{U}}$)
- Calculating determinant of $M[\phi]M[-\phi]$ with `python3`: *numpy.linalg.det(M)*
- Inverting matrix with `python3`: *numpy.linalg.inv(M)*

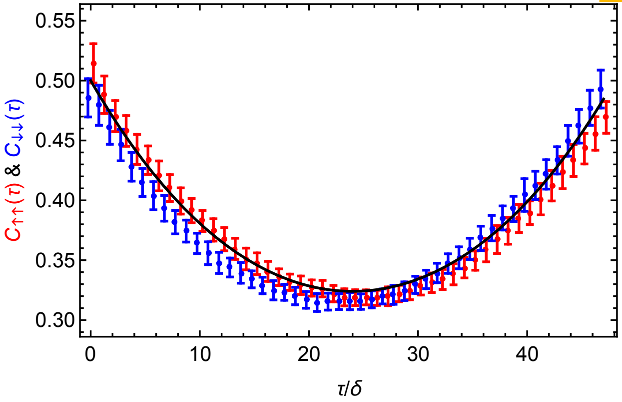

Figure: $C_{\uparrow\uparrow}(\tau)$ (red) and $C_{\downarrow\downarrow}(\tau)$ (blue) calculated from Monte Carlo integration for the one-site Hubbard Model. The parameters used for this calculation were $U/\kappa = 2$, $\kappa\beta = 2$, and $N_t = 48$. The number of Monte Carlo samples $N = 50000$. Shown errors are the bootstrap standard errors. The black line is the analytic result.