PHY604 Lecture 20

November 2, 2021

Review: Transformation method for changing distributions

- We have a source of random numbers *z* drawn from distribution *q*(*z*)
  - Probability of generating a number between *z* and *z*+d*z* is *q*(*z*)d*z*
- Now we choose a function *x* = *x*(*z*) whose distribution *p*(*x*) is the one we want
- We know that: $$p(x)dx = q(z)dz$$
- If our random numbers are drawn from a uniform distribution [0,1), *q*(*z*)=1 from 0 to 1, zero elsewhere
- Then:

$$\int_{-\infty}^{x(z)} p(x')dx' = \int_{0}^{z} dz' = z$$

- We need to do the integral on the left and then solve for *x*(*z*)
  - Not always possible

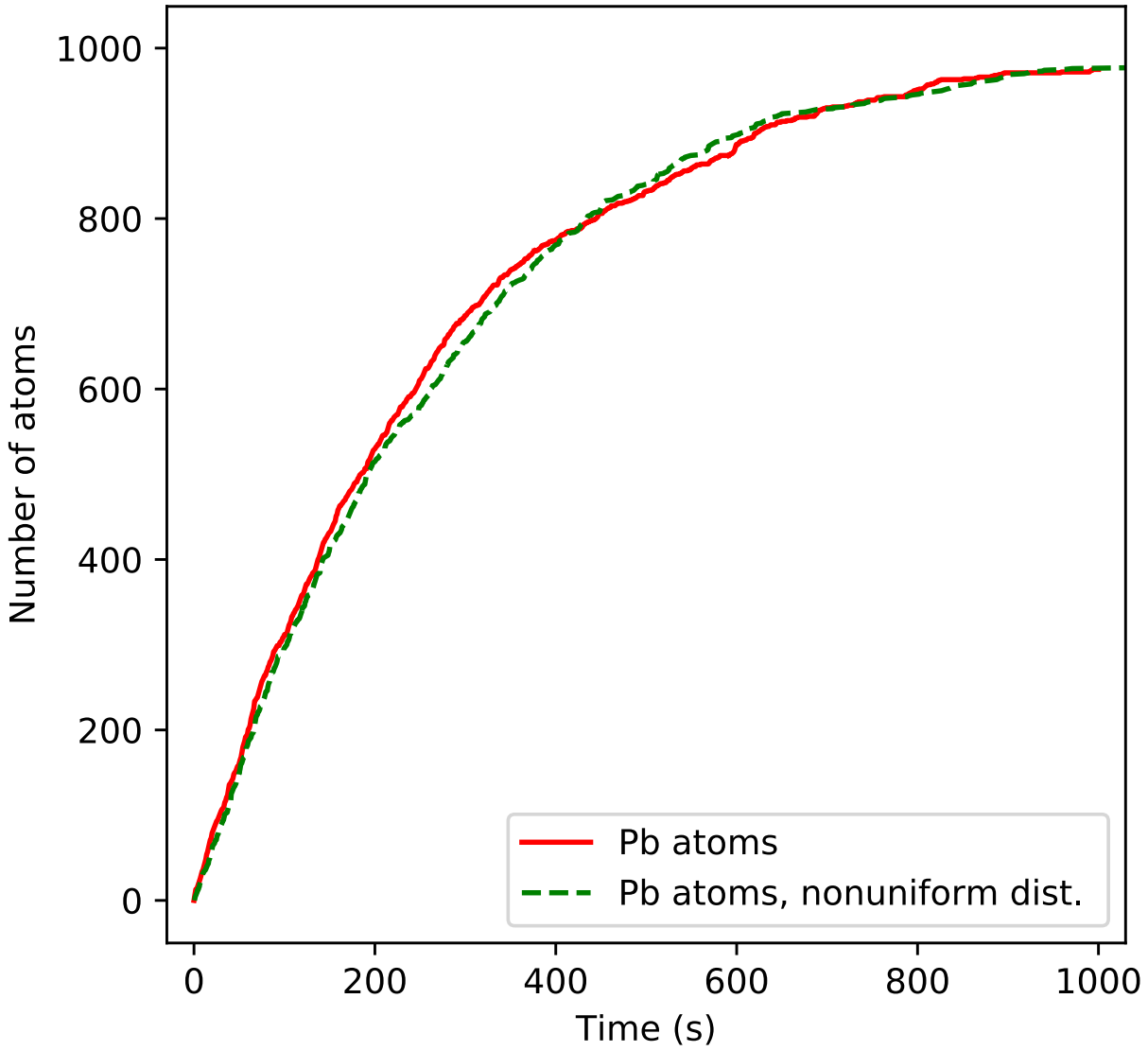
Review: Nonuniform distribution for decay example

- We can write the probability distribution for the decay example as

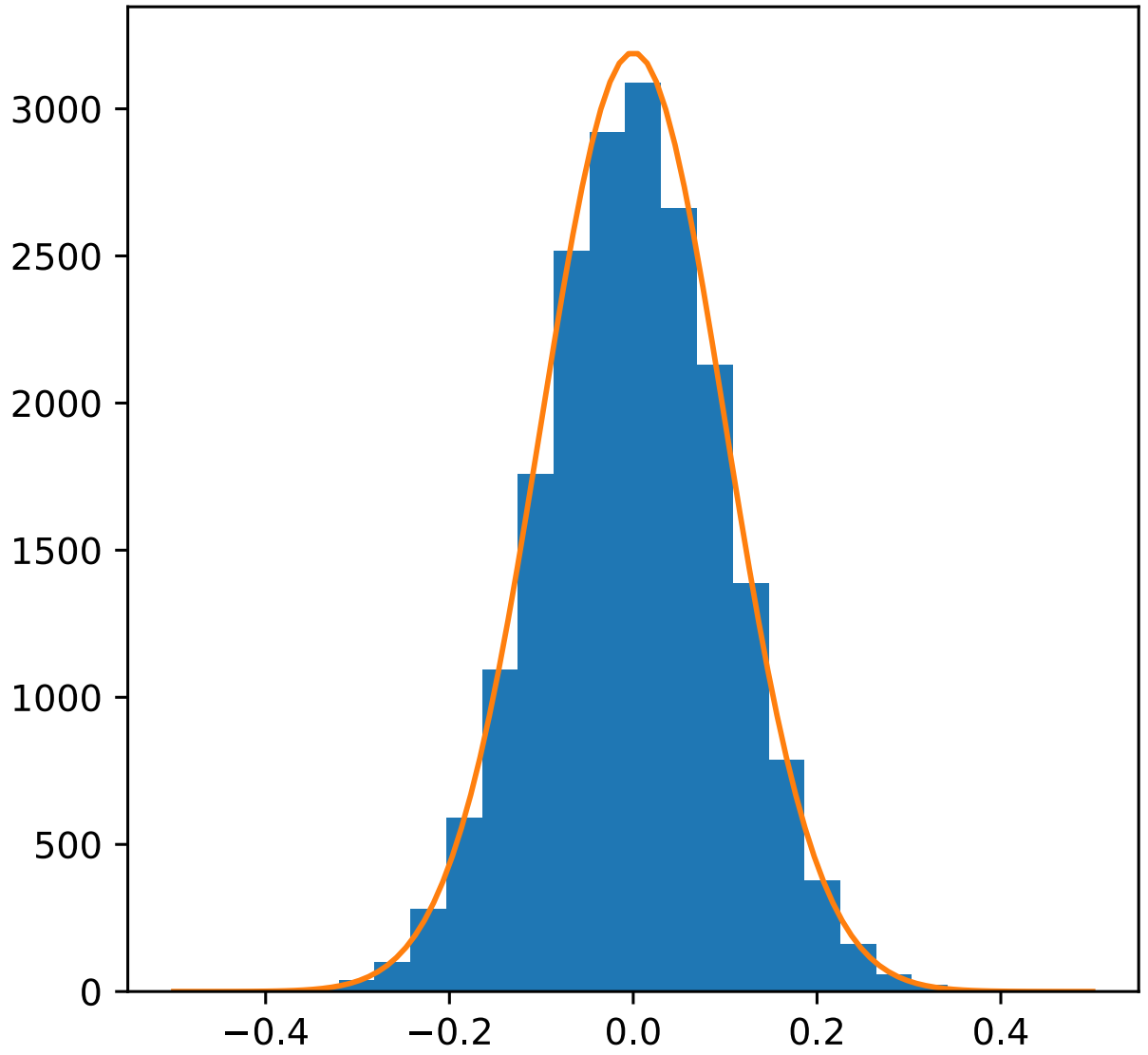
$$P(t)dt = 2^{-t/\tau}\frac{\ln 2}{\tau}dt = e^{-t\ln 2/\tau}\frac{\ln 2}{\tau}$$

- So:

$$x = -\frac{\tau}{\ln 2}\ln(1-z)$$



Example: Random numbers from Gaussian distribution

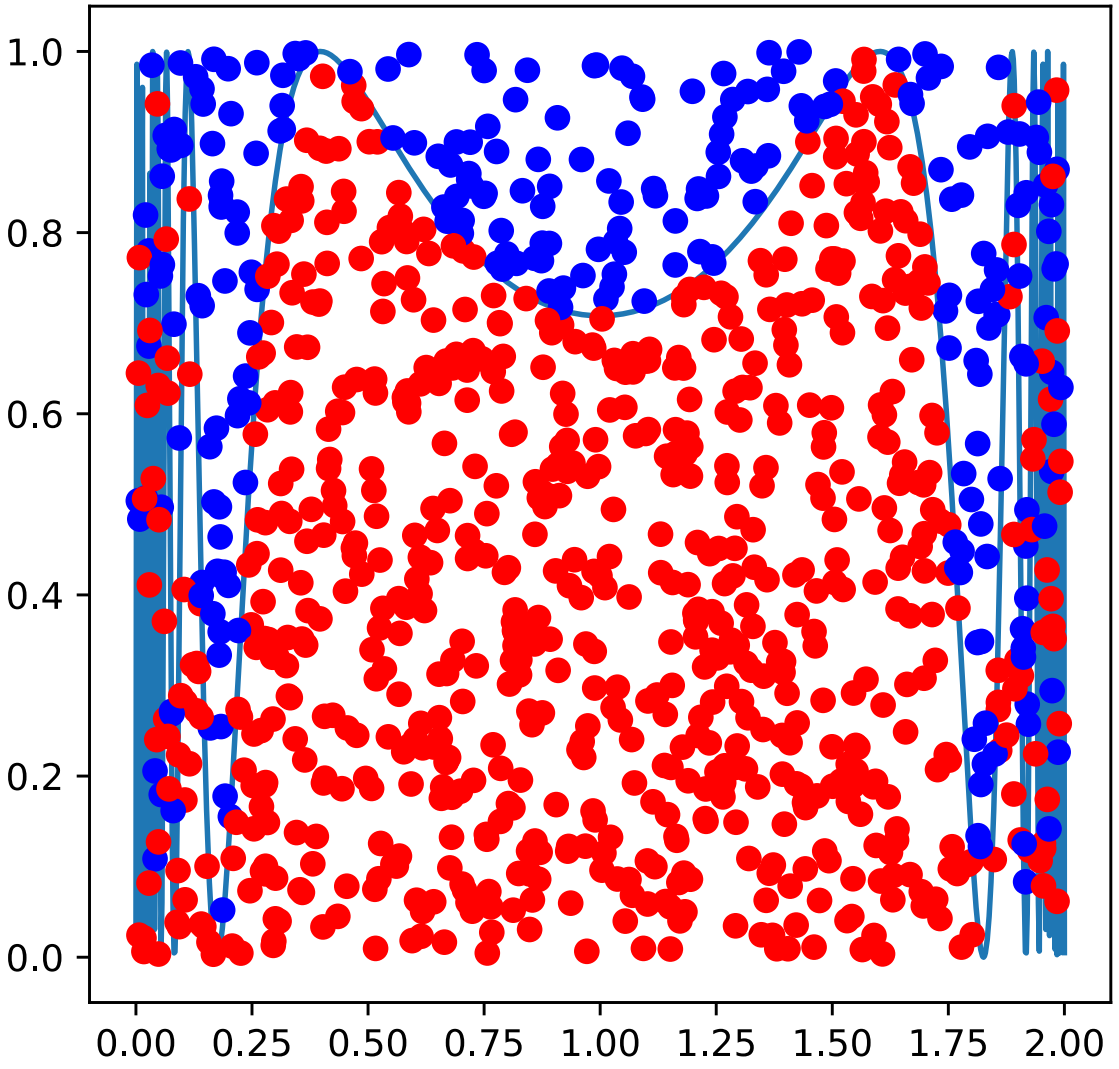


Monte Carlo Integration with random sampling

$$I = \int_0^2 \sin^2 \left[\frac{1}{x(2-x)} \right] dx$$

- Choose *N* random samples in the bounding rectangle with area *A*=2
- Check which lie under the curve
- Probability that point lies under the curve is $p = I/A$
- Fraction of points under the curve k/N should be approximately p
- So:

$$I \simeq \frac{kA}{N}$$



Review: Compare MC errors to quadrature rules

$$I_{\text{error}} = \sqrt{\text{var}k}\frac{A}{N} = \frac{\sqrt{I(A-I)}}{\sqrt{N}} \propto \frac{1}{\sqrt{N}}$$

- Errors for MC integration decrease like $N^{-1/2}$
- For the trapezoid rule, error was on the order of Δx^2, where Δx is the width of the integration slice:

$$\Delta x = \frac{b-a}{N}$$

- So, error decreases like N^{-2} much better than MC!
- For Simpson's rule, it decreases like N^{-4}

- **Monte Carlo methods should be used only when other methods break down!**

Today's lecture:
Monte Carlo integration and simulation

- More on Monte Carlo integration
- Monte Carlo simulation

Can we do better? Mean value method

- Consider general integration problem: $I = \int_a^b f(x)dx$

- Average value of *f* in the range between *b* and *a* is:

$$\langle f \rangle \equiv \frac{1}{b-a}\int_a^b f(x)dx = \frac{I}{b-a}$$

- So, we can get the integral by finding the average of *f*:

$$I = (b-a)\langle f \rangle$$

- We can estimate the average by measuring *f*(*x*) at *N* points chosen at random between *a* and *b*
- Then:

$$I \simeq \frac{(b-a)}{N}\sum_{i=1}^{N} f(x_i)$$

Errors of the mean value method

- Can estimate the error using the general theorem: **The variance on the sum of *N* independent random numbers is the sum of the variances of the individual numbers**
  - Holds no matter what the distribution is
- So:

$$\mathrm{var} f \equiv \langle f^2 \rangle - \langle f \rangle^2$$

- Where:

$$\langle f \rangle = \frac{1}{N} \sum_{i=1}^{N} f(x_i), \quad \langle f^2 \rangle = \frac{1}{N} \sum_{i=1}^{N} [f(x_i)]^2$$

- And:

$$I_{\mathrm{error}} = \frac{b-a}{N} \sqrt{N \mathrm{var} f} = (b-a) \frac{\sqrt{\mathrm{var} f}}{\sqrt{N}}$$

Still $N^{-1/2}$, but prefactor turns out to be smaller

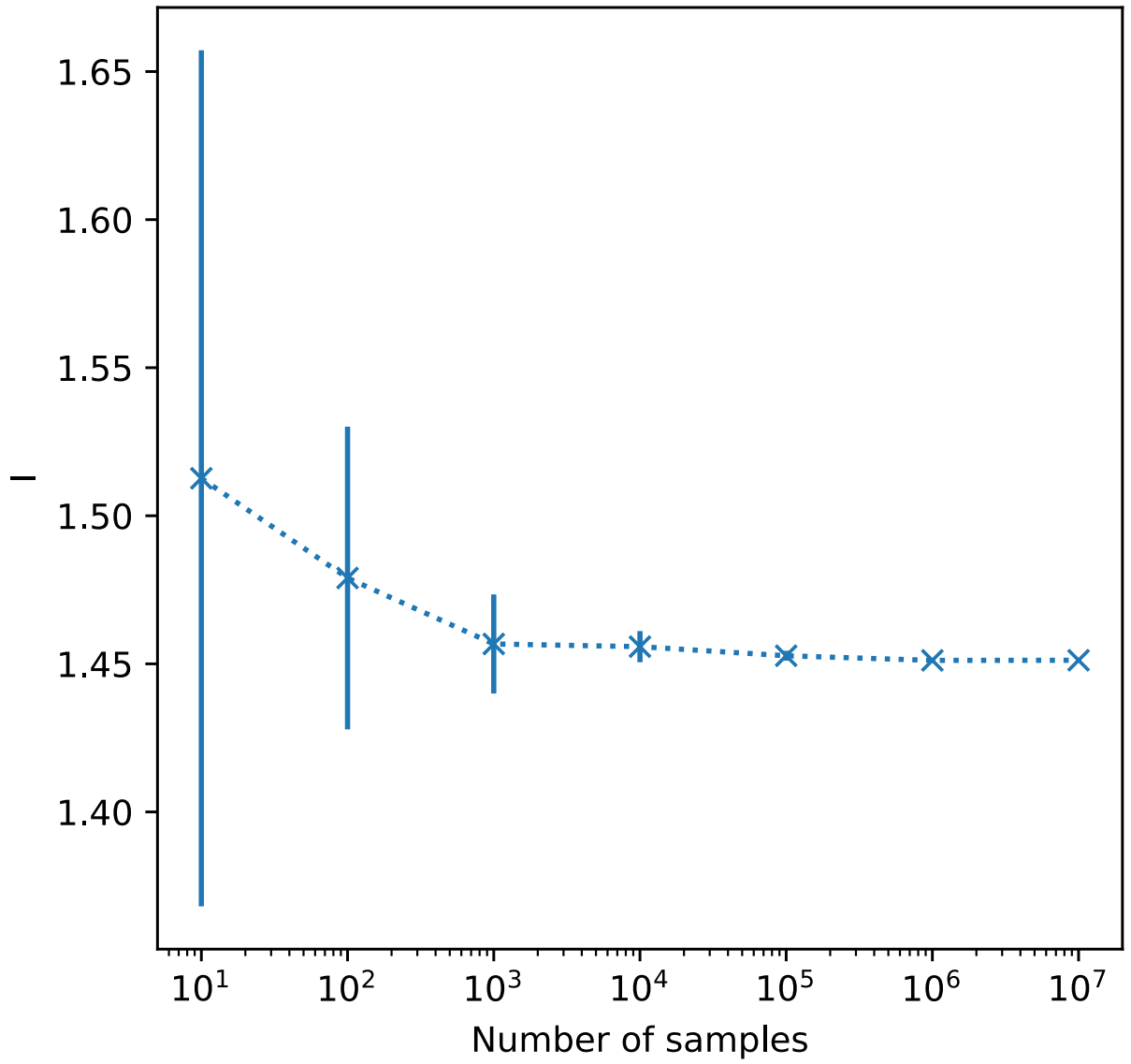
Mean value method

- Equation:

$$I = \int_0^2 \sin^2 \left[\frac{1}{x(2-x)} \right] dx$$

- Errors:

$$I_{\text{error}} = (b-a) \frac{\sqrt{\text{var} f}}{\sqrt{N}}$$



When to use Monte Carlo integration? Multi-dimensional integrals

- If we have an integral over many dimensions (> 4), grid sizes get very large, scale as N^d

- Monte Carlo integration can give reasonable results with many fewer points

- Straightforward to generalize methods discussed to more dimensions
  - E.g., mean value method

$$I \simeq \frac{V}{N} \sum_{i=1}^{N} f(\mathbf{r}_i)$$

Example: Volume of hypersphere

- Consider a hypersphere of unit radius in all dimensions:

$$f(\mathbf{r}) = \begin{cases} 1 & \text{if } \mathbf{r} \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

- Let's use the mean value method to compute the integral of a 10-dimensional hypersphere
  - Trapezoid rule with 100 samples per dimension: 10^{20} grid points!

- We can compare to the exact solution:

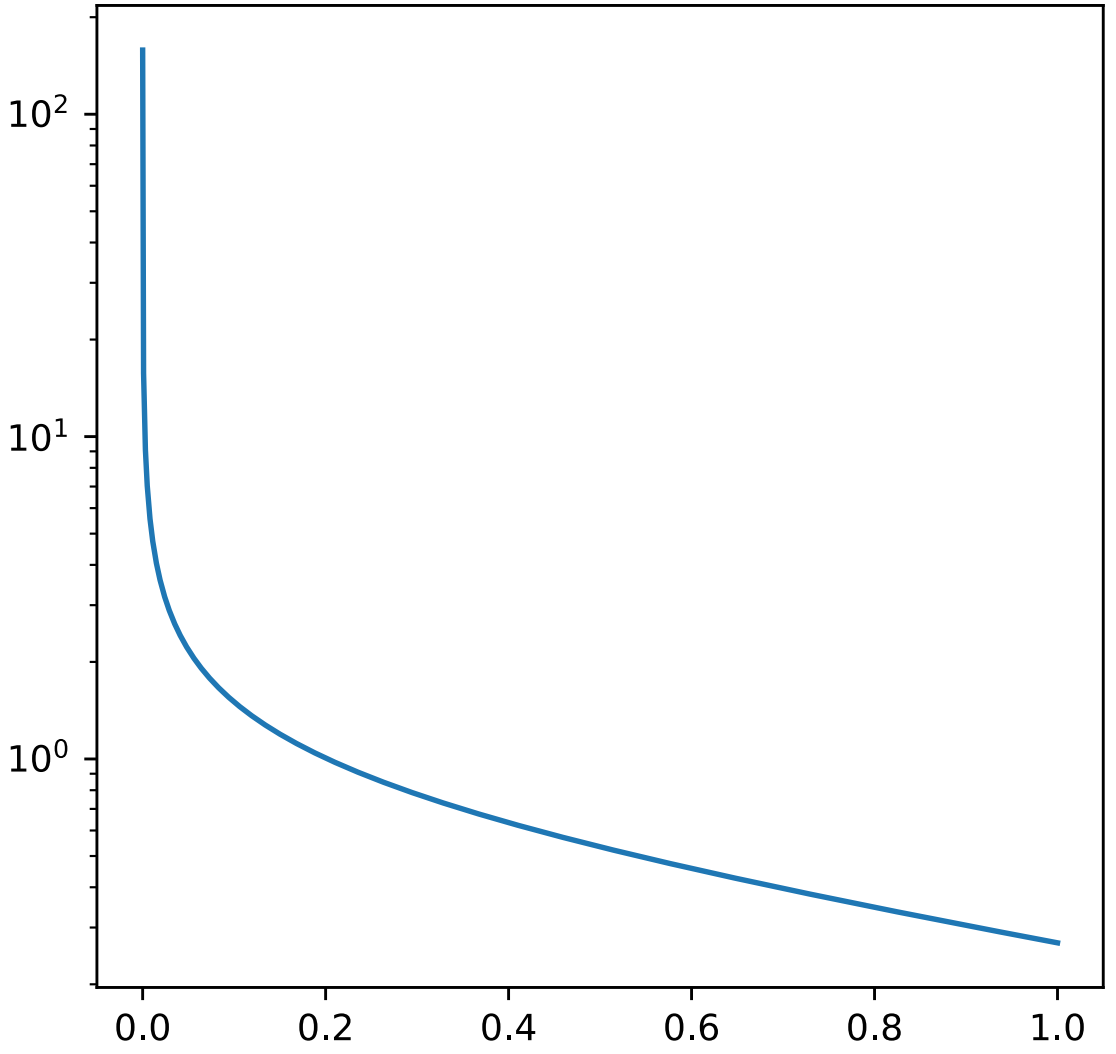
$$V_d(r) = \frac{\pi^{d/2}}{\Gamma\left(\frac{d}{2}+1\right)} r^d$$

Monte Carlo integration with divergences

- Monte Carlo integration fails for some pathological functions, e.g., those that contain divergences
- Consider:

$$I = \int_0^1 \frac{x^{-1/2}}{e^x + 1} dx$$

- Function diverges at *x*=0, but integral is finite
- E.g., for mean value method, will occasionally get a very large contribution
  - Estimate varies widely between runs



Importance sampling

- Can get around these issues by drawing points nonuniformly
- For a general function *g*(*x*) can define a weighted average:

$$\langle g \rangle_w = \frac{\int_a^b w(x) g(x) dx}{\int_a^b w(x) dx}$$

- *w*(*x*) is a weighting function
- If we want to solve a general 1D integral: $I = \int_a^b f(x) dx$
- We set *g*(*x*)=*f*(*x*)/*w*(*x*):

$$\left\langle \frac{f(x)}{w(x)} \right\rangle_w = \frac{\int_a^b f(x) dx}{\int_a^b w(x) dx} = \frac{I}{\int_a^b w(x) dx}$$

Importance sampling, 1D integral

- Thus, we have:

$$I = \left\langle \frac{f(x)}{w(x)} \right\rangle_w \int_a^b w(x)dx$$

- Equivalent to the mean value method, but from a weighted average

- How do we calculate the weighted average?

- Define probability density function as normalized *w*(*x*)

$$p(x) = \frac{w(x)}{\int_a^b w(x)dx}$$

- So

$$\langle g \rangle_w = \int_a^b p(x)g(x)dx$$

Importance sampling, 1D integral

- Now let's sample *N* random points in the interval with the distribution *p*(x). Then:

$$\sum_{i=1}^{N} g(x_i) \simeq \int_a^b N p(x) g(x) dx$$

- So:

$$\langle g \rangle_w = \int_a^b p(x) g(x) dx \simeq \frac{1}{N} \sum_{i=1}^{N} g(x_i)$$

- Where x_i are chosen from the distribution:

$$p(x) = \frac{w(x)}{\int_a^b w(x) dx}$$

Importance sampling, 1D integral

- Putting everything together:

$$I \simeq \frac{1}{N} \sum_{i=1}^{N} \frac{f(x_i)}{w(x_i)} \int_a^b w(x) dx$$

- Generalization of mean value method, which is where $w(x)=1$
- $w(x)$ can be any function that we choose
  - Can be chosen to remove pathologies in the integrand

- However, now we need to draw from a nonuniform distribution

Error on importance sampling method

- Error is given by:

$$I_{\text{error}} = \frac{\sqrt{\text{var}_w(f/w)}}{\sqrt{N}} \int_a^b w(x)dx$$

- Where:

$$\text{var}_w g = \langle g^2 \rangle_w - \langle g \rangle_w^2$$

- Still goes like $N^{-1/2}$

Importance sampling for pathological function

- Let's return to the integral: $I = \int_0^1 \frac{x^{-1/2}}{e^x + 1} dx$

- Choose: $w(x) = x^{-1/2}$
- Then: $f(x)/w(x) = (e^x + 1)^{-1}$
  - Finite and well-behaved over the range
- Probability distribution is:

$$p(x) = \frac{x^{-1/2}}{\int_0^1 x^{-1/2} dx} = \frac{1}{2\sqrt{x}}$$

- So, using the transformation method:

$$\int_0^x \frac{1}{2\sqrt{x'}} dx' = \sqrt{x} = z \quad \Longrightarrow \quad x = z^2$$

Importance sampling for pathological function

- So finally, we need to sample:

$$I \simeq \frac{1}{N}\sum_{i=1}^{N}\frac{f(x_i)}{w(x_i)}\int_a^b w(x)dx = \frac{1}{N}\sum_{i=1}^{N}\frac{1}{e^{x_i}+1}\int_0^1 \frac{1}{\sqrt{x}}dx = \frac{1}{N}\sum_{i=1}^{N}\frac{2}{e^{x_i}+1}$$

- With the distribution $x = z^2$

Today's lecture:
Monte Carlo integration and simulation

- More on Monte Carlo integration

- Monte Carlo simulation

Monte Carlo simulation

- Any computer simulation that uses random numbers to simulate physical process
- We saw a few examples already: radioactive decay and Rutherford scattering
- Used in every branch of physics
  - Particularly important in statistical mechanics and many-body physics

Monte Carlo simulation in stat mech

- Fundamental problem in statistical mechanics: Calculate expectation value of quantity of interest in thermal equilibrium

- Don’t know the exact state of the system, only probability of occupying state *i* with energy E_i

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

- Then average value of observable *X*:

$$\langle X \rangle = \sum_i X_i P(E_i)$$

States with large numbers

$$\langle X \rangle = \sum_i X_i P(E_i)$$

- Calculating this sum exactly can only be done in a few specific systems (e.g., harmonic oscillator)
- Numerically challenging: states are order Avogadro's number in size
- E.g., one mole of gas with two states: total number of states is $2^{10^{23}}$
- Instead, use Monte Carlo approach to evaluate the sum

Monte Carlo approach to expectation values

- We could choose *N* terms in the sum at random to add up:

$$\langle X \rangle \simeq \frac{\sum_{k=1}^{N} X_k P(E_k)}{\sum_{k=1}^{N} P(E_k)}$$

Needed to normalize the weighted average if not summing over *all* states

- This would not work well! Boltzmann probability is exponentially small for states $E_i \gg k_B T$

- Usually, most of the states are high energy, only a few contribute significantly

- **Need to use importance sampling!**

Importance sampling for thermal average

- Choose nonuniform distribution to focus on this small set
- Define weighted average over states:

$$\langle g \rangle_w \simeq \frac{\sum_i w_i g_i}{\sum_i w_i}$$

- We choose: $g_i = X_i P(E_i)/w_i$
- So:

$$\left\langle \frac{X_i P(E_i)}{w_i} \right\rangle_w = \frac{\sum_i w_i X_i P(E_i)/w_i}{\sum_i w_i} = \frac{\sum_i X_i P(E_i)}{\sum_i w_i} = \frac{\langle X \rangle}{\sum_i w_i}$$

- Or:

$$\langle X \rangle = \left\langle \frac{X_i P(E_i)}{w_i} \right\rangle_w \sum_i w_i$$

Importance sampling for thermal average

$$\langle X \rangle = \left\langle \frac{X_i P(E_i)}{w_i} \right\rangle_w \sum_i w_i$$

- Evaluate by selecting *N* states randomly with nonuniform distribution:

$$\langle X \rangle \simeq \frac{1}{N} \sum_{k=1}^{N} \frac{X_k P(E_k)}{w_k} \sum_i w_i$$

Summed over all states

Summed over *N* samples

- Still need to choose w_i to bias us towards high-probability samples
  - Also, so that sum over all states *i* can be evaluated analytically

Weights for importance sampling

- Simple choice: $w_i = P(E_i)$
- Sums to 1 over all by definition
- Then we have:

$$\langle X \rangle \simeq \frac{1}{N} \sum_{k=1}^{N} X_k$$

- Thus, choose *N* states in proportion to their Boltzmann weights, and average *X* over them

Markov chain Monte Carlo

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

- Partition function requires a sum over all states that we are trying to avoid
- Can use a Markov chain to choose states with probability $P(E_i)$ without knowing the partition function:
  - Start with a state *i*
  - Generate a new state *j* by making a small change to *i*
  - Choice of new state is determined probabilistically by a set of transition probabilities T_{ij} that give probability for changing from state *i* to *j*
- If we chose T_{ij} correctly, probability of visiting any state on a step of the Markov chain is $P(E_i)$!

Transition probabilities in the MC

- We must end up in some state on every MC step, so:

$$\sum_j T_{ij} = 1$$

- Choose transition probabilities such that:

$$\frac{T_{ij}}{T_{ji}} = \frac{P(E_j)}{P(E_i)} = \frac{e^{-\beta E_j}/Z}{e^{-\beta E_i}/Z} = e^{-\beta(E_j - E_i)}$$

- I.e., choosing particular ratio of the probability to go from *i* to *j*, and *j* to *i*

- Partition function cancels out!

Transition probabilities in the MC

- If we have correct probability of being in a given state at one step, we will have the correct probability for all later steps
- To see this:
  - Suppose we find a set of T_{ij}'s that satisfy the previous conditions
  - Suppose the probability to be in state *i* on one particular step is $P(E_i)$
  - Then, probability to be in state *j* on the next step is:

$$\sum_i T_{ij} P(E_i) = \sum_i T_{ji} P(E_j) = P(E_j) \sum_i T_{ji} = P(E_j)$$

- Once we get a Boltzmann distribution over states, we will keep it
  - Boltzmann distribution is a fixed point of the Markov chain
- Can also prove that we will converge to Boltzmann distribution
  - See, e.g., Appendix D of Newman

Metropolis-Hastings accept/reject

- Still have not worked out what elements of T_{ij} are
  - Actually, many possible choices
- Most common choice: Metropolis-Hastings algorithm:
  - Choose the change between *i* and *j* from specified set of possible changes
    - Can be, e.g., chosen at random, uniformly
  - Accept or reject the new state with acceptance probability:

$$P_a = \begin{cases} 1 & \text{if } E_j \leq E_i \\ e^{-\beta(E_j - E_i)} & \text{if } E_j > E_i \end{cases}$$

  - I.e., definitely accept if energy is lowered (or equal); may still accept if energy is increased

Transition probabilities under Metropolis-Hastings

- Total probability to move from *i* to given *j* (if $E_j > E_i$)

$$T_{ij} = \frac{1}{M} e^{-\beta(E_j - E_i)}$$

Probability we accept

Probability we choose *j*

Transition probabilities under Metropolis-Hastings

- If $E_j > E_i$:

$$T_{ij} = \frac{1}{M} e^{-\beta(E_j - E_i)}, \quad T_{ji} = \frac{1}{M} \quad \Longrightarrow \quad \frac{T_{ij}}{T_{ji}} = e^{-\beta(E_j - E_i)}$$

- If $E_j \leq E_i$:

$$T_{ij} = \frac{1}{M}, \quad T_{ji} = \frac{1}{M} e^{-\beta(E_i - E_j)} \quad \Longrightarrow \quad \frac{T_{ij}}{T_{ji}} = e^{-\beta(E_j - E_i)}$$

- Thus, both consistent with :

$$\frac{T_{ij}}{T_{ji}} = \frac{P(E_j)}{P(E_i)} = \frac{e^{-\beta E_j}/Z}{e^{-\beta E_i}/Z} = e^{-\beta(E_j - E_i)}$$

Some comments about the Metropolis algorithm

- Note that many steps will not change the system
  - Still need to include in the sum

- The number of possible moves *M*, must be the same when going from *i* to *j* as *j* to *i*

- Moves must be chosen to get you to every state
  - Move set for which all states are accessible is called ergodic

- Will generally take some (unknown) time to equilibrate to Boltzmann distribution

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

Example: 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:

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

Move set for ideal gas

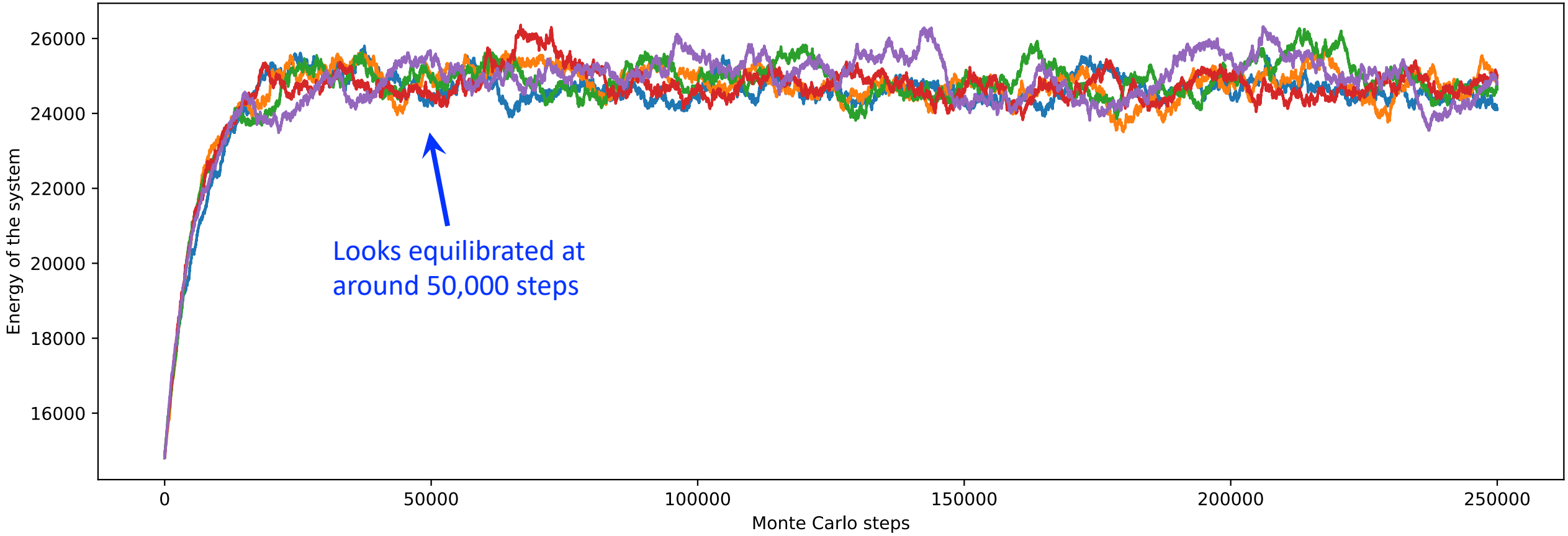
- Choose set of all moves of a single atom to one of the six "neighboring" states where n_x, n_y, or n_z differ by +/- 1
- Each Monte Carlo step, choose a random particle, chose a quantum number, change it by +/- 1
- Change in total energy just the change for single particle since there are no interactions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

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

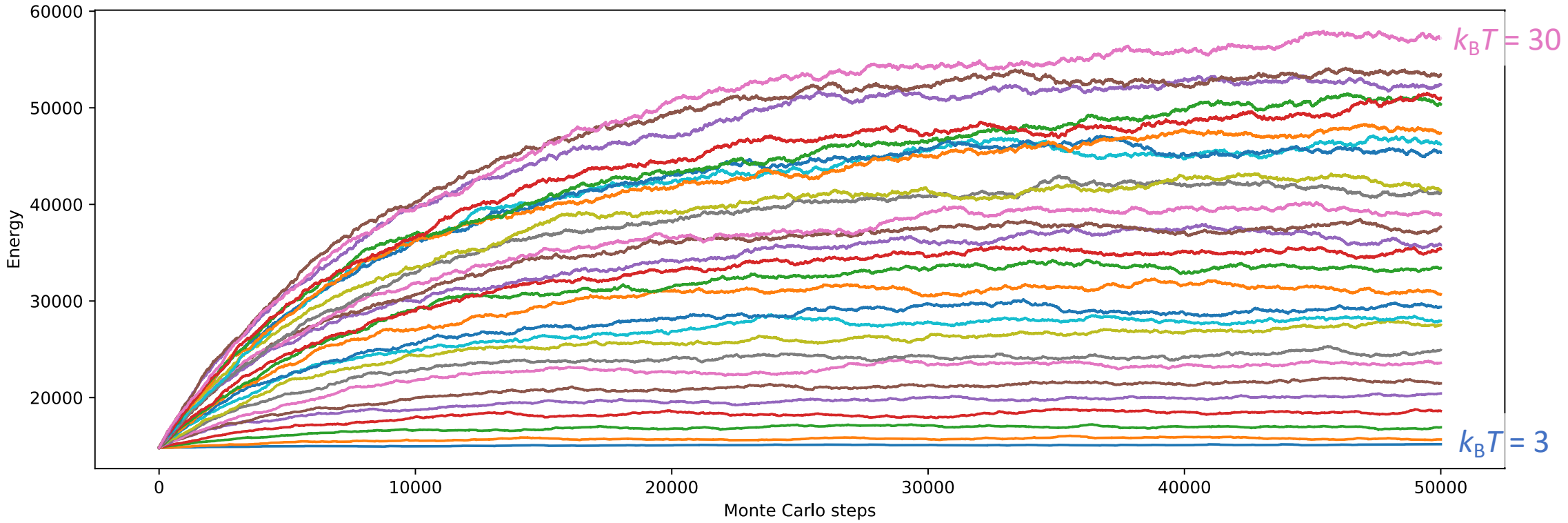
$$= \frac{\pi^2\hbar^2}{2mL^2}[(n_x \pm 1)^2 - n_x^2] = \frac{\pi^2\hbar^2}{2mL^2}(\pm 2n_x + 1)$$

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

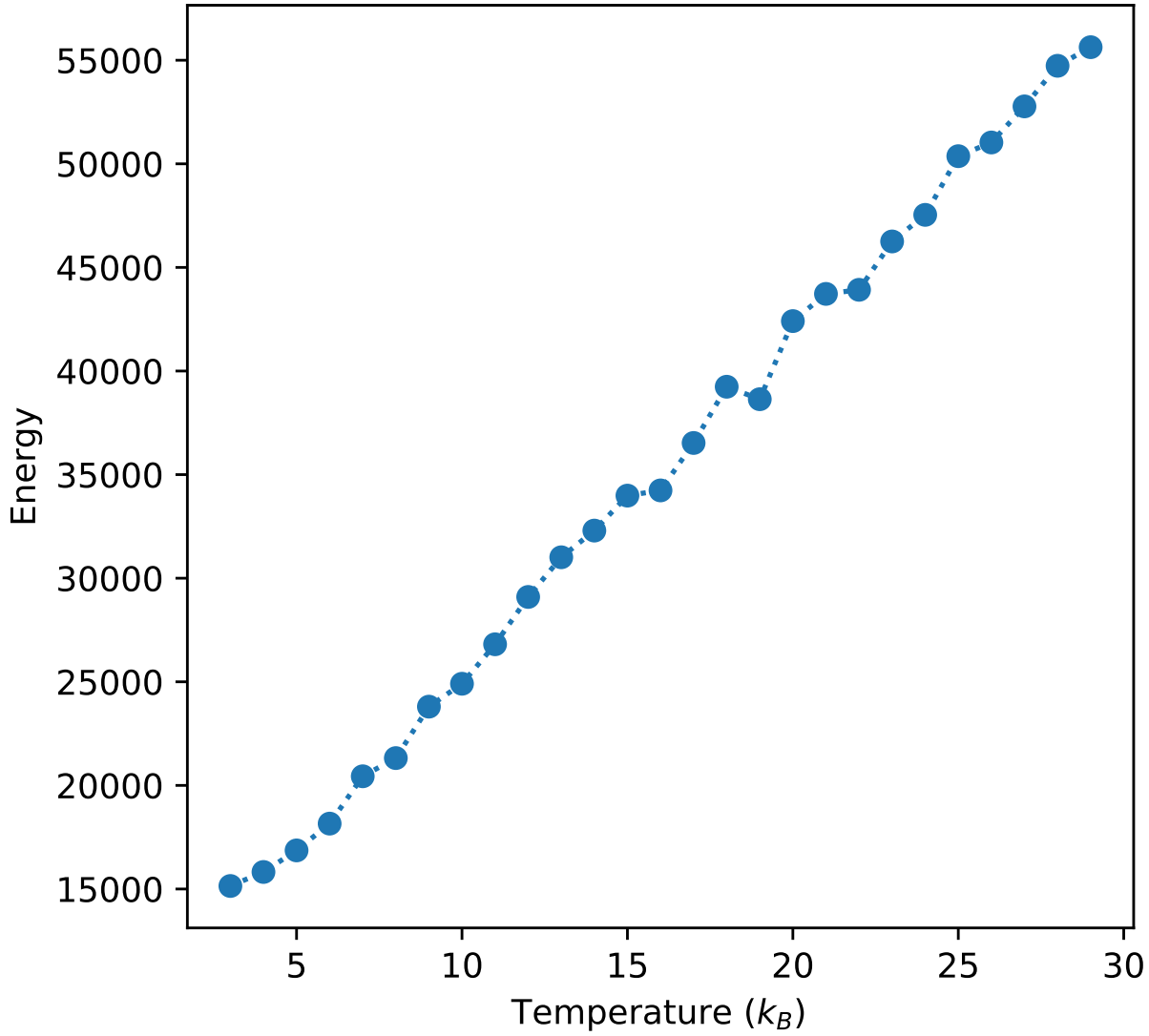
Monte Carlo simulation of ideal gas



Monte Carlo simulation of ideal gas: Dependence on T



Monte Carlo simulation of ideal gas: E vs. T



After class tasks and the rest of the semester

- Homework 5 is posted, due Nov. 11, 2021
- There will be one more homework (due date TBD)

- Final projects: See next slide

- Readings:
  - Newman Sec. 10.3

Final projects

- Topic is up to you:
  - Solving a physics problem with numerical methods discussed in class
  - Implementing a method/algorithm beyond what was discussed in class
  - A list of example topics will be provided
- To turn in (rubric will be provided):
  - Source code
  - Brief writeup (< 4 pages including figures and references)
    - In LaTeX
    - Include background/motivation, description of code, tests, and results
    - Rubric will be provided
- Presentations:
  - 15-minute talk + 5 min for questions
  - Can include demo of code