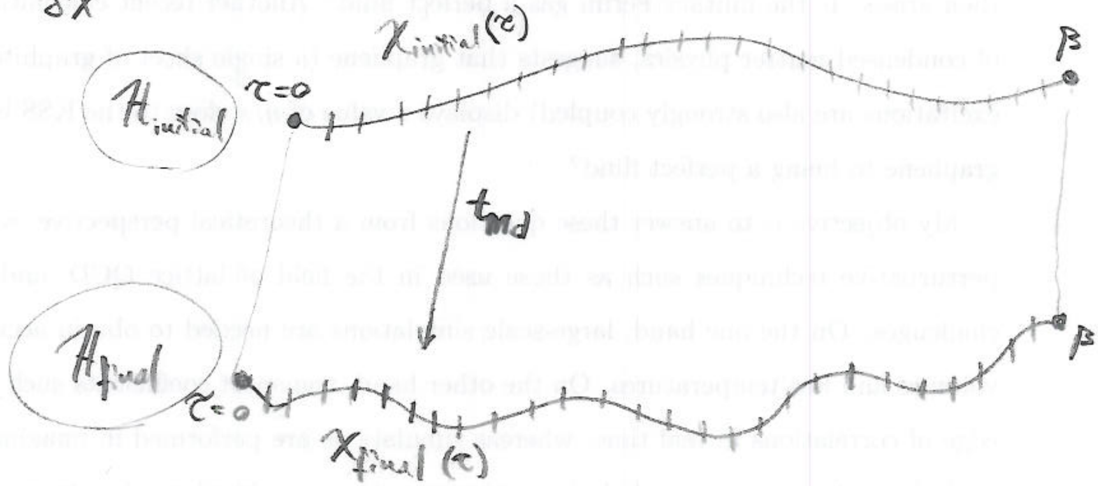
Recap from last time

- Inversion techniques for sparse matrices form a central part of many algorithms used to simulate the quantum many-fermion problem.

- Random updates are a slow way to explore configuration space. A better way is to define a molecular dynamics Hamiltonian and evolve globally using the corresponding equations of motion:

$$\begin{cases} \dot{x} = \dfrac{\delta H}{\delta \pi} \\ \dot{\pi} = -\dfrac{\delta H}{\delta x} \end{cases} \qquad H = \sum_i \frac{\pi_i^2}{2} + S_E[x]$$



and perform a Metropolis accept/reject step with H_{initial} and H_{final}.

- Let's now put these two together!

Hybrid Monte Carlo for the fermion many-body problem.

Our starting point will be, as always, the partition function:

$$Z = \int \mathcal{D}\psi_s^\dagger \mathcal{D}\psi_s \, e^{-S_E[\psi_s^\dagger, \psi_s]}$$

Let us assume now that we have used an "auxiliary field" or "Hubbard-Stratonovich" transformation to represent the interaction:

$$Z = \int \mathcal{D}\psi_s^\dagger \mathcal{D}\psi_s \int \mathcal{D}\sigma \, e^{-S_g[\sigma]} \, e^{-\int d^4x\, d^4x' \sum_{s=1,2} \psi_s^\dagger(x) M_{xx'}[\sigma] \psi_s(x')}$$

$$= \int \mathcal{D}\sigma \, e^{-S_g[\sigma]} \operatorname{Det} M_\uparrow[\sigma] \operatorname{Det} M_\downarrow[\sigma] =$$

Assume $\uparrow$ & $\downarrow$ are completely equivalent

$$= \int \mathcal{D}\sigma \, e^{-S_g[\sigma]} \operatorname{Det}\left[M^\dagger M\right] =$$

$$= \int \mathcal{D}\sigma \, e^{-S_g[\sigma]} \int \mathcal{D}\phi^\dagger \mathcal{D}\phi \, e^{-\int \phi^\dagger (M^\dagger M)^{-1}_{[\sigma]} \phi}$$

impossibly complicated object! very expensive to compute!

"pseudofermions" (bosonic but with anti-periodic boundary conditions)

both are done stochastically!

(but differently in practice, can you guess why?)

- Let's introduce π and write down the resulting path integral:

$$\mathcal{Z} = \int D\pi D\sigma \int D\varphi^\dagger D\varphi \; e^{-\mathcal{H}[\pi,\sigma,\varphi^\dagger,\varphi]}$$

$$\boxed{\begin{aligned} \mathcal{H} &= \sum_i \frac{\pi_i^2}{2} + S_E[\sigma,\varphi^\dagger,\varphi] \\ S_E &= S_g[\sigma] + \int \varphi^\dagger (M^T M)^{-1}_{[\sigma]} \varphi \end{aligned}}$$

Strategy:
- sample φ at fixed σ (a)
- sample σ at fixed φ (b)

(a) $$\int D\varphi^\dagger D\varphi \; e^{-\int \varphi^\dagger (M^T M)^{-1} \varphi} = \int D\xi^\dagger D\xi \; e^{-\xi^\dagger \xi}$$

$$\underbrace{\varphi^\dagger M^{-1}}_{\xi^\dagger} \underbrace{M^{T^{-1}} \varphi}_{\xi}$$

we know how to sample this

→ use gaussian RNG

↓

→ compute $\begin{cases} \varphi = M^T \xi \\ \varphi^\dagger = M \xi^\dagger \end{cases}$

→ go to (b) !

(b) We have φ; use gaussian RNG to get π and start the Molecular dynamics evolution.

(Q:) what evolves with MD? What sets the dynamics? Can you write down the equations of motion?

• Let's write down the equations of motion:

$$\frac{\partial}{\partial t_{md}} \quad \dot{\sigma}(x,\tau) = \frac{\delta H}{\delta \Pi(x,\tau)} = \Pi(x,\tau)$$

$$\dot{\Pi}(x,\tau) = -\frac{\delta H}{\delta\sigma(x,\tau)} = -\underbrace{\frac{\delta S_g}{\delta\sigma(x,\tau)}}_{\text{easy}} + \underbrace{\frac{\delta}{\delta\sigma(x,\tau)}\left[\int \varphi^+ \left(M^T M[\sigma]\right)^{-1}\varphi\right]}_{\text{what do we do with this?}}$$

("pseudofermion force")

$i,j,k \leftrightarrow$ spacetime indices

$$\frac{\delta}{\delta\sigma_k}\left[\sum_{ij}\varphi_i^+ \left(M^T M\right)^{-1}_{ij}\varphi_j\right] = \sum_{ij}\varphi_i^+ \frac{\delta\left(M^T M\right)^{-1}_{ij}}{\delta\sigma_k}\varphi_j = \circledast$$

How do we deal w/ this?

$$\left(M^T M\right)^{-1}\cdot\left(M^T M\right) = 1$$

$$\frac{\partial}{\partial\lambda}\left[\left(M^T M\right)^{-1}\right] M^T M + \left(M^T M\right)^{-1}\frac{\partial}{\partial\lambda}\left(M^T M\right) = 0 \Rightarrow$$

$$\Rightarrow \frac{\partial}{\partial\lambda}\left[\left(M^T M\right)^{-1}\right] = -\left(M^T M\right)^{-1}\frac{\partial\left(M^T M\right)}{\partial\lambda}\left(M^T M\right)^{-1}$$

$$\boxed{\circledast = -\sum_{ij}\eta_i^+ \frac{\partial\left(M^T M\right)_{ij}}{\partial\sigma_k}\eta_j}$$

This we can do!

$$\boxed{\eta = \left(M^T M\right)^{-1}\varphi}$$

Inversion needed at every step!

(Given φ and σ, find $\eta = \left(M^T M[\sigma]\right)^{-1}\varphi$)

More about inversion strategies

- We talked about dense vs. sparse matrices.
- We talked about direct vs. iterative solvers.
- Let us talk about our specific case in more detail.
  - We need to invert $M^T M$. What are its main properties?
    - Real (complex)
    - symmetric (hermitian)
    - positive definite! (why?)

What can we say about $(M^T M)^{-1}$?

CG. is the best method for this case

(Think eigenvalues of M, M^T & $M^T M$)

- It's important (central) to be able to invert $M^T M$ as fast as possible. What determines how fast we can do this?

  - Condition number → ratio of largest to smallest eigenvalue.

→ What's the condition number of the identity matrix? 1

→ What's the condition number of the matrix A below? ∞

$$A = \begin{pmatrix} 2 & -1 & & & -1 \\ -1 & 2 & -1 & & 0 \\ & & \ddots & & \\ & 0 & & \ddots & \\ -1 & & & -1 & 2 \end{pmatrix}$$

→ Can we do anything to improve the condition number without changing the problem? Yes! Preconditioning!

It's essential!