LATTICE METHODS FOR STRONGLY INTERACTING SYSTEMS

Lecture 3: Fermions, fermions, fermions!

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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:

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

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

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

Now we can evaluate the coherent state matrix elements:

$$\langle\psi_{t+1}|e^{-\sum_{ji}\tilde{\kappa}_{jk}a_j^\dagger a_k\pm i\sum_j\phi_jn_j}|\psi_t\rangle =$$
$$e^{-\sum_{ji}\tilde{\kappa}_{jk}\psi_{j,t+1}^\dagger\psi_{k,t}\pm i\sum_j\phi_j\psi_{j,t+1}^\dagger\psi_{j,t}}e^{\sum_i\psi_{i,t+1}^\dagger\psi_{i,t}}+\mathcal{O}(\delta^2)$$
$$=e^{-\sum_{ji}\tilde{\kappa}_{jk}\psi_{j,t+1}^\dagger\psi_{k,t}+\sum_j(1\pm i\phi_j)\psi_{j,t+1}^\dagger\psi_{j,t}}+\mathcal{O}(\delta^2)$$

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,

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

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!

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

Observables $\hat{O}$ with the PI

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

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

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,

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

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

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

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

Therefore our fermion correlator is

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

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

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.: $|\psi\rangle \rightarrow |\psi_\uparrow \psi_\downarrow\rangle$
- 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 $\mathcal{Z}$

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

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

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 $\vec{\phi} = (\phi_0\ ,\ \phi_1\ ,\ \dots,\ \phi_{N_t-1})$
- 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)*

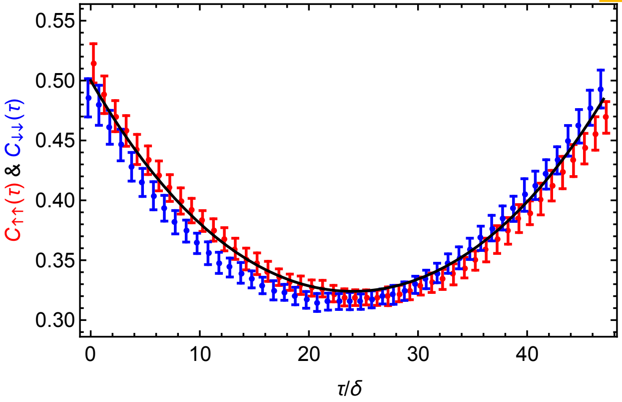


Figure: $C_{\uparrow\uparrow}(\tau)$ (red) and $C_{\downarrow\downarrow}(\tau)$ (blue) calculated from Monte Carlo integration for the one-site Hubbard Model. The parameters used for this calculation were $U/\kappa = 2$, $\kappa\beta = 2$, and $N_t = 48$. The number of Monte Carlo samples $N = 50000$.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

Show me the quarks!

- Let's reverse the situation, and now consider a theory with only fermions and no gauge fields

$$L_F = \overline{\psi}(x)\left(\gamma_\mu \partial_\mu + m\right)\psi(x)$$

$$\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$$

$$\overline{\psi}(x) = \psi^{*T}\gamma_0$$

Note: no covariant derivative!

- The propagator for these fermions is simply the inverse of the kernel, which in momentum space is

$$G_F \propto \frac{1}{\gamma_\mu p_\mu + m + i\varepsilon} = \frac{\gamma_\mu p_\mu - m}{p^2 + m^2 + i\varepsilon}$$

LET'S LOOK AT THE FERMION PROPAGATOR ON A LATTICE

- The Lagrangian now becomes

$$\partial_\mu \psi(x) = \frac{\psi(x+\hat{\mu}) - \psi(x-\hat{\mu})}{2a}$$

$$S_F = \sum_{x,y} \overline{\psi}(x) K_{xy} \psi(y)$$

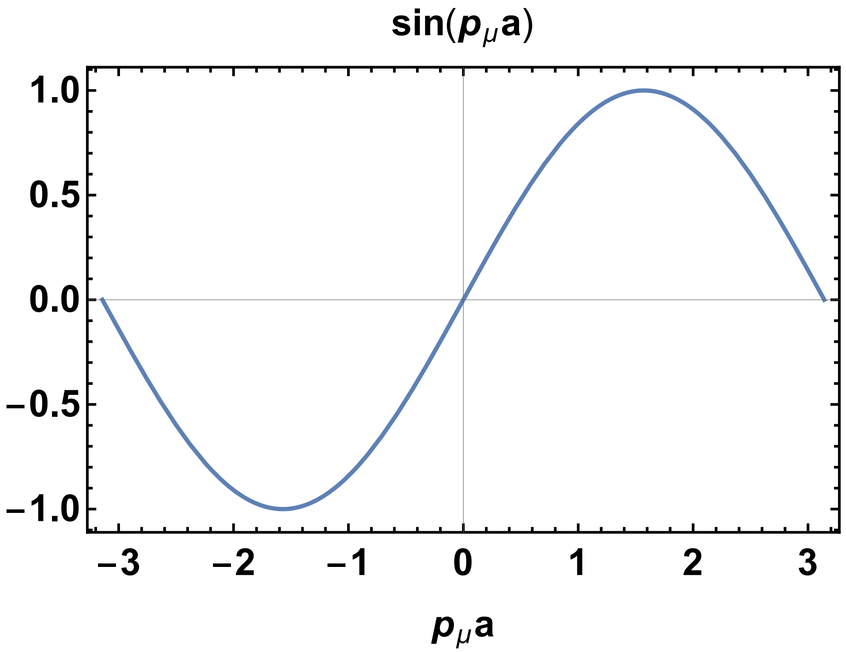
$$K_{xy} = \sum_\mu \frac{\gamma_\mu}{2a}\left(\delta_{x,y+\hat{\mu}} - \delta_{x,y-\hat{\mu}}\right) + m\delta_{x,y}$$

- Does the propagator, in the limit $a \rightarrow 0$, give the correct expression in the momentum representation?

$$G_F = \lim_{a\to 0} K^{-1} \propto \frac{\gamma_\mu \dfrac{\sin(p_\mu a)}{a} - m}{\sum_\mu \left(\dfrac{\sin(p_\mu a)}{a}\right)^2 + m^2}$$

$$G_F = \lim_{a\to 0} K^{-1} \propto \frac{\gamma_\mu \dfrac{\sin(p_\mu a)}{a} - m}{\sum_\mu \left(\dfrac{\sin(p_\mu a)}{a}\right)^2 + m^2}$$

- For $p \to 0$, one gets the correct expression
- For $|p| \to \pi/2$, one also gets the correct expression (near the corners of the Brillouin zones (BZ))!
  - We get more than one correct solution
    - In d-dimensions, we get 2^d allowed solutions, only one of which is relevant in the continuum limit
  - "Fermion doubling problem"
- There is a physical realization of this doubling—the lattice is trying to preserve chiral symmetry
  - Chiral symmetry $\leftrightarrow$ fermion doubling
- Can/should we remedy this?



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Wilson fermions

- We can use Wilson fermions

$$S_W = S_F - \frac{r}{2}a^2 \sum_{x,y} \overline{\psi}(x)\left(\partial_\mu\right)^2 \psi(y)$$

$$G_F = \lim_{a\to 0} K^{-1} \propto \frac{\gamma_\mu \dfrac{\sin(p_\mu a)}{a} - m(p)}{\sum_\mu \left(\dfrac{\sin(p_\mu a)}{a}\right)^2 + m(p)^2} \quad ; \quad m(p) = m + \frac{2r}{a}\sum_\mu \sin\left(\frac{p_\mu a}{2}\right)^2$$

$$m(0) = m \quad ; \quad m\left(\frac{\pi}{2}\right) = \infty$$

- Wait—can we just arbitrarily add terms to our lattice lagrangian?
    - Yes—as long as we obtain the correct continuum limit (e.g. just like in our YM example of last lecture)
    - But we lost chiral symmetry

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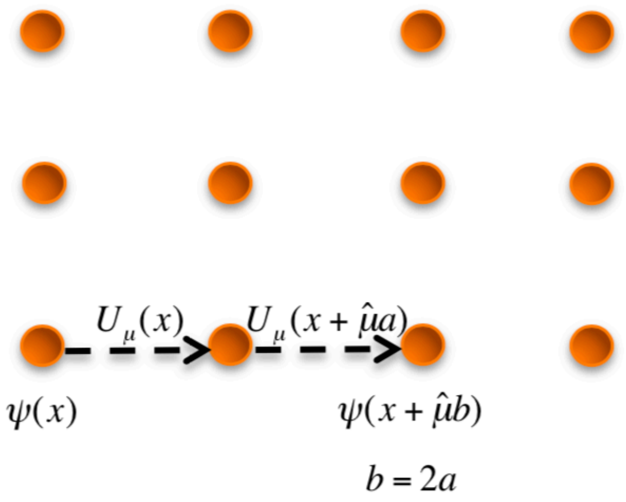
Staggered fermions

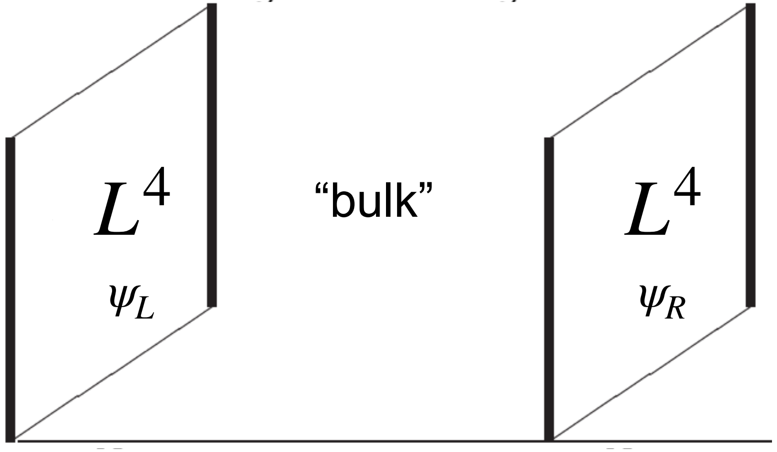
- What if we just forced the fermion field to live in a world where the BZ was different?



- In the staggered formalism, the fermion BZs are never actually probed—i.e. (almost) no doublers!
  - Only works with even number of flavors of fermions
  - Preserves certain aspects of chiral symmetry (but not all)
  - Does it have the correct continuum limit???

THE FIFTH DIMENSION—AND NO, I'M NOT TALKING ABOUT THE MOVIE (THOUGH I DID LIKE THE MOVIE TOO!)

- The *Nielson-Ninomiya* theorem in LQCD essentially tells us that when dealing with fermions on a lattice, exact chiral symmetry comes hand-in-hand with fermion doublers (tastes) in any number of dimensions
- In the 90s it was discovered that one could formulate a lattice theory in 5-dimensions where doublers and the like existed, but the underlying 4-dimensional world retained fermions with "exact" chiral symmetry BUT W/O doublers!
  - Domain-Wall fermions (Kaplan)
  - Overlap fermions
- Drawbacks
  - Very computationally demanding!



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A second look at QCD, this time with Fermions

- Okay, so here's the full-fledged QCD lagrangian using Wilson fermions, for example:

$$S_{QCD} = S_G[U] + S_{F,W}[U,\overline{\psi},\psi]$$

$$S_G[U] = \frac{6}{g^2}\sum_P \left(1 - P_{\mu\nu}\right)$$

$$S_{F,W}[U,\overline{\psi},\psi] = (m+4r)\sum_x \overline{\psi}(x)\psi(x)$$

$$-\frac{1}{2}\sum_{x,\mu}\left(\overline{\psi}(x)(r-\gamma_\mu)U_\mu(x)\psi(x+a\hat{\mu}) + \overline{\psi}(x+a\hat{\mu})(r-\gamma_\mu)U_\mu^{*T}(x)\psi(x)\right)$$

Okay, so I skipped a couple of steps in deriving the expression on the previous page

- First off, I expressed everything in terms of dimensionless quantities

$$\psi \to \frac{1}{a^{3/2}}\psi \quad ; \quad m \to \frac{1}{a} m$$

$$\partial_\mu \to \frac{1}{a}\partial_\mu$$

- Used the covariant derivative in the fermion action

$$D_\mu = \partial_\mu + igA_\mu(x)$$

- Re-expressed coupling of fermions with gauge fields using link variables

SO WE INTEGRATE OUT THE FERMION FIELDS

$$\int d[U]d[\overline{\psi}]d[\psi]e^{-S_g[U]-S_F[U,\overline{\psi},\psi]}$$

$$=\int d[U]d[\overline{\psi}]d[\psi]e^{-S_g[U]-\overline{\psi}M[U]\psi}$$

$$=\int d[U]\det\big(M[U]\big)e^{-S_g[U]}$$

Function of gauge links U
and consists of real numbers!

Problem #4 (easy):

Show that for Wilson fermions, have

$$M_{ij}[U] = (m + 4r)\delta_{ij} - \frac{1}{2}\sum_{\mu>0}\Big((r - \gamma_\mu)U_\mu(i)\delta_{i+a\hat{\mu},j} + (r - \gamma_\mu)U_\mu^{*T}(i - a\hat{\mu})\delta_{i-a\hat{\mu},j}\Big)$$

Problem #5 (easy):

What is the dimension of $M_{ij}[U]$?

So that's it! We can now simulate QCD, right?

- We just need to generate gauge configurations with probability distribution proportional to

$$P \propto \det\left(M[U]\right)e^{-S_G[U]} = e^{-S_G[U]+\log(\det(M[U]))}$$

- M in our case is no ordinary, run-of-the-mill matrix
  - Non-local
  - It's big
  - Can be ill-conditioned
- The upshot: calculating the determinant of M is the most time-consuming aspect when generating configurations

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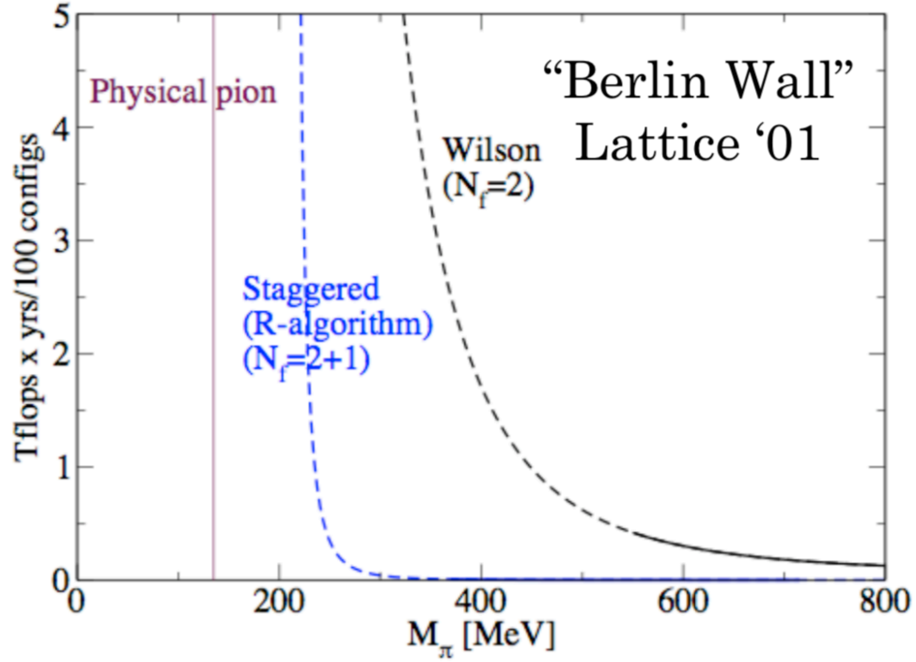
But computers are much faster now, right?

- Yes, but even with advances in computer technology, simulating dynamical fermions is never easy!
  - Condition number of matrix increases as mass of quarks decreases, or equivalently, $m_\pi^{lattice} \to m_\pi^{phys.}$

L = 2.5 fm, T = 2L, a = 0.09 fm



$$\text{cost} \sim \frac{V^{1\leftrightarrow 5/4}}{m_\pi^{5\leftrightarrow 6} a^7}$$

Ukawa Lat01

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THE FALL OF THE BERLIN WALL

- Great advancements in algorithms:
  - Hybrid Monte Carlo
  - Smarter pre-conditioners
  - Deflation methods

$$\text{cost} \sim \frac{V^{1\leftrightarrow 5/4}}{m_\pi^{5\leftrightarrow 6} a^7} \rightarrow \frac{V^{1\leftrightarrow 5/4}}{m_\pi^2 a^6}$$

Ukawa 08,
Sugar 08

- Greater theoretical control
  - Finite-volume Effective Field Theories
  - Finite-volume many-body techniques

- And yes, faster computers

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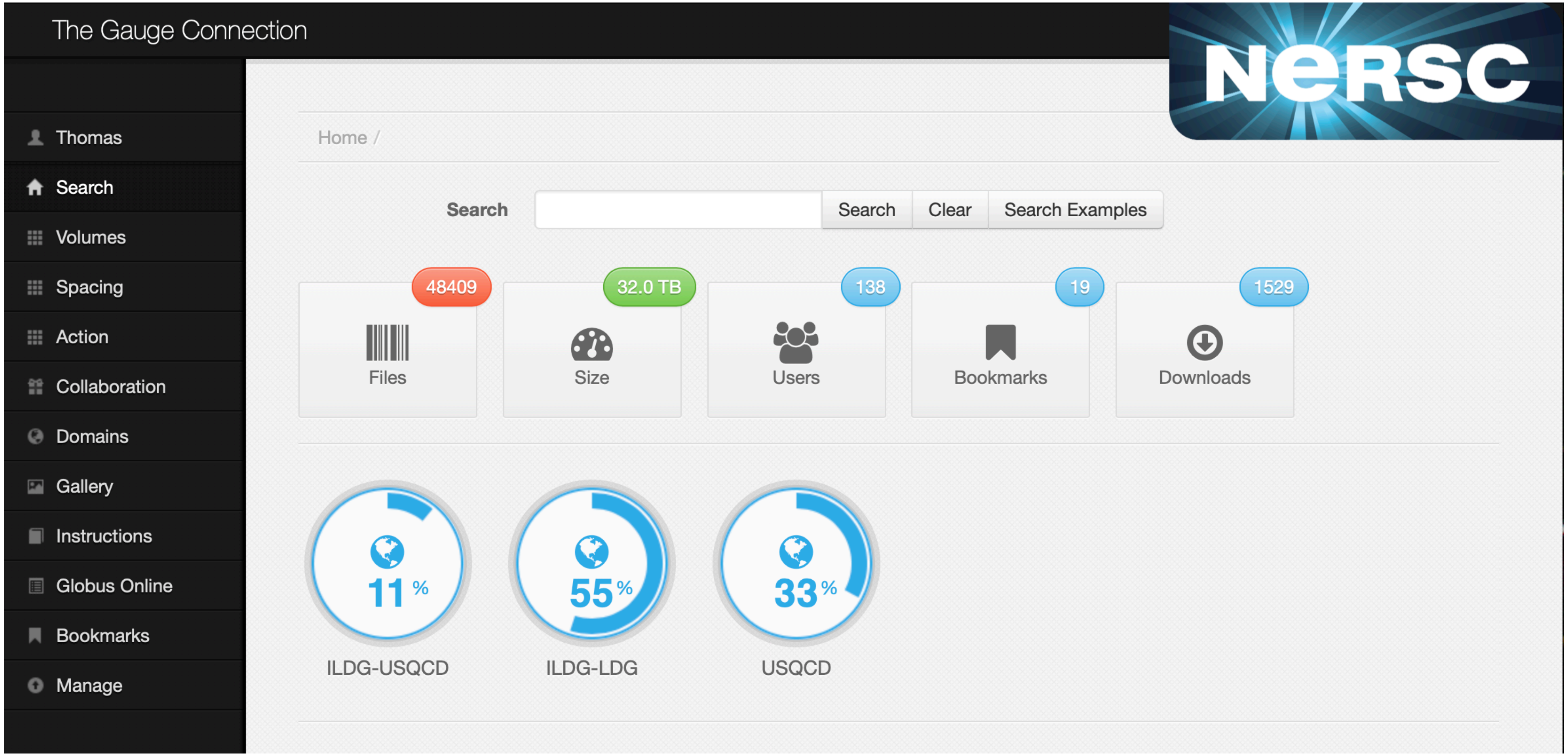
So do you have a big computer? Yes?

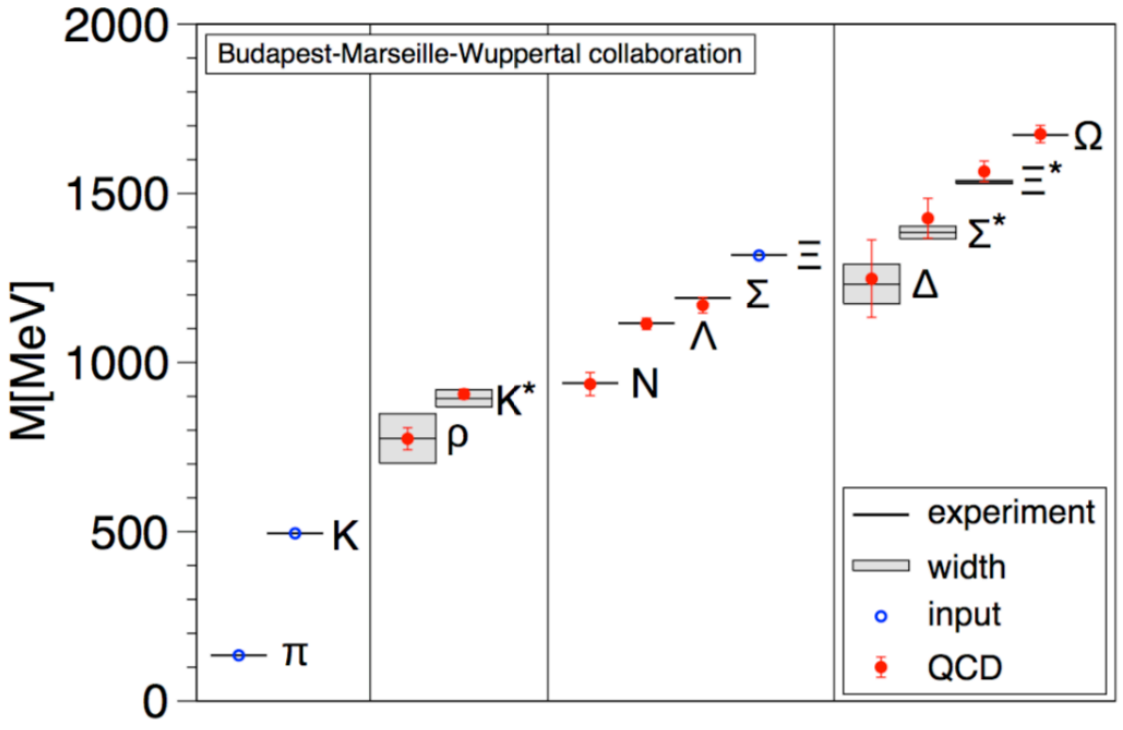
- Go to http://usqcd.jlab.org/usqcd-docs/chroma/ and download *chroma* (and it's supporting software)
  - Supported under SciDac-2
  - And of course, there are other LQCD codes on the market
- There are decent tutorials that show you how the code works and how to run it

You can also download full fledged lattice configurations

- Go to http://qcd.nersc.gov/
  - Set up an account (it's free)



Exactly how are the masses measured in LQCD?



$$\left\langle O^{\{A\}}(t)\right\rangle = \frac{\int d[U]O^{\{A\}}(t)\det\left(M[U]\right)e^{-S_g[U]}}{\int d[U]\det\left(M[U]\right)e^{-S_g[U]}} = \sum_i C_i e^{-E_i^{\{A\}}t}$$

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Let's look at the Pion as an example

- The operator in this case is of the form

$$O^{\{A\}}(t) = \sum_x \overline{\pi^+(x,t)}\ \pi^+(0,0)$$

$$= \sum_x \underbrace{\overline{\left(\psi_u(x,t)\gamma_5\overline{\psi}_d(x,t)\right)}}_{\text{“Interpolating } \textbf{\textit{sink}} \text{ field”}}\ \underbrace{\psi_u(0,0)\gamma_5\overline{\psi}_d(0,0)}_{\text{“Interpolating } \textbf{\textit{source}} \text{ field”}}$$

Sum over all lattice sites to project onto zero momentum

“Interpolating ***sink*** field”

“Interpolating ***source*** field”

- The interpolating fields have the same quantum numbers as the charged pion
  - Isospin = 1
  - Strangeness = 0
  - Negative parity
  - Color singlet

WE USE THE RULES FROM THE PREVIOUS LECTURE TO CALCULATE THE EXPECTATION VALUE OF THIS OPERATOR

$$\left\langle \sum_x \overline{\pi^+(x,t)}\ \pi^+(0,0) \right\rangle = \left\langle \sum_x \overline{\left(\psi_u(x,t)\gamma_5\overline{\psi}_d(x,t)\right)}\ \psi_u(0,0)\gamma_5\overline{\psi}_d(0,0) \right\rangle$$

Contract a là Wick's theorem

$$= \sum_x \left\langle tr\ \gamma_5 M_u^{-1}(x,0,t)\gamma_5 M_d^{-1}(x,0,t) \right\rangle$$

$$= \frac{1}{N_{cfg}} \sum_{U\in\{U\}} \sum_x \mathrm{tr}\, \gamma_5 M_u^{-1}[x,0,t,U]\gamma_5 M_d^{-1}[x,0,t,U]$$

By definition, the lowest eigenvalue is defined as the mass of the pion

$$\left\langle \overline{\pi^+}(t)\,\pi^+(0) \right\rangle \equiv C_\pi(t) = \sum_i C_i e^{-E_i t} \xrightarrow{t>>1} C_0 e^{-m_\pi t}$$

$$M_{eff}(t) = \log\left(\frac{C_\pi(t)}{C_\pi(t+1)} \right) \xrightarrow{t>>1} m_\pi$$

And of course the interpolating operators can be generalized

$$\mathrm{K}^+(x,t) = \psi_u(x,t)\gamma_5\overline{\psi}_s(x,t)$$

Kaon interpolating field

$$N(x,t) = \varepsilon_{abc}\psi_u^a(x,t)\left(\psi_u^{bT}(x,t)C\gamma_5\psi_d^c(x,t)\right)$$

Proton interpolating field

Ensures color neutrality

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As you might have guessed, we can do many particles

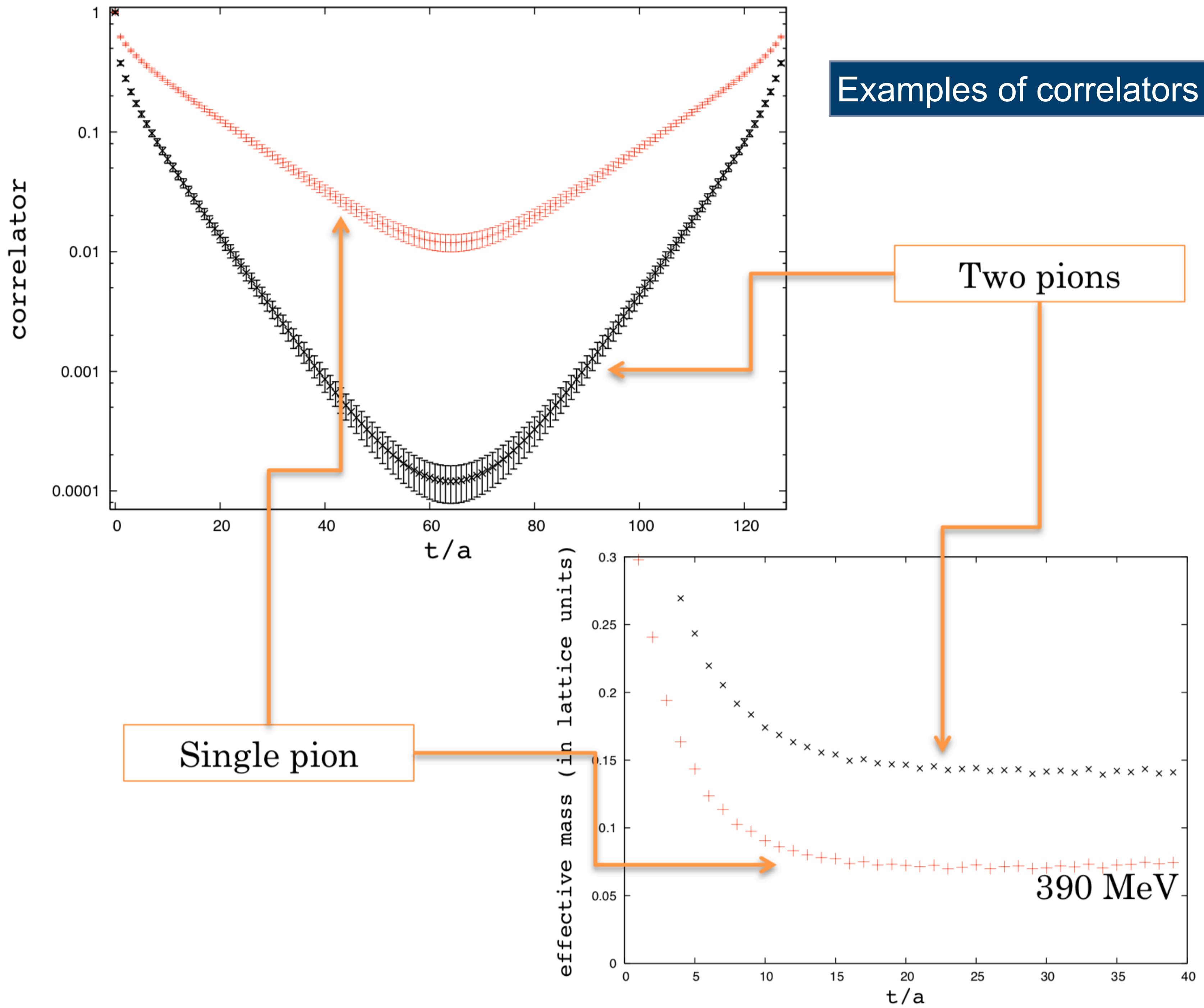
- For example, two pions need four interpolating fields

$$C_{\pi\pi}(t) = \sum_{x,y} \left\langle \overline{\pi^+}(x,t)\overline{\pi^+}(y,t)\pi^+(0,0)\pi^+(0,0) \right\rangle$$

Zero CM momentum state

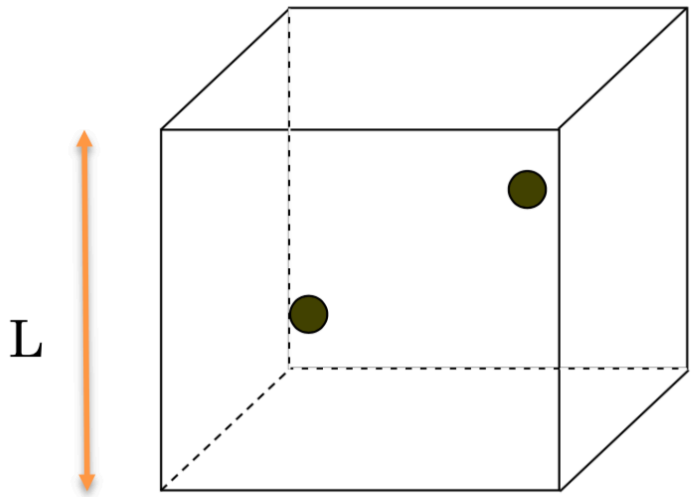
- And for three pions, we need six interpolating operators, and so on . . .

Examples of correlators from real LQCD calculations



Okay, we can get energies, but what's that good for?

- Since the beginning of time, it has been known that the non-relativistic eigenenergies E_{nrel} of two particles in a box can be related to their masses and scattering amplitudes



"Lüscher's formula"

$$\frac{1}{L} S\left(\frac{E_{nrel}}{\varepsilon_0}\right) = p\cot(\delta(p))$$

$$E_{nrel} = \frac{p^2}{2\mu} \quad ; \quad \varepsilon_0 = \frac{1}{2\mu L^2}$$

Assumption: range of interaction << L

$$S(x) = \lim_{\Lambda\to\infty} 4\pi \sum_{\vec{n}}^{|\vec{n}|<\Lambda} \frac{1}{4\pi^2\vec{n}^2 - x} - 4\Lambda$$

3-d zeta function

$$\vec{n} = (n_x, n_y, n_z)$$

Comm. Math. & Phys., 105, 153 (1986)

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Typically the interacting momentum p is small

Effective range

$$p\cot(\delta(p)) = -\frac{1}{a} + \frac{r}{2}|p|^2 + O(p^3)$$

Effective Range Expansion

Scattering length

There is no restriction to the size of this of the scattering length!!!

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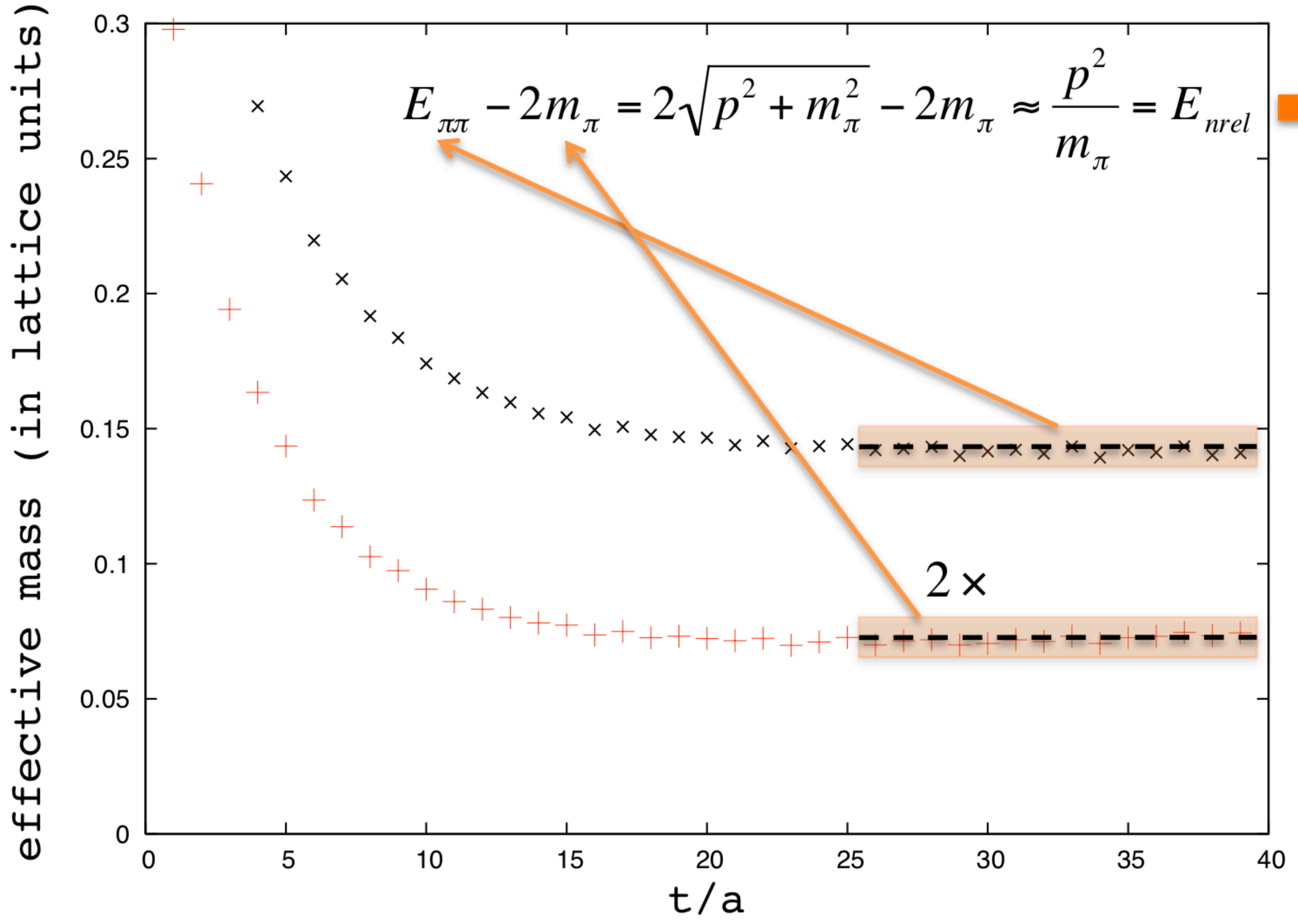
LQCD ALLOWS US TO CALCULATE E_{NREL} !



$$\frac{1}{L} S\left(\frac{E_{nrel}}{\varepsilon_0}\right)$$

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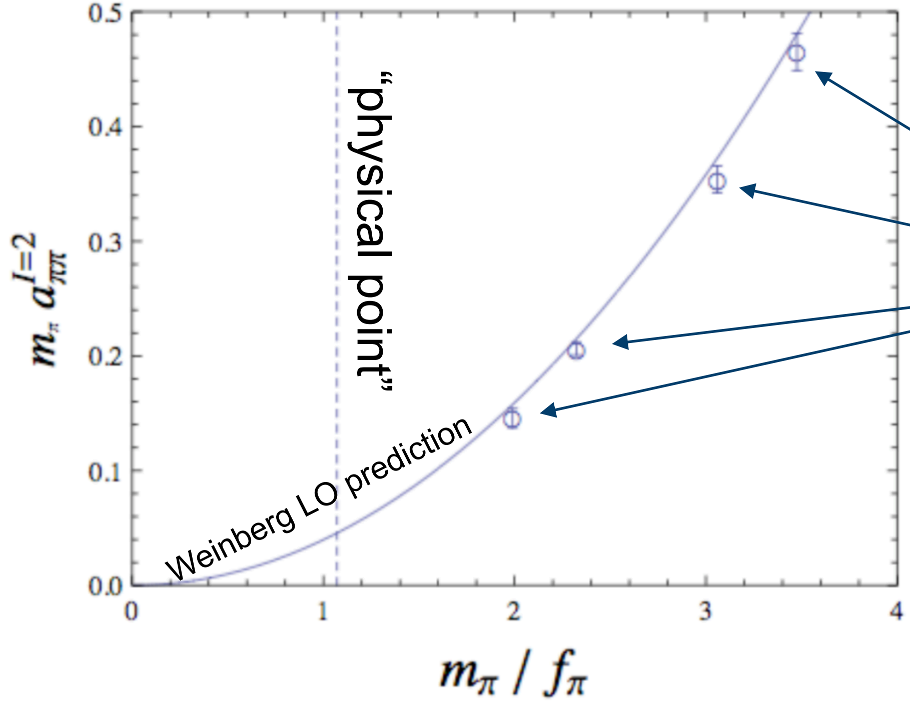
WE CAN USE THESE RELATIONS TO CALCULATE THE SCATTERING LENGTH BETWEEN TWO CHARGED PIONS, FOR EXAMPLE



Finite-volume correction term that vanishes as $b \to 0$

$$m_\pi\, a_{\pi\pi}^{I=2}(b \neq 0) = \frac{m_\pi^2}{8\pi f_\pi^2}\left\{1 + \frac{m_\pi^2}{16\pi^2 f_\pi^2}\left[3\log\left(\frac{m_\pi^2}{\mu^2}\right) - 1 - l_{\pi\pi}^{I=2}(\mu) - \frac{\tilde{\Delta}_{ju}^4}{6m_\pi^4}\right]\right\}$$

b is now the lattice spacing

Lattice measured quantities

Low-energy constant (LEC)

Chen et al. hep/lat 0611003

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LET'S "TALK THE TALK"

Anatomy of a LQCD calculation

Mixed action calculation

Gauge generation

Measurements

"(2+1+1) Wilson-Clover action + Domain-wall valence fermions"

<u># of quarks</u>
"2" : up/down deg.
1 strange quark
1 charm quark

<u>Type of Fermion/Gauge discretisation</u>
Staggered-Iwasaki
Twisted-mass
Domain-wall
etc. . .

<u>Type of Fermion discretisation</u>
Twisted-mass
Wilson
Staggered
etc. . .

SO WHERE DOES LQCD GO FROM HERE?

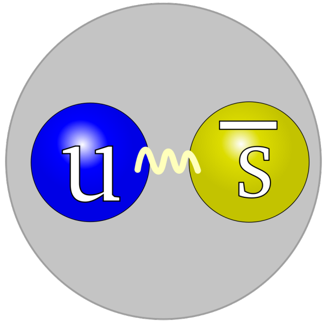
Calculations at physical point opens new opportunities. . .

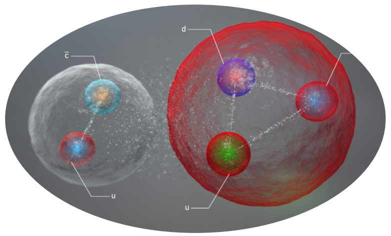
- Probing the interactions between nucleons and hyperons
  - Poorly constrained empirically
  - Relevant to matter at extreme conditions
    - Compact astrophysical objects (think neutron stars!)

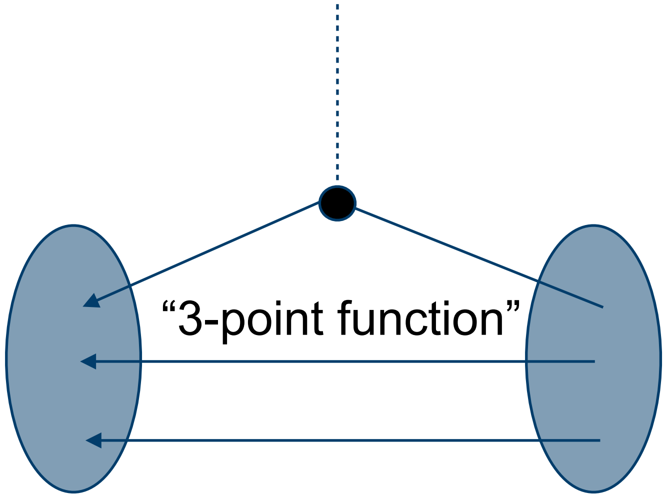
- Tackling QCD exotica
  - Everything Prof. Guo has been talking about!
  - see Prof. Zou's talk

- Constraining BSM physics
  - Need to pin down hadronic component
  - Nuclear matrix element
  - e.g. nEDM, muon g-2 etc. . .
  - see Dr. Gupta's talk. . . :(
  - see talks by Agadjanov, Petschlies

- Tackling the "sign problem"
  - See my talk on Friday! :)







LATTICE QCD CAN ONLY CALCULATE “OBSERVABLES”

A word of warning. . .

- Energy levels (e.g. masses, binding energies)
- ERE parameters (e.g. scattering lengths, effective ranges $\in$ phase shifts)
- If an experiment can measure it, then (in principle) LQCD can calculate it
- Question: Is a potential an observable?

SOME REFERENCES, IN CASE I DIDN'T SCARE YOU AWAY. . .

Lattice Gauge Theories, An Introduction—H. Rothe

Lattice QCD for Novices—*P. Lepage hep- lat-0506036v1 Quarks,*

Gluons, and Lattices—M. Cruetz

Introduction to Quantum Field Theories—J. Smit

Introduction to Lattice QCD—R. Gupta hep-lat/ 9807028

QCD on the Lattice—C. Gattringer and C. Lang