PHY604 Lecture 22

November 9, 2021

Review: Steps of Markov chain Monte Carlo:

- 1. Choose random starting state
- 2. Choose a move uniformly at random from set of moves
- 3. Calculate the acceptance probability
- 4. Accept or reject the move
- 5. Measure *X* in current state, add to sum
- 6. Go back to step 2

Review: Ideal gas

- Consider the quantum states of a particle or atom of mass *m* in cubic box of length *L*
- Energy of one particle given by:

Quantum numbers from 1 to infinity.

$$E(n_x, n_y, n_z) = \frac{\pi^2 \hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$$

- Ideal gas: no interactions between particles
  - Energy is sum of individual particles:

$$E = \sum_{i=1}^{N} E(n_x^{(i)}, n_y^{(i)}, n_z^{(i)})$$

Review: Move set for ideal gas

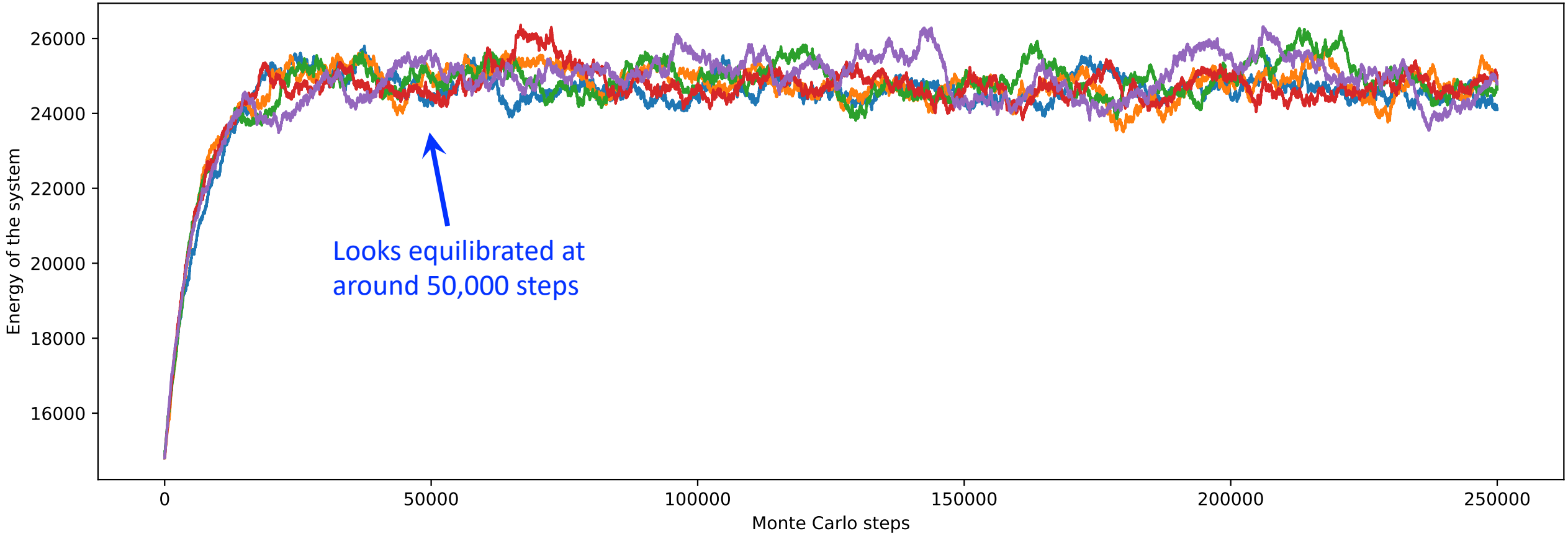
- Choose set of all moves of a single atom to one of the six "neighboring" states where n_x, n_y, or n_z differ by +/- 1
- Each Monte Carlo step, choose a random particle, chose a quantum number, change it by +/- 1
- Change in total energy just the change for single particle since there are no interactions
  - E.g., increase or decrease n_x of atom *i* by one:

$$\Delta E = \frac{\pi^2\hbar^2}{2mL^2}[(n_x \pm 1)^2 + n_y^2 + n_z^2] - \frac{\pi^2\hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2)$$

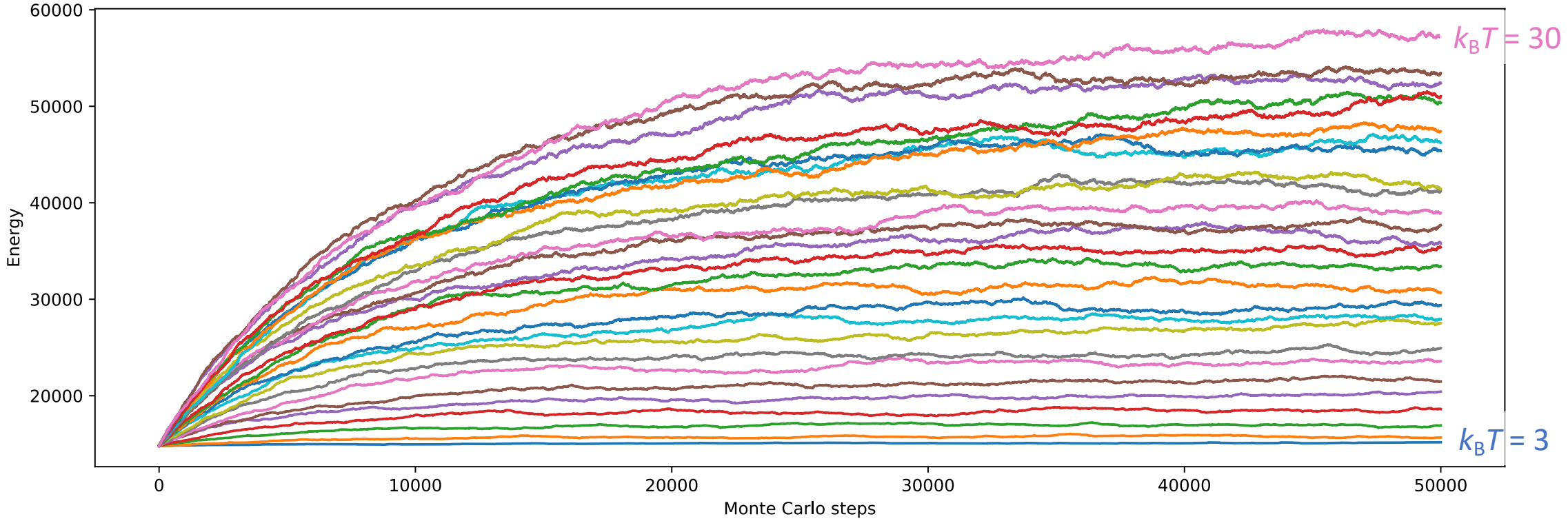
$$= \frac{\pi^2\hbar^2}{2mL^2}[(n_x \pm 1)^2 - n_x^2] = \frac{\pi^2\hbar^2}{2mL^2}(\pm 2n_x + 1)$$

- Note: Reject moves that try to make $n < 1$

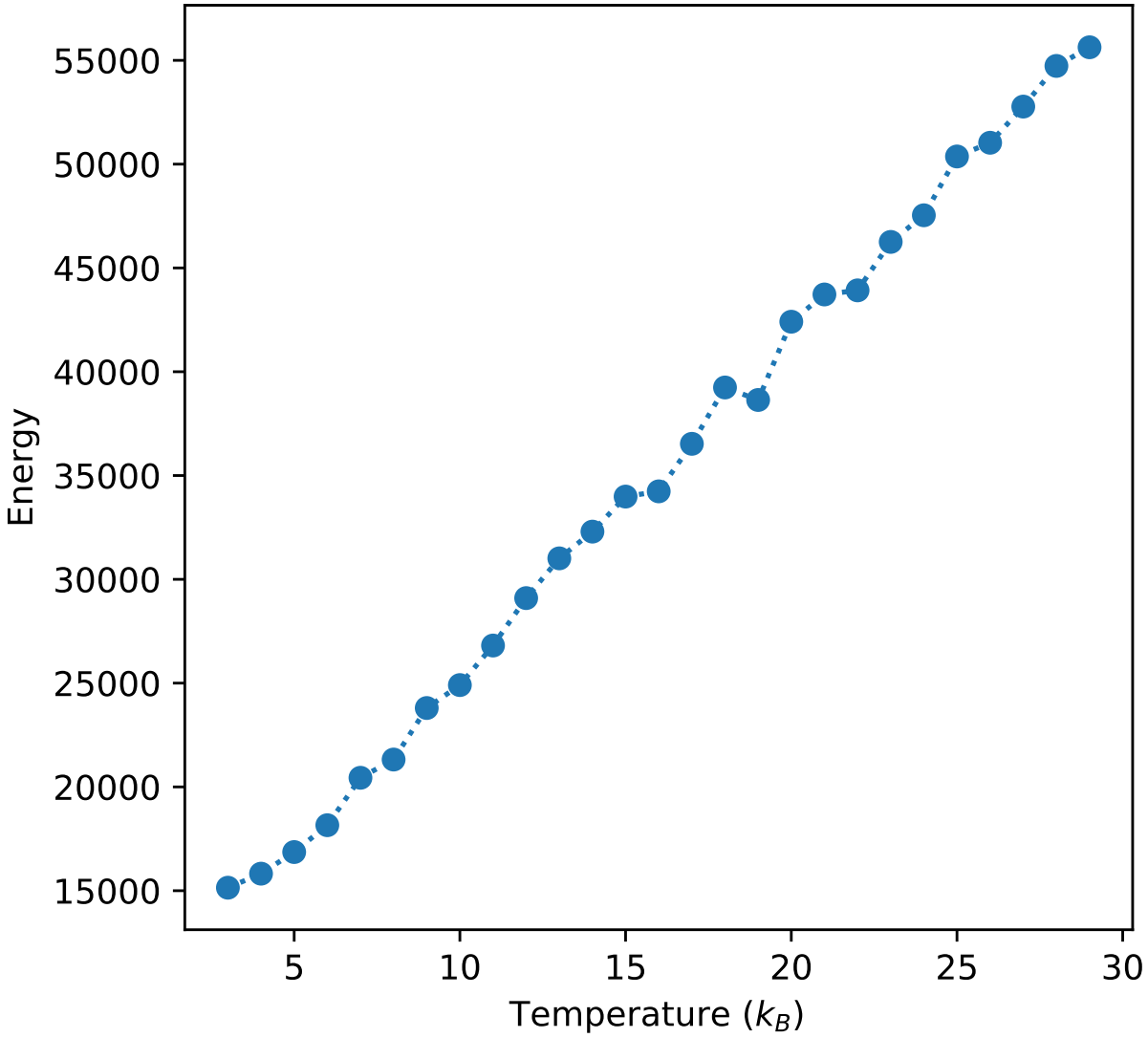
Review: Monte Carlo simulation of ideal gas



Review: Monte Carlo simulation of ideal gas: Dependence on T



Review: Monte Carlo simulation of ideal gas: E vs. T



Review: The Ising model

- The Ising model is a classic model in statistical physics for describing magnetic systems

- Describe a magnetic material as classical spins on a lattice
  - Spins can only point up or down
  - Energy is given by:

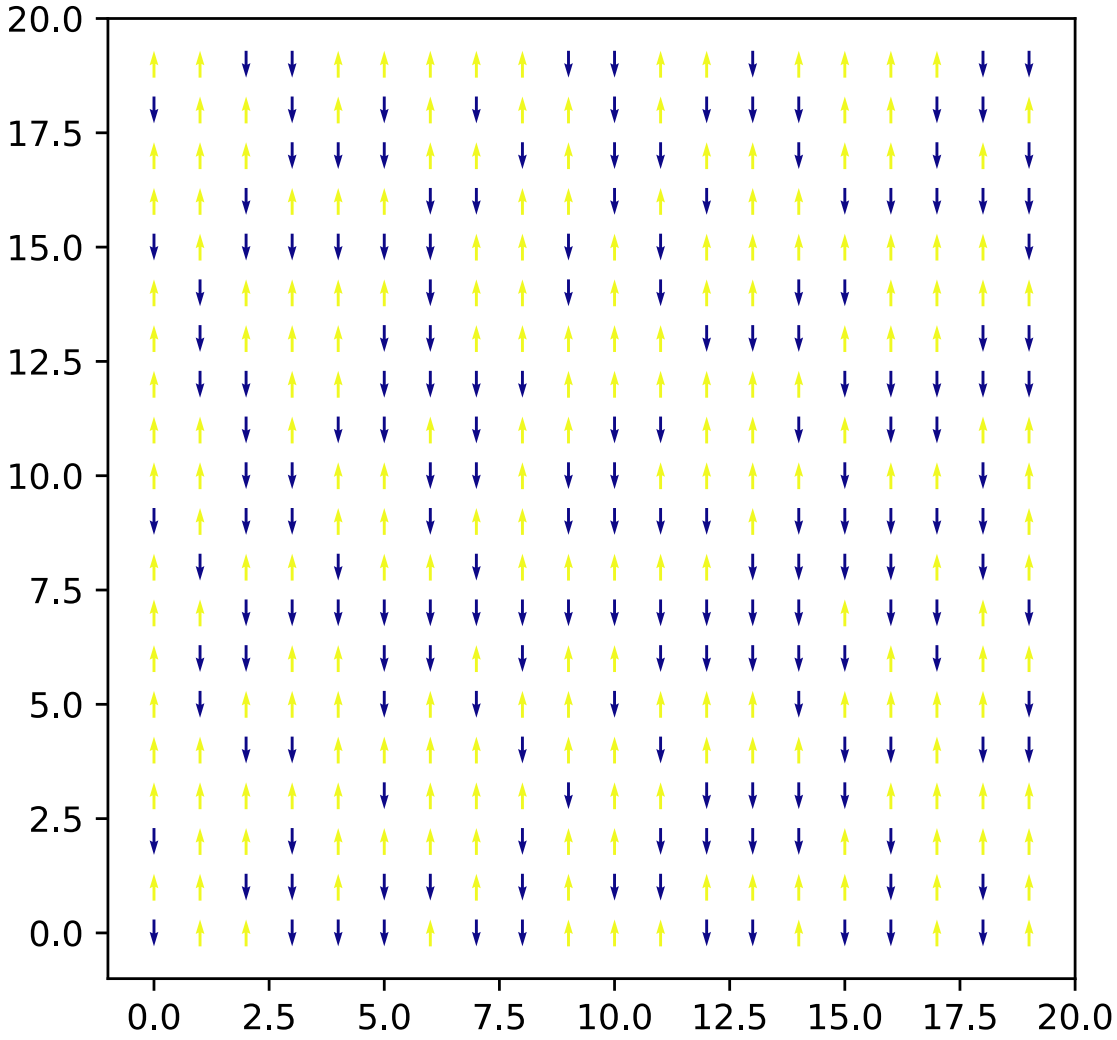
$$E = -J \sum_{\langle i,j \rangle} s_i s_j$$

  - Where $\langle i, j \rangle$ indicate neighboring spins
  - *J* is the interaction strength
    - If J > 0 aligned spins are preferred
    - If J < 0 antialigned spins are preferred

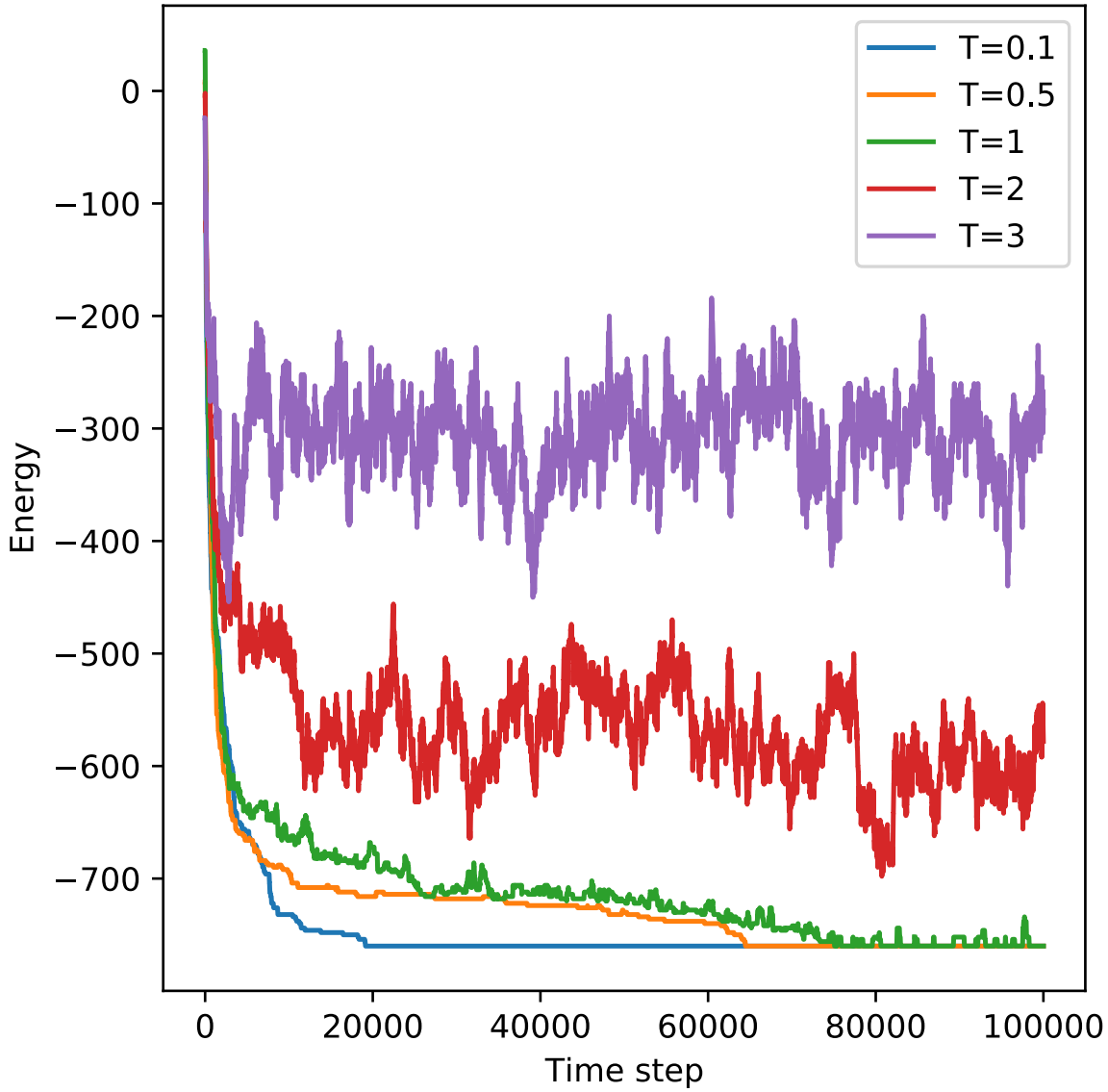
Review: Monte Carlo simulation: Ising model on square lattice

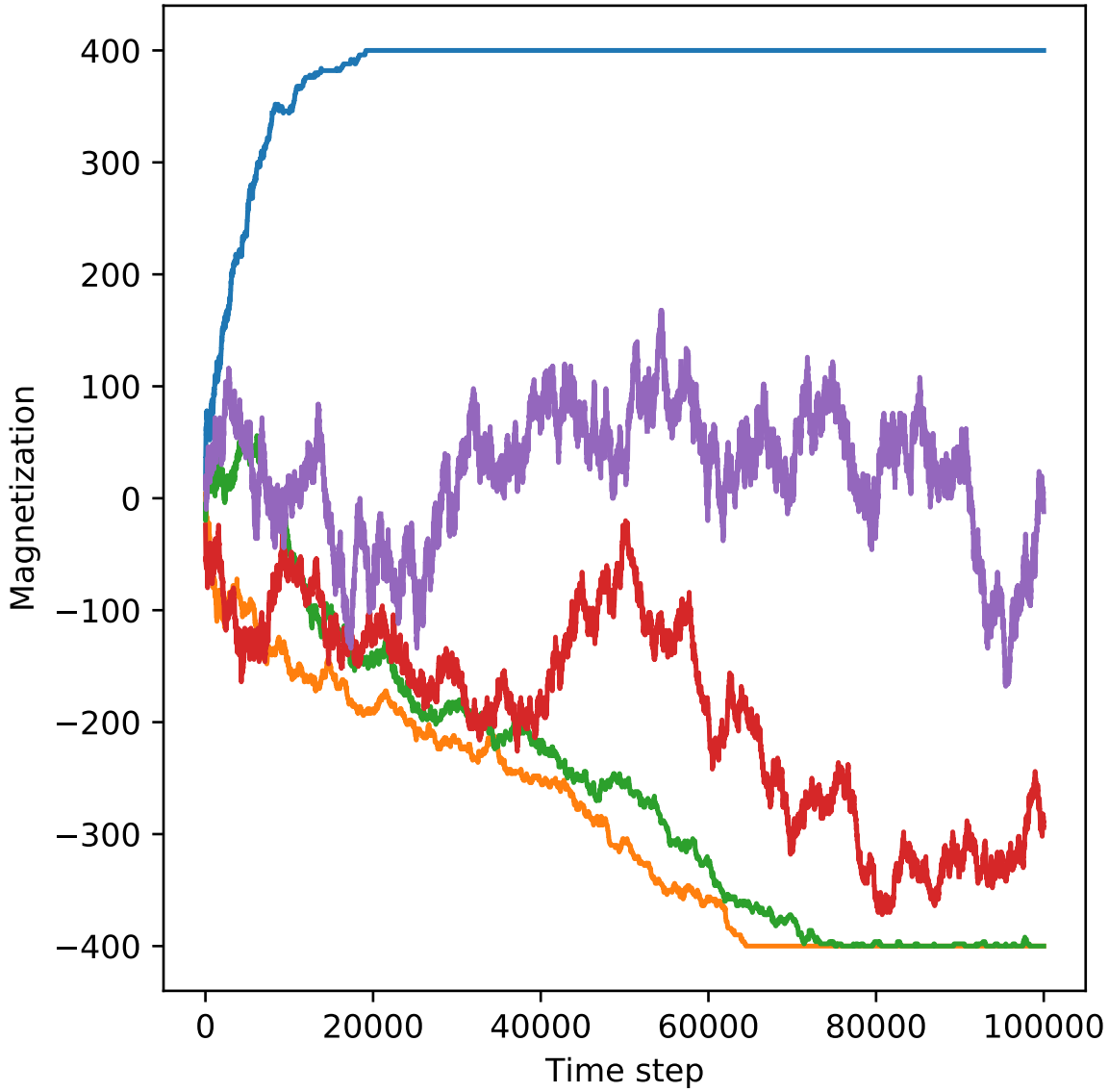
- 20 x 20 square lattice of spins
- Initialized randomly
- Move set: Flip a random spin
  - If it lowers the energy, accept
  - If it raises the energy, accept with Boltzmann probability
- Can also monitor magnetization

$$M = \sum_i s_i$$

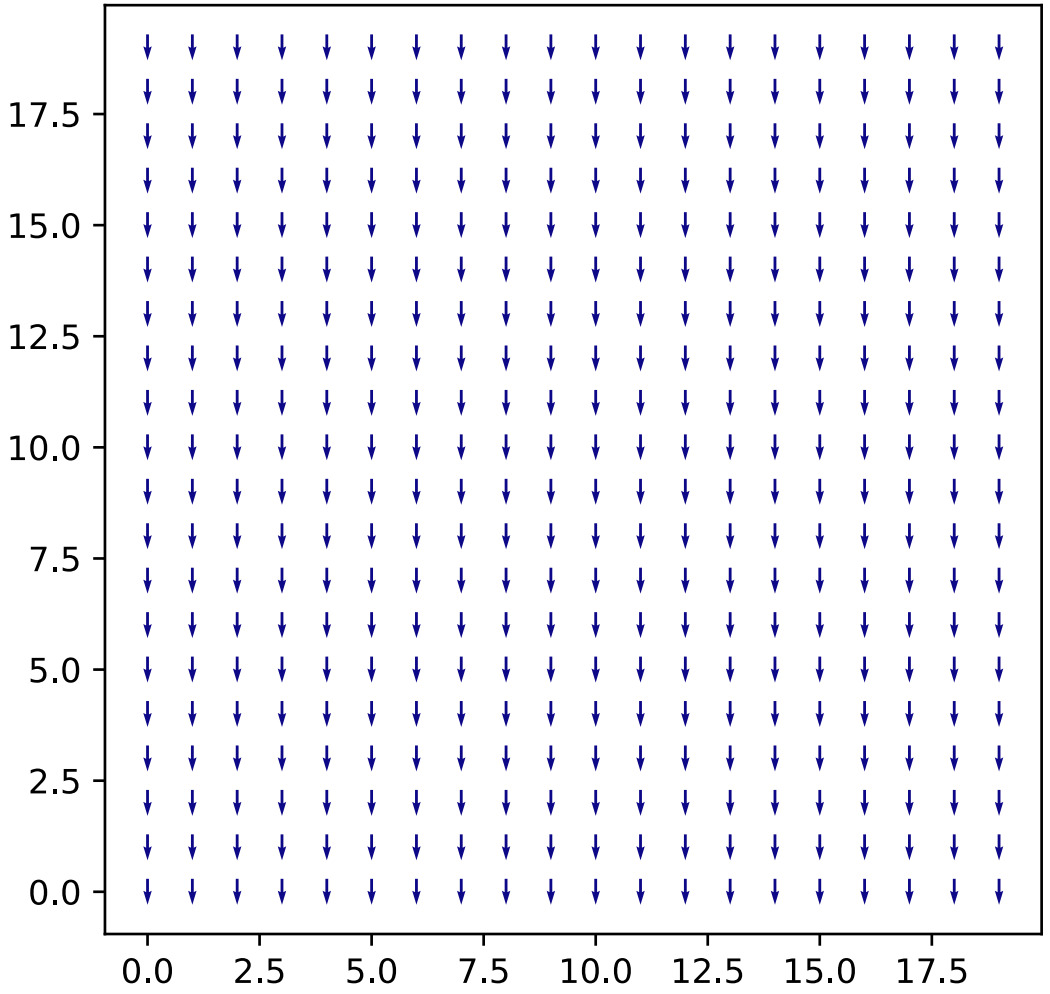


Review: Ising model on square lattice versus T

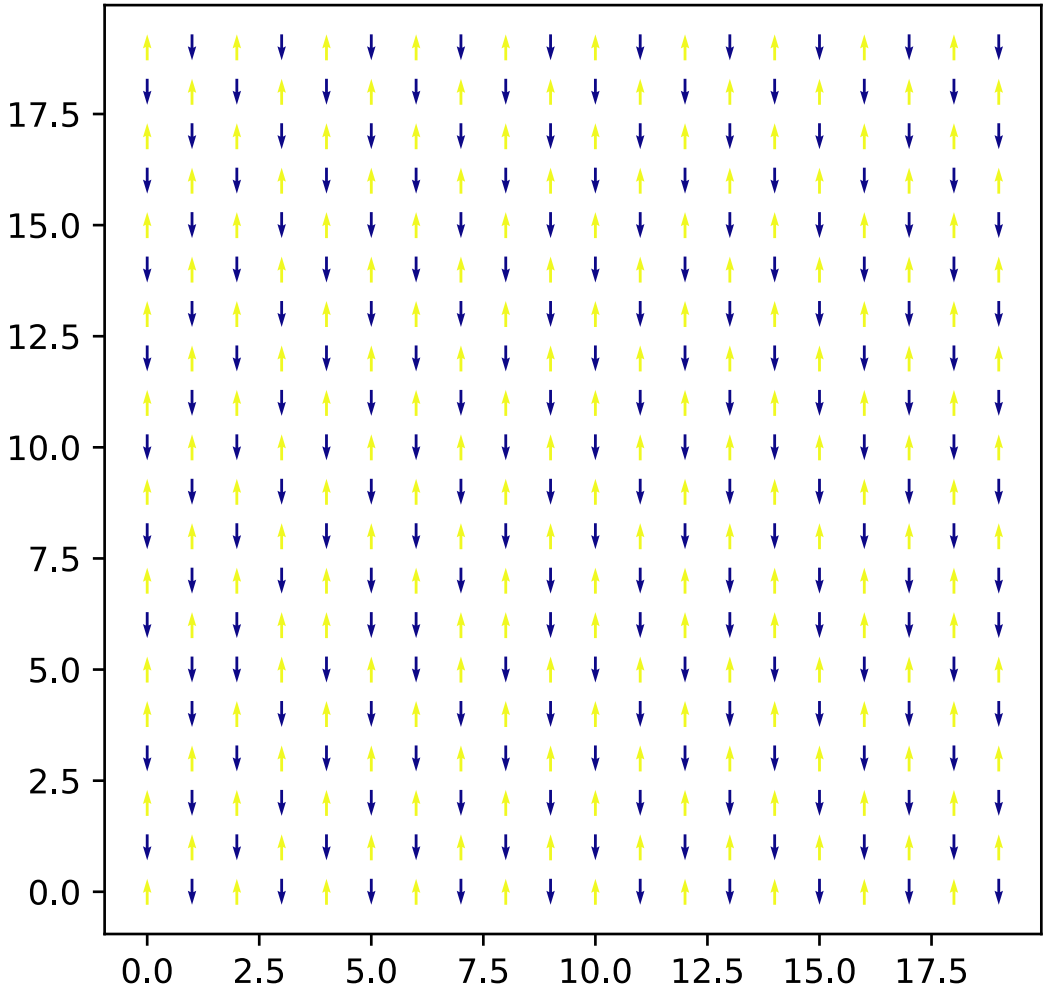




Ferromagnetic for J > 0,



Antiferromagnetic for J < 0



Today's lecture:
Simulated annealing, QMC

- Simulated Annealing
  - Travelling salesman problem
- Quantum Monte Carlo
- Genetic algorithms

Simulated annealing (Newman Sec. 10.4)

- Monte Carlo methods can also be used for numerical optimization
- Optimization methods discussed so far only give local minima
- Global optimization problems are very challenging
- Simulated annealing borrows ideas from statistical physics/materials science to tackle this problem
  - Annealing: Heat treatment of materials to remove defects by allowing atoms to move to their equilibrium structure

Statistical mechanics for optimization

- Recall the Boltzmann probability:

$$P(E_i) = \frac{e^{-\beta E_i}}{Z}, \qquad Z = \sum_i e^{-\beta E_i}$$

- Assume we have single, unique ground state
- Choose energy scale so that the ground state configuration is 0 energy
- If we cool the system to $T = 0$, then the probability distribution is:

$$P(E_i) = \begin{cases} 1 & \text{if } E_i = 0 \\ 0 & \text{if } E_i > 0 \end{cases}$$

- By cooling the system, we can find the ground state

Statistical mechanics for optimization

- We can use the same strategy (cooling the system) for finding the minimum of a function
  - Take the value of the function to be the “energy”
  - Take the values of independent variables to define a state of the system

- But how can we avoid getting trapped in a local minima?
  - Energy of all nearby states are higher in energy, will not accept moves for low T

- Solution: “Anneal” by cooling slowly so system can find its way to the global minimum
  - Guaranteed to converge to global minimum if we cool slowly enough (often not possible)

Simulated annealing approach

- Choose $k_B T$ to be significantly greater than the typical energy change from a singe Monte Carlo move
  - Then:

$$\beta(E_j - E_i) \ll 1 \quad \Longrightarrow \quad P_a \simeq 1$$

  - Most moves accepted, state of the system rapidly randomized

- Make a cooling "schedule," e.g.:

$$T = T_0 e^{-t/\tau}$$

- Choice of τ require some trial and error, slower cooling is more likely to find ground state, but simulation takes longer

Example: Travelling salesman problem

- Find the shortest route that visits a given set of locations on a map
- One of the most famous optimization problems (NP hard)
- We will assume the salesman can travel between the *N* points on the map in straight lines (i.e., the world is flat)
  - *N* cities are chosen at random in a 2D square of unit length
- Want to minimize total distance travelled over the tour:

$$D = \sum_{i=0}^{N-1} |\mathbf{r}_{i+1} - \mathbf{r}_i|$$

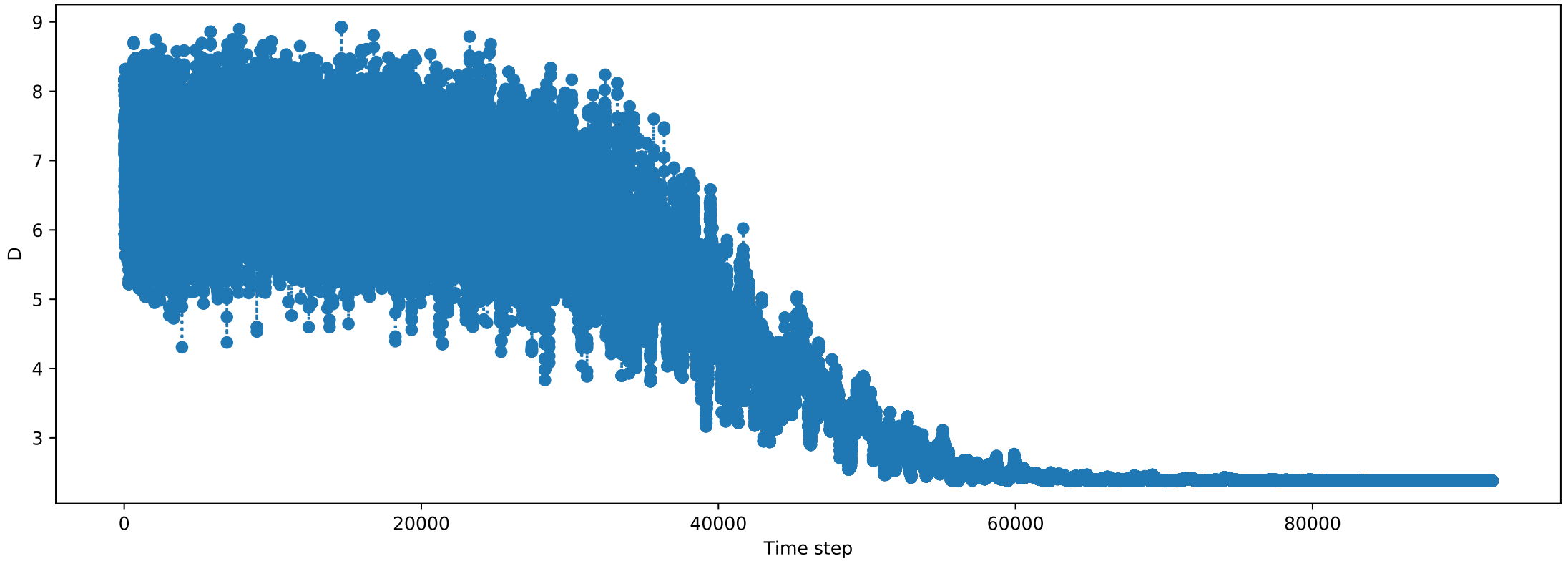
Markov chain Monte Carlo for traveling salesman

$$D = \sum_{i=0}^{N-1} |\mathbf{r}_{i+1} - \mathbf{r}_i|$$

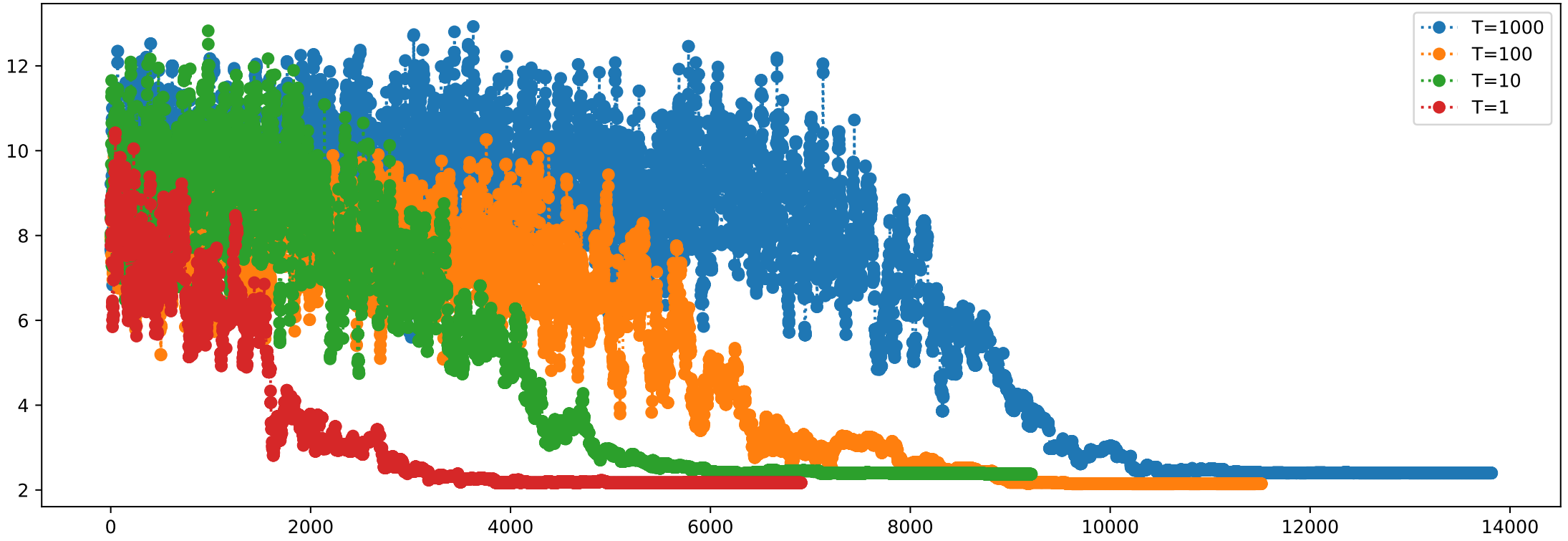
- Minimize *D* over set of all possible tours

- First set up an initial tour
- Then choose from set of moves: Swap pairs of cities
  - Accept if swap shortens the tour
  - If it lengthens the tour, accept with Boltzmann probability, energy replaced by distance D

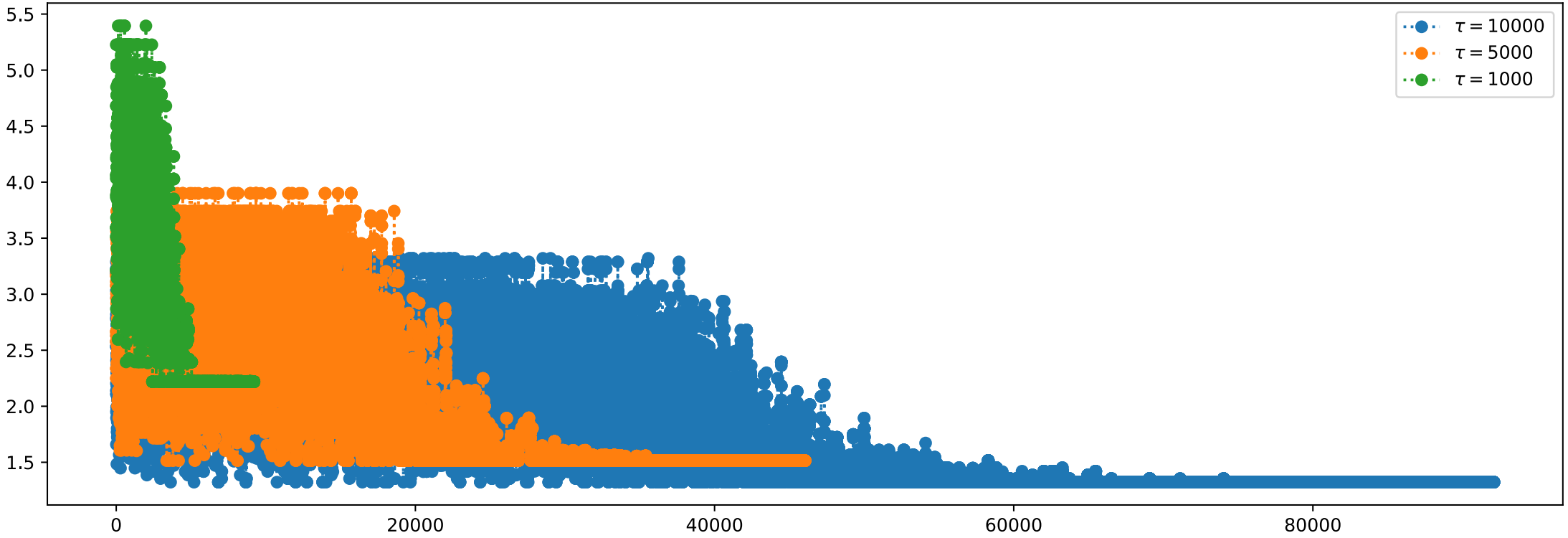
Simulated annealing for traveling salesman



Simulated annealing for traveling salesman: Different starting temperatures



Simulated annealing for traveling salesman: Different cooling rates temperatures



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Quantum Monte Carlo (Pang Sec. 10.5)

- So far, we have studied classical systems
- Monte Carlo algorithm can be generalized to study quantum systems
- Most direct generalization of the Metropolis algorithm: Variational quantum Monte Carlo
- We will just introduce some basic concepts in QMC and show how what we learned on classical systems transfers

General many-body quantum problem:

- We are seeking approximate solutions of the Hamiltonian:

$$H = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m_i} \nabla_i^2 + U_{\text{ext}}(\mathbf{r}_i) \right] + \sum_{i>j} V(\mathbf{r}_i, \mathbf{r}_j)$$

Kinetic energy

External potential

Electron-electron interaction

General many-body quantum problem:

- We are seeking approximate solutions of the Hamiltonian:

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- Time-independent many-body Schrödinger equation

$$H\Psi_n(\mathbf{R}) = E_n \Psi_n(\mathbf{R})$$

- $\mathbf{R}=(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)$ is the positions of all particles

- In general, cannot obtain analytic solution for more than two particles
- Numerically exact solutions are also limited to few particles

The many-body ground state

- Often, we would like to study the ground state of the system
- In that case, we can make use of the variational principle
  - Any other state has higher energy than the ground state
  - Introduce a trial state Φ to approximate the ground state, and minimize with respect to some set of parameters α_i

$$E[\alpha_i] = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} \geq E_0$$

- Minimize by taking parameters in the Euler-Lagrange equation

$$\frac{\delta E[\alpha_i]}{\delta \alpha_i} = 0$$

Variational minimization of many-body ground state

- We can write:

$$E[\alpha_i] = \frac{\int \Phi^\dagger(\mathbf{R}) H \Phi(\mathbf{R}) d\mathbf{R}}{\int |\Phi(\mathbf{R}')|^2 d\mathbf{R}'} \equiv \int \mathcal{W}(\mathbf{R}) \mathcal{E}(\mathbf{R}) d\mathbf{R}$$

- Where:

$$\mathcal{W}(\mathbf{R}) = \frac{|\Phi(\mathbf{R})|^2}{\int |\Phi(\mathbf{R}')|^2 d\mathbf{R}'}, \qquad \mathcal{E}(\mathbf{R}) = \frac{1}{\Phi(\mathbf{R})} H \Phi(\mathbf{R})$$

Distribution function

Local energy of specific **R**

Variational minimization of many-body ground state

- We can write:

$$E[\alpha_i] = \frac{\int \Phi^\dagger(\mathbf{R}) H \Phi(\mathbf{R}) d\mathbf{R}}{\int |\Phi(\mathbf{R}')|^2 d\mathbf{R}'} \equiv \int \mathcal{W}(\mathbf{R}) \mathcal{E}(\mathbf{R}) d\mathbf{R}$$

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- If we know these, we can evaluate the expression via Monte Carlo
- Then vary α_i to minimize $E[\alpha_i]$

The trial wavefunction

- Common choice for trial wavefunctions:

$$\Phi(\mathbf{R}) = D(\mathbf{R})e^{-U(\mathbf{R})}$$

- $D(\mathbf{R})$ is a constant for bosons and a Slater determinant of single-particle orbitals for fermion systems
- $U(\mathbf{R})$ is ”Jastrow factor”:

$$U(\mathbf{R}) = \sum_{i=1}^{N} u_i(\mathbf{r}_i) + \sum_{i>j}^{N} u_2(\mathbf{r}_i, \mathbf{r}_j) + \dots$$

Comes from the interaction of particles with external potential

Comes from the interparticle interactions

The trial wavefunction

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- The key to the method is to choose a trial wavefunction that contains the necessary physics

Procedure for variational QMC

- 1. Choose a basis of single-particle orbitals
- 2. For fermions, construct Slater determinant (by a linear combination of atomic orbitals, or a by single-particle method like Hartree-Fock or DFT)
- 3. Determine the interparticle interactions
- 4. Perform Metropolis steps, e.g., by altering particle positions $\mathbf{r}_i$
- 5. Use as the probability in the Markov chain: $\mathcal{W}(\mathbf{R}) = \frac{|\Phi(\mathbf{R})|^2}{\int |\Phi(\mathbf{R}')|^2 d\mathbf{R}'}$
- 6. Accumulate average energy via local energy: $E = \frac{1}{M} \sum_{m=1}^{M} \mathcal{E}(\mathbf{R}_m)$

Diffusion Monte Carlo with Green's functions

- Variational Monte Carlo limited by trail wave function. Can we go beyond this to find the exact ground state?

- Diffusion Monte Carlo: Treat the ground state of the Schrödinger equation as the stationary solution of a diffusion equation
  - We used this approach before for solving the Poisson equation

- Diffusion equation in this case is "imaginary time Schrödinger equation":

$$\frac{\partial \Phi(\mathbf{R}, t)}{\partial t} = -(H - E_c)\Phi(\mathbf{R}, t)$$

- E_c is adjustable energy offset

Green's function:

- At a later time, the wave function is:

$$\Phi(\mathbf{R}, t+\tau) = \int G(\mathbf{R}, \mathbf{R}'; \tau)\Phi(\mathbf{R}', t)d\mathbf{R}'$$

- Where *G* is the Green's function, obeys the same equation of the wavefunctions (with a delta function initial condition):

$$\left[\frac{\partial}{\partial t} - (H - E_c)\right] G(\mathbf{R}, \mathbf{R}'; \tau) = \delta(\mathbf{R} - \mathbf{R}')\delta(\tau)$$

- Or:

$$G(\mathbf{R}, \mathbf{R}'; \tau) = \langle \mathbf{R}| \exp[-\tau(H - E_c)]|\mathbf{R}'\rangle$$

Projecting onto the ground state

- We now use the expansion in terms of eigenfunctions of *H,* Ψ_i with eigenvalues E_i:

$$\exp(-\tau H) = \sum_i |\Psi_i\rangle \exp(-\tau E_i) \langle \Psi_i|$$

- The the Green's function can be written:

$$G(\mathbf{R}, \mathbf{R}'; \tau) = \sum_i \Psi_i(\mathbf{R}) \exp[-\tau(E_i - E_c)] \Psi_i^*(\mathbf{R}')$$

- Choose an initial state, e.g., the trial wavefunction from variational QMC:

$$\Phi(\mathbf{R}, 0) = \Phi_{\text{init}}(\mathbf{R})$$

Projecting onto the ground state

- Now we take τ to infinity:

$$\lim_{\tau\to\infty} \langle \mathbf{R}|e^{-\tau(H-E_c)}|\Phi_{\text{init}}\rangle$$

$$= \lim_{\tau\to\infty} \int G(\mathbf{R},\mathbf{R}';\tau)\Phi_{\text{init}}(\mathbf{R}')d\mathbf{R}'$$

$$= \lim_{\tau\to\infty} \sum_i \Psi_i(\mathbf{R})e^{-\tau(E_i-E_c)}\langle\Psi_i|\Phi_{\text{init}}\rangle$$

$$= \lim_{\tau\to\infty} \left(\Psi_0(\mathbf{R})e^{-\tau(E_0-E_c)}\langle\Psi_0|\Phi_{\text{init}}\rangle + \sum_{i=1} \Psi_i(\mathbf{R})e^{-\tau(E_i-E_c)}\langle\Psi_i|\Phi_{\text{init}}\rangle \right)$$

- Adjusting E_c to E_0 suppresses the second term, giving us the ground state
  - As long as there is some overlap with our initial state

Wait, what is the Green's function?

$$G(\mathbf{R}, \mathbf{R}'; \tau) = \sum_i \Psi_i(\mathbf{R}) \exp[-\tau(E_i - E_c)] \Psi_i^*(\mathbf{R}')$$

- We don't know the eigenstates/eigenvalues *a priori*
- Let consider the the imaginary time Schrödinger equation with no potential

$$\frac{\partial \Phi(\mathbf{R}, t)}{\partial t} = \frac{1}{2} \nabla^2 \Phi(\mathbf{R}, t)$$

- We have solved this problem before with a delta function initial condition! Just the linear diffusion equation.
  - At later times it is a Gaussian
  - In this case, we are in 3*N* dimensions

$$G_d(\mathbf{R}, \mathbf{R}'; \tau) = (2\pi\tau)^{-3N/2} \exp\left[-\frac{|\mathbf{R} - \mathbf{R}'|^2}{2\tau}\right]$$

Suzuki-Trotter decomposition and birth/death

- Can show that the effect of the potential on the Green's function is approximately (for small τ):

$$G(\mathbf{R},\mathbf{R}';\tau) \simeq (2\pi\tau)^{-3N/2} \exp\left[-\frac{|\mathbf{R}-\mathbf{R}'|^2}{2\tau}\right] \exp\left[-\tau\frac{V(\mathbf{R})+V(\mathbf{R}')-2E_c}{2}\right]$$

- Can treat the factor:

$$P = \exp\left[-\tau\frac{V(\mathbf{R})+V(\mathbf{R}')-2E_c}{2}\right]$$

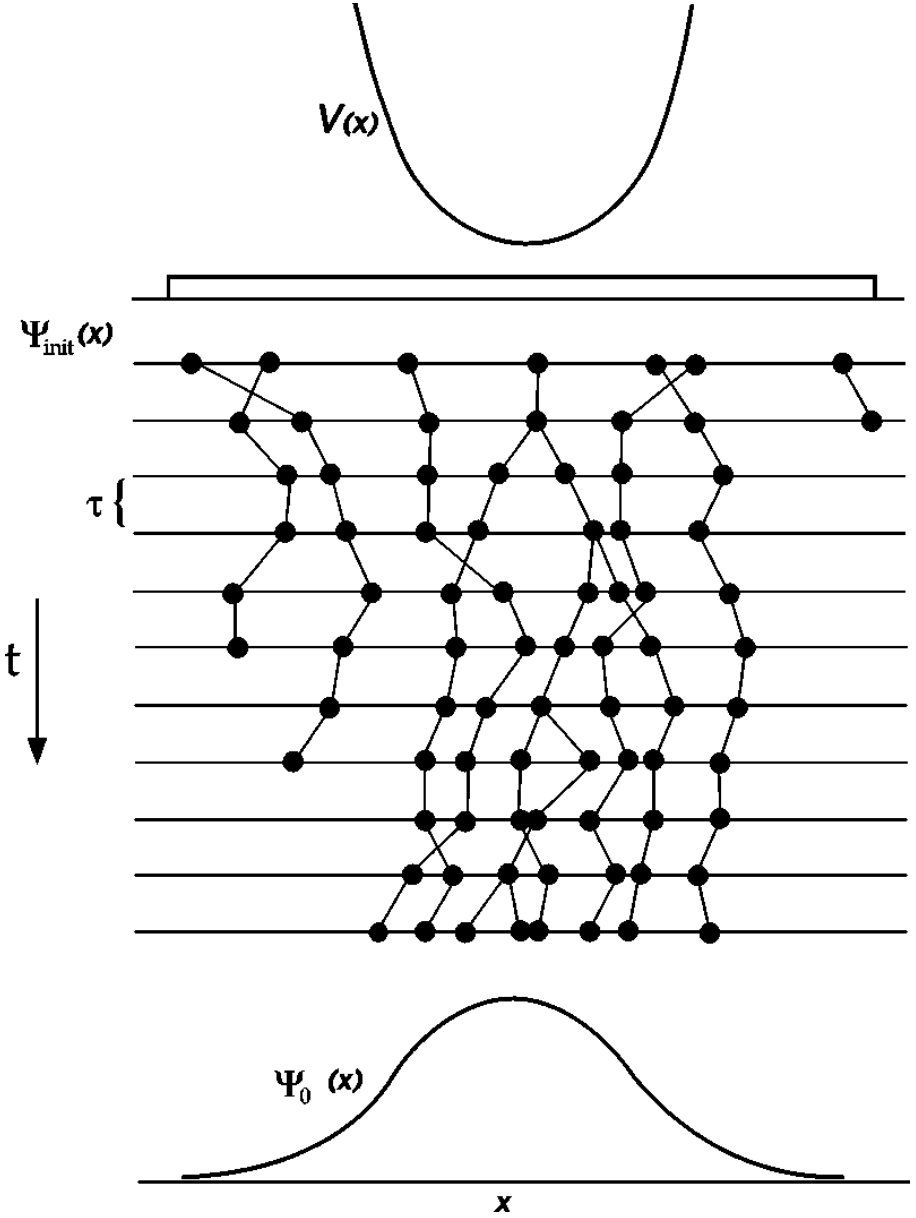
- As a reweighting of the free-particle Green's function
- Can be used to kill random walkers that enter high-potential areas of Hilbert space (see next slide)

Markov chain for QMC

- To do the Metropolis algorithm, we first create an ensemble of independent configurations: "random walkers"

- Propagate based on the diffusion part of Green's function G_d
  - As we showed, will propagate to ground state over time

- Use *P* as a "branching" probability distribution to choose whether:
  - Walker is killed
  - Walker continues its propagation
  - Walker continues its propagation and an additional one is spawned



Rev. Mod. Phys. 73 (2001)

Importance sampling in QMC

- Note that P exponentially suppresses propagation into high-potential areas, and potential may vary quickly and significantly
- We can make this more efficient with importance sampling
- Construct a “probability-like” function:

$$F(\mathbf{R}, t) = \Phi(\mathbf{R}, t)\Psi(\mathbf{R})$$

- Where Ψ is a trial wave function, e.g., from variational QMC
- This satisfies the diffusion equation:

$$\frac{\partial F}{\partial t} = \frac{1}{2}\nabla^2 F - \nabla \cdot F\mathbf{U} + [E_c - \mathcal{E}(\mathbf{R})]F$$

- Where we have a “drift” velocity: $U = \nabla \ln \Psi(\mathbf{R})$
- And we see again the local energy: $\mathcal{E}(\mathbf{R}) = \frac{1}{\Psi(\mathbf{R})} H\Psi(\mathbf{R})$

Modified Green's function

- Can show that the new Green's function is:

$$G(\mathbf{R},\mathbf{R}';\tau) \simeq (2\pi\tau)^{-3N/2} \exp\left[-\frac{[\mathbf{R}-\mathbf{R}'-\tau\mathbf{U}(\mathbf{R}')]^2}{2\tau}\right]$$
$$\times \exp\left[-\tau\frac{\mathcal{E}(\mathbf{R})+\mathcal{E}(\mathbf{R}')-2E_c}{2}\right]$$

- The drift velocity pushes random walkers towards areas of high density of the trial wave function

- If the trial wavefunction is good, the local energy is approximately constant, so second term does not vary too rapidly

Sign problem and fixed node approximation

- We have a crucial issue not yet discussed: Probabilistic methods like MC assume that probability distributions are positive
- Because we require wavefunctions of fermions to be antisymmetric, they cannot be positive everywhere
  - Need to assign a sign to the walkers, may change as they move through configuration space
- This leads to the fermion sign problem: If we sample over many configurations, we will get approximately zero
  - Gives decaying signal to noise ratio rather than the other way around

- Fixed node approximation: Take the zeros of trial wavefunction to be fixed and prevent walkers from changing sign

Importance sampling and the fixed node approximation

- Recall the Green's function we got from importance sampling:

$$G(\mathbf{R},\mathbf{R}';\tau) \simeq (2\pi\tau)^{-3N/2} \exp\left[-\frac{[\mathbf{R}-\mathbf{R}'-\tau\mathbf{U}(\mathbf{R}')]^2}{2\tau}\right]$$
$$\times \exp\left[-\tau\frac{\mathcal{E}(\mathbf{R})+\mathcal{E}(\mathbf{R}')-2E_c}{2}\right]$$

- Drift velocity carries walkers away from nodal surface
- Local energy also diverges near the nodal surface
- So, this importance sampling helps enforce the fixed node approximation
  - Walkers can still traverse a node if the time step is too big

One more issue: Approximation for Green's function poor near nodes

- Our approximation for the Green's function is not good when the drift velocity and local energy become large
- Could take smaller time steps to make sure we are pushed away from nodes
- Alternative approach: One more accept/reject step:
  - Accept propagation with probability:

$$w(\mathbf{R}', \mathbf{R}, \tau) = \frac{\Psi(\mathbf{R}')^2 G(\mathbf{R}', \mathbf{R}; \tau)}{\Psi(\mathbf{R})^2 G(\mathbf{R}, \mathbf{R}'; \tau)}$$

- This actually improves the approximation to the Green's function by enforcing a key property of the exact Green's function: detailed balance

Procedure for diffusion QMC

- 1. Perform a variational Monte Carlo simulation to optimize variational parameters in trial wave function.
- 2. Use the wavefunction from step 1 to generate an initial ensemble of configurations
- 3. Update with drift term and random walk χ: $\mathbf{R}' = \mathbf{R} + \mathbf{U}\tau + \chi$
- 4. Reject any step that crosses a node.
- 5. Accept the move with probability:

$$w(\mathbf{R}', \mathbf{R}, \tau) = \frac{\Psi(\mathbf{R}')^2 G(\mathbf{R}', \mathbf{R}; \tau)}{\Psi(\mathbf{R})^2 G(\mathbf{R}, \mathbf{R}'; \tau)}$$

- 6. Create a new ensemble of walkers using branching probability *P*
- 7. Measure local energy
- 8. Update E_c by averaging local energy over configurations **R** and **R'**

Some comments on QMC

- Quantum Monte Carlo is often the standard for accuracy for numerical calculations of solids and molecules

- It is at the basis of many other methods in condensed-matter physics
  - I.e., density-functional theory approximations rely on QMC of homogeneous electron gas
  - Solvers for embedding methods such as dynamical mean-field theory use ”continuous time” QMC

- The key to an efficient accurate scheme is how to deal with the sign problem

Today's lecture:
Simulated annealing, QMC

- Simulated Annealing
  - Travelling salesman problem
- Quantum Monte Carlo
- Genetic algorithms

Genetic Algorithms (Pang Ch. 11)

- We saw in the case of simulated annealing:
  - Finding global minima is difficult
  - We can use inspiration from physics in solving unrelated problems in optimization

- Genetic algorithms are techniques for optimization inspired by biology
  - Create “organisms” that store a set of chromosomes
  - Create new organisms by mixing the genes of parents, and allowing for mutations

Steps for the genetic algorithm

- The problem: find the global minimum of multi-variable function $g(r_1,r_2,\ldots,r_n)$

- 1. Create a gene pool, i.e., an initial population of configurations
  - Configurations are values of variables
  - Can be binary or continuous
- 2. Selection: Choose members to be parents
- 3. Crossover: Produce offspring by mixing their genes
  - Parent chromosomes are cut into segments, exchanged, and joined together
- 4. Mutation: Create random changes to the chromosomes
- 5. In all of the steps above, make sure the configurations with lowest cost (evaluation of g) survive

Example: the Thompson problem

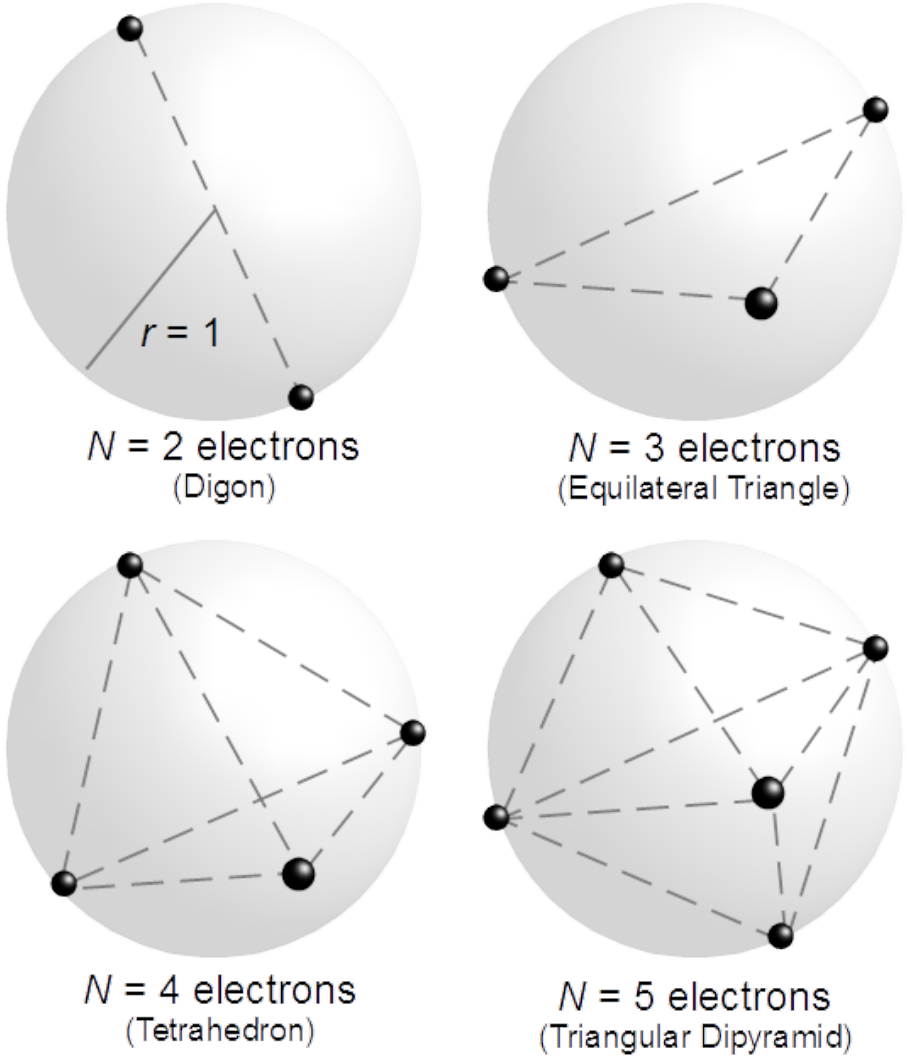
- Consider placing like charges on a unit sphere
- What is the optimal arrangement to reduce the electrostatic energy:

$$U = \frac{q^2}{4\pi\epsilon_0} \sum_{i>j=1}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

- Inspired by J.J. Thompson's "plum pudding model" for atoms

Solutions to the Thompson problem

N	E_1	Symmetry	$\left\|\sum \mathbf{r}_i\right\|$	v_3	v_4	v_5	v_6	v_7	v_8	e	f_3	f_4	θ_1	Equivalent polyhedron
2	0.500000000	$D_{\infty h}$	0	–	–	–	–	–	–	2	–	–	180.000°	digon
3	1.732050808	D_{3h}	0	–	–	–	–	–	–	3	2	–	120.000°	triangle
4	3.674234614	T_d	0	4	0	0	0	0	0	6	4	0	109.471°	tetrahedron
5	6.474691495	D_{3h}	0	2	3	0	0	0	0	9	6	0	90.000°	triangular dipyramid
6	9.985281374	O_h	0	0	6	0	0	0	0	12	8	0	90.000°	octahedron
7	14.452977414	D_{5h}	0	0	5	2	0	0	0	15	10	0	72.000°	pentagonal dipyramid
8	19.675287861	D_{4d}	0	0	8	0	0	0	0	16	8	2	71.694°	square antiprism
9	25.759986531	D_{3h}	0	0	3	6	0	0	0	21	14	0	69.190°	triaugmented triangular prism
10	32.716949460	D_{4d}	0	0	2	8	0	0	0	24	16	0	64.996°	gyroelongated square dipyramid
11	40.596450510	C_{2v}	0.013219635	0	2	8	1	0	0	27	18	0	58.540°	edge-contracted icosahedron
12	49.165253058	I_h	0	0	0	12	0	0	0	30	20	0	63.435°	icosahedron (geodesic sphere $\{3,5+\}_{1,0}$)
13	58.853230612	C_{2v}	0.008820367	0	1	10	2	0	0	33	22	0	52.317°	
14	69.306363297	D_{6d}	0	0	0	12	2	0	0	36	24	0	52.866°	gyroelongated hexagonal dipyramid
15	80.670244114	D_3	0	0	0	12	3	0	0	39	26	0	49.225°	
16	92.911655302	T	0	0	0	12	4	0	0	42	28	0	48.936°	
17	106.050404829	D_{5h}	0	0	0	12	5	0	0	45	30	0	50.108°	double-gyroelongated pentagonal dipyramid
18	120.084467447	D_{4d}	0	0	2	8	8	0	0	48	32	0	47.534°	
19	135.089467557	C_{2v}	0.000135163	0	0	14	5	0	0	50	32	1	44.910°	
20	150.881568334	D_{3h}	0	0	0	12	8	0	0	54	36	0	46.093°	
21	167.641622399	C_{2v}	0.001406124	0	1	10	10	0	0	57	38	0	44.321°	
22	185.287536149	T_d	0	0	0	12	10	0	0	60	40	0	43.302°	



https://en.wikipedia.org/wiki/Thomson_problem

After class tasks and the rest of the semester

- Homework 5 due Nov. 11, 2021
- There will be **no homework 6**
- Final projects: Send topics by Nov. 11
- First draft of first two sections of writeup due Nov. 18

- Readings:
  - Simulated annealing: Newman Sec. 10.4
  - QMC:
    - Pang Secs. 10.5, 10.6
    - https://journals.aps.org/rmp/abstract/10.1103/RevModPhys.73.33
    - https://journals.aps.org/prb/abstract/10.1103/PhysRevB.16.3081
  - Genetic algorithms:
    - https://en.wikipedia.org/wiki/Thomson_problem
    - Pang Ch. 11