The Monte Carlo Method in Quantum Mechanics

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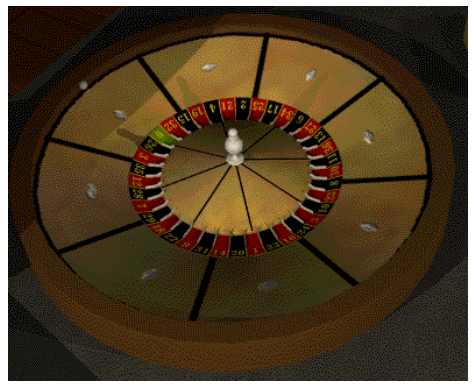


Overview

- **will present a detailed description of a Monte Carlo calculation of a simple quantum mechanical system**
  - the 1-dim simple harmonic oscillator
- **you should be able to do the calculation after this talk!**
  - that's how easy it is
- **outline:**
  - different view of quantum mechanics → path integrals
  - simple Monte Carlo integration
  - importance sampling using Markov chains
  - lattice quantum chromodynamics (QCD)

Transition amplitudes in quantum mechanics

- **key quantity in quantum mechanics → transition amplitude**

$$Z(b,a) \equiv \langle x_b(t_b) | x_a(t_a) \rangle$$

  - $Z(b,a)$ is the probability amplitude for a particle to go from a point x_a at time t_a to the point x_b and time t_b
- **in this talk, shall work in the Heisenberg picture**
  - state vectors are stationary $|\psi\rangle$
  - operators and their eigenvectors evolve with time

$$x(t) = e^{iHt/\hbar}\, x(0)\, e^{-iHt/\hbar}$$
$$|x(t)\rangle = e^{iHt/\hbar}\, |x(0)\rangle$$

- **shift Hamiltonian so ground state energies are zero**

$$H\ |\phi_n(t)\rangle = E_n\ |\phi_n(t)\rangle \quad E_0 = 0$$
$$|\phi_0(t)\rangle = |\phi_0(0)\rangle \equiv |0\rangle$$

Vacuum saturation

- take $t_a = -T$ and $t_b = T$ in the limit $T \to (1 - i\epsilon)\infty$

$$\begin{aligned}
\langle x_b(T)|x_a(-T)\rangle &= \langle x_b(0)|e^{-iHT/\hbar}\ e^{iH(-T)/\hbar}|x_a(0)\rangle \\
&= \sum_{n=0}^{\infty} \langle x_b(0)|\phi_n(0)\rangle\langle\phi_n(0)|x_a(0)\rangle\ e^{-2iE_nT/\hbar} \\
&\to \langle x_b(0)|0\rangle\langle 0|x_a(0)\rangle
\end{aligned}$$

inserting a complete set of energy eigenstates and using $E_{n+1} \geq E_n,\ E_0 = 0$ assuming nondegenerate vacuum

- possibility of probing ground state (vacuum) properties

Vacuum expectation values

- **now apply limit $T \to (1-i\epsilon)\infty$ to more complicated amplitude**

$$
\begin{aligned}
& \langle x_b(T)|x(t_2)x(t_1)|x_a(-T)\rangle \\
= \; & \langle x_b(0)|e^{-iHT/\hbar}\; x(t_2)x(t_1)\; e^{-iHT/\hbar}|x_a(0)\rangle \\
= \; & \sum_{n,m} \langle x_b(0)|\phi_n(0)\rangle\langle\phi_n(0)|x(t_2)x(t_1)|\phi_m(0)\rangle\langle\phi_m(0)|x_a(0)\rangle \\
& \qquad \times e^{-i(E_n+E_m)T/\hbar} \\
\to \; & \langle x_b(0)|0\rangle\langle 0|x(t_2)x(t_1)|0\rangle\langle 0|x_a(0)\rangle
\end{aligned}
$$

- **hence, vacuum expectation values from**

$$
\langle 0|x(t_2)x(t_1)|0\rangle = \lim_{T\to(1-i\epsilon)\infty} \frac{\langle x_b(T)|x(t_2)x(t_1)|x_a(-T)\rangle}{\langle x_b(T)|x_a(-T)\rangle}
$$

- **result generalizes to higher products of position operator**

Observables from correlation functions

- **all observables can be extracted from the correlation functions (vacuum expectation values)**
- **example: energies of the stationary states**

$$\begin{aligned}\langle 0|x(t)x(0)|0\rangle &= \langle 0|e^{iHt/\hbar}x(0)e^{-iHt/\hbar}x(0)|0\rangle \\ &= \sum_n \langle 0|x(0)e^{-iHt/\hbar}|\phi_n(0)\rangle\langle\phi_n(0)|x(0)|0\rangle \\ &= \sum_n |\langle 0|x(0)|\phi_n(0)\rangle|^2 e^{-iE_nt/\hbar}\end{aligned}$$

- **similarly for more complicated correlation functions**

$$\begin{aligned}\langle 0|x^2(t)x^2(0)|0\rangle &= \langle 0|e^{iHt/\hbar}x^2(0)e^{-iHt/\hbar}x^2(0)|0\rangle \\ &= \sum_n |\langle 0|x^2(0)|\phi_n(0)\rangle|^2 e^{-iE_nt/\hbar}\end{aligned}$$

- **but difficult to extract energies E_n from above *oscillatory* functions → much easier if we had *decaying* exponentials**

The imaginary time formalism

- can get decaying exponentials if we rotate from the ***real*** to the ***imaginary*** axis in time (Wick rotation) $t \to -i\tau$

$$\begin{aligned} \langle 0|x(t)x(0)|0\rangle &= \sum_n |\langle 0|x(0)|\phi_n(0)\rangle|^2 e^{-E_n\tau/\hbar} \\ &\overset{\tau\to\infty}{\longrightarrow} |\langle 0|x(0)|0\rangle|^2 + |\langle 0|x(0)|\phi_1(0)\rangle|^2 e^{-E_1\tau/\hbar} \end{aligned}$$

- later, we will see that this imaginary time formalism provides another important advantage for Monte Carlo applications

Quantum mechanics and path integrals

- **in the 1940's, Feynman developed an alternative formulation of quantum mechanics (his Ph.D. thesis)**
  - Richard Feynman, Rev Mod Phys **20**, 367 (1948)

- **quantum mechanical law of motion:**
  - probability amplitude from *sum over histories*

$$Z(b,a) \sim \sum_{\substack{\text{all paths } x(t) \\ \text{from } a \text{ to } b}} \exp\left(iS[x(t)]/\hbar\right)$$

- **all paths contribute to the probability amplitude, but with different *phases* determined by the *action*** $S[x(t)]$
- **<u>classical limit</u>: when small changes in path yield changes in action large compared to** $\hbar$ **, phases cancel out and path of least action** $\delta S = 0$ **dominates sum over histories**

Defining the path integral

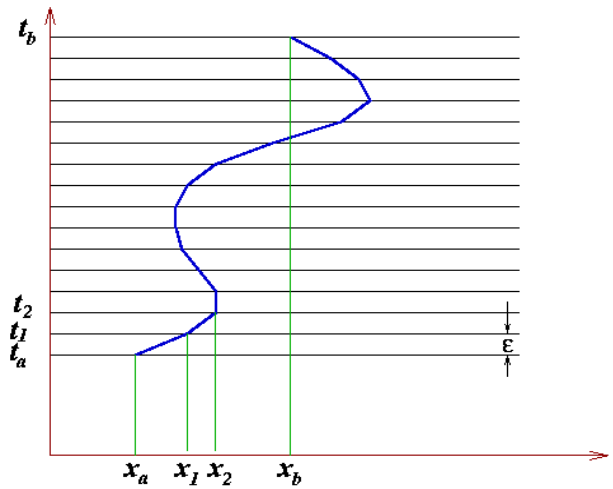
- action = time integral of Lagrangian (kinetic – potential energy)

$$S = \int dt\ L(x, \dot{x}) = \int dt\ (K - U)$$

- divide time into steps of width ε where $N\varepsilon = t_b - t_a$
- path integral is defined as

$$Z(b,a) = \lim_{\varepsilon \to 0} \frac{1}{A} \int_{-\infty}^{\infty} \frac{dx_1}{A} \frac{dx_2}{A} \cdots \frac{dx_{N-1}}{A}\ e^{iS[x(t)]/\hbar}$$

where A is a normalization factor depending on ε



The simple harmonic oscillator

- **kinetic and potential energy of a simple harmonic oscillator of mass m and frequency ω**

$$K = \tfrac{1}{2}m\dot{x}^2 \qquad U = \tfrac{1}{2}m\omega^2 x^2$$

- **action is given by**

$$S[x(t)] = \int_{t_a}^{t_b} dt \ \left(\tfrac{1}{2}m\dot{x}^2 - \tfrac{1}{2}m\omega^2 x^2\right)$$

- **classical equations of motion**

$$\delta S = 0 \quad \Rightarrow \quad \ddot{x}_{\mathrm{Cl}} + \omega^2 x_{\mathrm{Cl}} = 0$$

- **value of action for the classical path $T = t_b - t_a$**

$$S_{\mathrm{Cl}} = \frac{m\omega}{2\sin(\omega T)}\left[(x_a^2 + x_b^2)\cos(\omega T) - 2x_a x_b\right]$$

- **to calculate path integral, write path as deviation from classical path**

$$x(t) = x_{\mathrm{Cl}}(t) + \chi(t) \qquad \chi(t_a) = \chi(t_b) = 0$$

Path integral of simple harmonic oscillator

- **amplitude can then be written as**

$$Z(b,a) = F(T)\exp(iS_{\rm cl}/\hbar)$$

$$F(T) = \int_0^0 \mathcal{D}\chi \ \exp\left\{\frac{im}{2\hbar}\int_0^T dt\ (\dot{\chi}^2-\omega^2\chi^2)\right\}$$

- **partition time into discrete steps of length ε and use midpoint prescription**

$$\int_0^0 \mathcal{D}\chi = \frac{1}{A}\int_{-\infty}^{\infty}\left(\prod_{l=1}^{N-1}\frac{d\chi_l}{A}\right) \qquad A=\left(\frac{2\pi i\hbar\varepsilon}{m}\right)^{1/2}$$

$$\int_0^T dt(\dot{\chi}^2-\omega^2\chi^2) = \frac{1}{\varepsilon}\sum_{j=0}^{N-1}\left[(\chi_{j+1}-\chi_j)^2-\frac{\varepsilon^2\omega^2}{4}(\chi_{j+1}+\chi_j)^2\right]$$

$$F(T) = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{N/2}\int_{-\infty}^{\infty}\left(\prod_{l=1}^{N-1}d\chi_l\right)\exp\left\{\frac{im}{2\hbar\varepsilon}\chi_j M_{jk}\chi_k\right\}$$

Gaussian integration

- **a multivariate Gaussian integral remains**

$$F(T) = \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{N/2} \int_{-\infty}^{\infty} \left(\prod_{l=1}^{N-1} d\chi_l\right) \exp\left\{\frac{im}{2\hbar\varepsilon}\chi_j M_{jk}\chi_k\right\}$$

where M **is a symmetric** $(N-1)\times(N-1)$ **matrix**

$$M = \begin{bmatrix} 2 & -1 & 0 & 0 & \cdots \\ -1 & 2 & -1 & 0 & \cdots \\ 0 & -1 & 2 & -1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix} - \frac{\varepsilon^2\omega^2}{4} \begin{bmatrix} 2 & 1 & 0 & 0 & \cdots \\ 1 & 2 & 1 & 0 & \cdots \\ 0 & 1 & 2 & 1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

- **Gaussian integrals are easily evaluated**

$$F(T) = \left(\frac{m}{2\pi i\hbar\varepsilon \det M}\right)^{1/2}$$

Amplitude for simple harmonic oscillator

- **using a few tricks**

$$\begin{aligned}\lim_{\substack{\varepsilon\to 0\\ N\to\infty}} \varepsilon \det M &= \lim_{\substack{\varepsilon\to 0\\ N\to\infty}} \varepsilon \frac{1}{2i\omega\varepsilon}((1+i\omega\varepsilon)^N - (1-i\omega\varepsilon)^N) \\ &= \lim_{\substack{\varepsilon\to 0\\ N\to\infty}} \frac{1}{2i\omega}\left(\left(1+\frac{i\omega T}{N}\right)^N - \left(1-\frac{i\omega T}{N}\right)^N\right) \\ &= \frac{1}{2i\omega}\left(e^{i\omega T} - e^{-i\omega T}\right) = \frac{\sin\omega T}{\omega}.\end{aligned}$$

- **final result for the path integral**

$$Z(b,a) = \left(\frac{m\omega}{2\pi i\hbar \sin(\omega T)}\right)^{1/2} \exp(iS_{\mathrm{Cl}}/\hbar)$$

$$S_{\mathrm{Cl}} = \frac{m\omega}{2\sin(\omega T)}\left[(x_a^2 + x_b^2)\cos(\omega T) - 2x_a x_b\right]$$

Evolution of Gaussian wave packet

- **for initial wave packet at time $t_a = 0$ with probability dist.**

$$|\phi(x_a, t_a)|^2 = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x_a - \bar{x})^2}{2\sigma^2}\right)$$

- **probability amplitude at later time t_b**

$$\begin{aligned}\phi(x_b, t_b) &= \int_{-\infty}^{\infty} dx_a \; Z(b,a) \; \phi(x_a, 0) \\ &= \left(\frac{-im\omega(2\pi)^{-3/2}}{\hbar\sigma \sin(\omega t_b)}\right)^{1/2} \int_{-\infty}^{\infty} dx_a \; e^{iS_{\mathrm{cl}}/\hbar} \; e^{-(x_a - \bar{x})^2/(4\sigma^2)}\end{aligned}$$

- **final result for probability dist.: Gaussian with width s**

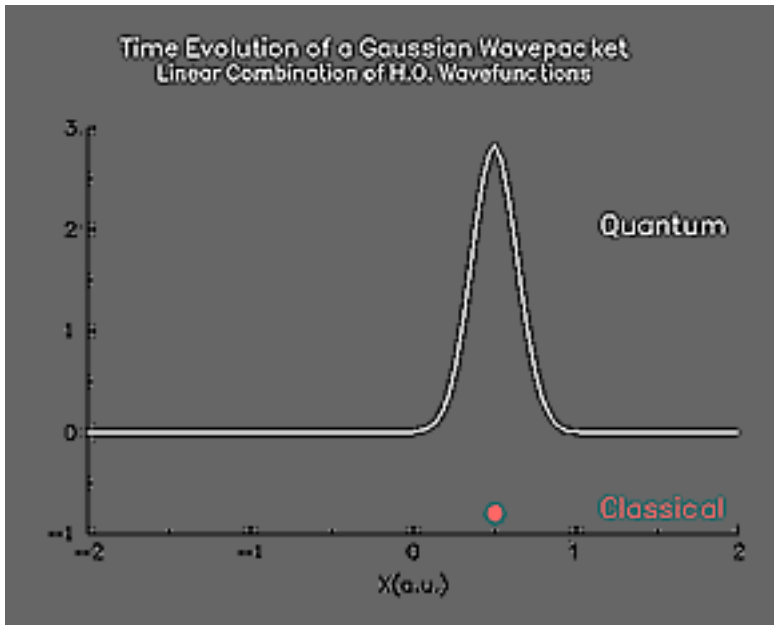
$$|\phi(x_b, t_b)|^2 = \frac{1}{s\sqrt{2\pi}} \exp\left(-\frac{(x_b - \bar{x}\cos(\omega t_b))^2}{2s^2}\right)$$

- **new width given by**

$$s = \sigma\left\{\cos^2(\omega t_b) + \frac{\hbar^2}{4m^2\omega^2\sigma^4}\sin^2(\omega t_b)\right\}^{1/2}$$

Visualization

- **time evolution of a Gaussian wave packet for a simple harmonic oscillator**



mass m=1g/mol= 1.66×10^{-27} kg

$\omega=3\times10^{14}$ radians/sec

initial wave packet:

center at 0.5 au

RMS spread 0.14 au

1 au (atomic unit)

= 0.529 angstrom

probability distribution shown

(in inverse a.u.)

- **completely calculated using path integrals → did *not* use Schrodinger equation**

Other probability amplitudes

- **so path integrals give us simple transition amplitudes**

$$\langle x_b(t_b)|x_a(t_a)\rangle = \int_a^b \mathcal{D}x \;\; \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt \;\; L(x,\dot{x})\right\}$$

- **but this important result generalizes to more complicated amplitudes**

$$\begin{aligned} & \langle x_b(t_b)| \;\; x(t_2) \;\; x(t_1) \;\; |x_a(t_a)\rangle \\ = & \int_a^b \mathcal{D}x \;\; x(t_2)x(t_1) \;\; \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b} dt \;\; L(x,\dot{x})\right\} \end{aligned}$$

for $t_a < t_1 < t_2 < t_b$

Path integrals in imaginary time

- **in the imaginary time formalism, paths contribute to sum over histories with real exponential weights (not phases)**

$$\langle x_b(\tau_b)|\ x(\tau_2)\ x(\tau_1)\ |x_a(\tau_a)\rangle$$
$$= \int_a^b \mathcal{D}x\ x(\tau_2)x(\tau_1)\ \exp\left\{-\frac{1}{\hbar}\int_{\tau_a}^{\tau_b} d\tau\ L(x,\dot{x})\right\}$$

- **classical path gets highest weighting**
- **note that weights are *real* and *positive* since action is real**
  - this fact will be crucial for the Monte Carlo method

Vacuum expectation values from path integrals

- **obtain correlation functions (vacuum expectation values) from ratios of path integrals**

$$\langle 0|x(\tau_2)x(\tau_1)|0\rangle = \lim_{T\to\infty} \frac{\langle x_b(T)|x(\tau_2)x(\tau_1)|x_a(-T)\rangle}{\langle x_b(T)|x_a(-T)\rangle}$$

$$= \frac{\int_a^b \mathcal{D}x\ x(\tau_2)x(\tau_1)\exp\left\{-\frac{1}{\hbar}\int_{-\infty}^{\infty} d\tau L(x,\dot{x})\right\}}{\int_a^b \mathcal{D}x\ \exp\left\{-\frac{1}{\hbar}\int_{-\infty}^{\infty} d\tau L(x,\dot{x})\right\}}$$

- **generalizes to more complicated correlation functions**
  - *any* correlation function can be computed using path integrals

Examples for the simple harmonic oscillator

- **evaluating path integrals as before, the following correlation functions can be obtained** $(\tau_1 \leq \tau_2 \leq \tau_3 \leq \tau_4)$

$$\begin{aligned}
\langle 0|x(\tau_1)|0\rangle &= 0 \\
\langle 0|x(\tau_2)x(\tau_1)|0\rangle &= \frac{\hbar}{2m\omega} e^{-\omega(\tau_2-\tau_1)} \\
\langle 0|x(\tau_4)x(\tau_3)x(\tau_2)x(\tau_1)|0\rangle &= \left(\frac{\hbar}{2m\omega}\right)^2 e^{-\omega(\tau_4-\tau_1)} \\
&\quad \times \left[e^{-\omega(\tau_2-\tau_3)} + 2e^{-\omega(\tau_3-\tau_2)}\right]
\end{aligned}$$

- **comparison with spectral representation tells us**

$$\langle 0|x(\tau)x(0)|0\rangle = \frac{\hbar}{2m\omega} e^{-\omega\tau}$$

$$\Rightarrow E_1 - E_0 = \hbar\omega \qquad |\langle 1|x(0)|0\rangle|^2 = \frac{\hbar}{2m\omega}$$

Another example in SHO

- **excite vacuum with $x(\tau)^2$ operator**

$$\langle 0|x^2(\tau)x^2(0)|0\rangle = \left(\frac{\hbar}{2m\omega}\right)^2 (1+2e^{-2\omega\tau}).$$

- **compare with spectral representation at large time separations**

$$\begin{aligned}\lim_{\tau\to\infty}\langle 0|x^2(\tau)x^2(0)|0\rangle &= |\langle 0|x^2(0)|0\rangle|^2 \\ &+ |\langle 2|x^2(0)|0\rangle|^2\ e^{-(E_2-E_0)t/\hbar} + \ldots \\ &= \left(\frac{\hbar}{2m\omega}\right)^2 (1+2e^{-2\omega\tau})\end{aligned}$$

- **interpretation:**

$$E_2 - E_0 = 2\hbar\omega$$

$$|\langle 0|x^2(0)|0\rangle|^2 = \left(\frac{\hbar}{2m\omega}\right)^2 \qquad |\langle 2|x^2(0)|0\rangle|^2 = 2\left(\frac{\hbar}{2m\omega}\right)^2$$

One last example in SHO

- **to determine expectation value of $x(0)^2$ in first-excited state**

$$\langle 0|x(\tau)\ x^2(\tfrac{1}{2}\tau)\ x(0)|0\rangle = 3\left(\frac{\hbar}{2m\omega}\right)^2\ e^{-\omega\tau}$$

- **compare with spectral interpretation at large times**

$$\lim_{\tau\to\infty}\langle 0|x(\tau)x^2(\tfrac{1}{2}\tau)x(0)|0\rangle$$
$$= |\langle 0|x(0)|1\rangle|^2\langle 1|x^2(0)|1\rangle\ e^{-(E_1-E_0)\tau/\hbar} + \ldots$$

since $\langle 0|x(0)|0\rangle = \langle 0|x(\tau)|0\rangle = 0$

- **by inspection and using previously derived results**

$$\langle 1|x^2(0)|1\rangle = \frac{3\hbar}{2m\omega}.$$

Pause for reflection

- observables in quantum mechanics can be extracted from the correlation functions (vacuum expectation values)
- imaginary time formalism is a great trick for assisting in such extractions
- correlation functions can be computed via path integrals

$$\langle 0|x(\tau_2)x(\tau_1)|0\rangle = \frac{\int_a^b \mathcal{D}x\ x(\tau_2)x(\tau_1)\exp\left\{-\frac{1}{\hbar}\int_{-\infty}^{\infty} d\tau L(x,\dot{x})\right\}}{\int_a^b \mathcal{D}x\ \exp\left\{-\frac{1}{\hbar}\int_{-\infty}^{\infty} d\tau L(x,\dot{x})\right\}}$$

The die is cast?

- **in rare situations, the path integrals can be computed exactly**
  - simple harmonic oscillator, free particle
- **sometimes the action can be written**

$$S = S_0 + gS_I$$

  - S_0 describes the free motion of the particles
  - path integrals using S_0 are Gaussian and can be exactly computed
  - S_I describes the interaction of the particles, but the coupling g is small
  - compute in perturbation theory as expansion in g
- **however, if interactions are *not weak***
  - usually must resort to Monte Carlo methods
    - for example, quantum chromodynamics (QCD)

Simple Monte Carlo integration

- **basic theorem of Monte Carlo integration**

$$\int_V f(\vec{x})\; d^D x \approx V\langle f\rangle \pm V\sqrt{\frac{\langle f^2\rangle - \langle f\rangle^2}{N}}$$

$$\langle f\rangle \equiv \frac{1}{N}\sum_{i=1}^{N} f(\vec{x}_i) \qquad \langle f^2\rangle \equiv \frac{1}{N}\sum_{i=1}^{N} f(\vec{x}_i)^2$$

where $\vec{x}_1, \ldots, \vec{x}_N$ are N points chosen *independently* and at *random* with uniform probability distribution throughout D-dimensional volume V

- **justified by the central limit theorem**
- **in the limit $N \to \infty$, MC estimate tends to normal distribution, uncertainty tends to standard deviation**

Pseudorandom number generators

- **MC integration requires random numbers**
- **but computers are deterministic!!**
- **clever algorithms can produce sequences of numbers which *appear* to be random (pseudorandom)**
  - uniform deviates between 0 and 1

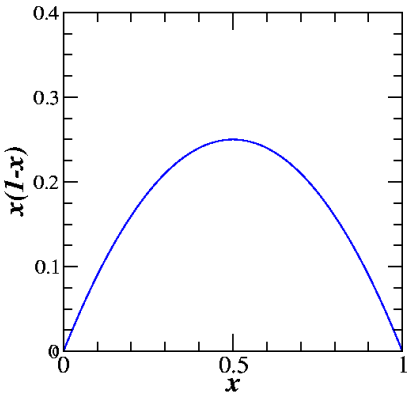
- **example: the Mersenne twister**
  - *http://www.math.sci.hiroshima-u.ac.jp/~m-mat/MT/emt.html*
  - currently holds the record for longest period $2^{19937}-1$
  - very fast, passes all standard tests (Diehard) for good RNG
- **devising good RNG's is a science in itself**
  - most utilize modulus function, bit shifting, shuffling

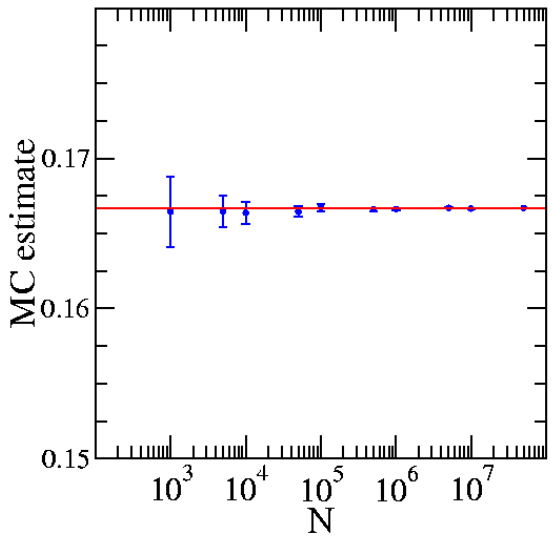
One-dimensional example

- **simple example**

$$\int_0^1 x(1-x)\ dx = \frac{1}{6} = 0.166666\cdots$$

- **plot of integrand and some Monte Carlo estimates**





- **not efficient for 1-dim integrals**

Importance sampling

- **importance sampling can greatly improve efficiency of Monte Carlo integration**
  - recall simple integration

$$\int_0^1 f(x)dx \approx \frac{1}{N}\sum_{j=1}^{N} f(x_j) \qquad x_j \text{ chosen with uniform probability between 0 and 1}$$

  - choose weighting function $g(x) > 0$ so $h(x) = \frac{f(x)}{g(x)}$ is as close as possible to a constant

$$\int_0^1 f(x)dx = \int_0^1 h(x)g(x)dx \approx \frac{1}{N}\sum_{j=1}^{N} h(x_j)$$

    where now x_j chosen with probability density $g(x)$
- **but how do we choose $g(x)$ for multi-dimensional complicated integral?**

Markov chains

- **use the elements of a *Markov chain* generated by a Markov process for our importance sampling!!**
- **sequence of configurations $C_1, C_2, \ldots$ generated one after another using transition probability $P(C_i \to C_j)$ satisfying**
  - strong ergodicity (usually only need weak version)
    $$P(C_i \to C_j) > 0 \text{ for any two } i, j$$
  - normalization $\sum_C P(C' \to C) = 1$
  - stable equilibrium (fixed point)
    $$\sum_C P_{\text{eq}}(C)\ P(C \to C') = P_{\text{eq}}(C')$$
- **starting with any configuration C_0, will eventually generate configurations with probability distribution $P_{\text{eq}}(C)$**

Detailed balance

- **crucial observation:**
  - last condition holds if transition probability satisfies *detailed balance*:

$$P_{\text{eq}}(C)\ P(C \to C') = P_{\text{eq}}(C')\ P(C' \to C)$$

for every pair C and C'

- **for our path integrals, we need to generate paths with probability distribution**

$$P_{\text{eq}}(x) = \frac{e^{-S[x]/\hbar}}{\int_a^b \mathcal{D}x'\ e^{-S[x']/\hbar}}$$

  - in imaginary time formalism, path integral weight is real and positive → probability interpretation for Monte Carlo

What's the catch?

- **Monte Carlo estimates require statistically *independent* random configurations, but configurations generated by a Markov process *do depend* on previous elements in chain**
  - this dependence is known as autocorrelation
- **this autocorrelation can actually be measured!**
  - for any observable (integrand) O_i, the autocorrelation can be defined by

$$\frac{\langle O_i O_{i+1} \rangle - \langle O_i \rangle^2}{\langle O_i^2 \rangle - \langle O_i \rangle^2}$$

i refers to sequence in the Markov chain

  - highly correlated → value near 1
  - independent → value near 0
- **dependence decreases as distance between elements increases in the chain**
  - do not use every element in chain for "measurements"
  - skip some number of elements between measurements

The Metropolis algorithm

- **one of the simplest Markov chain updating algorithms is the Metropolis method**
  - for current configuration C, propose a new configuration C' with some transition probability $P_0(C \to C')$ satisfying the microreversibility requirement
    $$P_0(C \to C') = P_0(C' \to C)$$
  - compute the change in the action
    $$\delta S \equiv S(C') - S(C)$$
  - accept the new configuration with probability
    $$\min\left(1, e^{-\delta S/\hbar}\right)$$
- **this simple algorithm satisfies detailed balance**
- **useful for *local* updating so changes to action are small**
- **probability normalization never enters in the calculation!**

Discretization of SHO action

- **action of harmonic oscillator (imaginary time formalism)**

$$S[x(\tau)] = \int_{\tau_a}^{\tau_b} d\tau \ \left(\tfrac{1}{2}m\dot{x}^2 + \tfrac{1}{2}m\omega^2 x^2\right)$$

- **discretize time** $N\varepsilon = \tau_b - \tau_a$ **for Monte Carlo evaluation**

$$\frac{S}{\hbar} = \frac{m\varepsilon}{2\hbar}\sum_{j=0}^{N-1}\left[\left(\frac{x_{j+1}-x_j}{\varepsilon}\right)^2 + \omega^2\left(\frac{x_{j+1}+x_j}{2}\right)^2\right]$$

- **choose** ε **so discretization errors sufficiently small**
- **introduce dimensionless parameters**

$$x_k = d_k\sqrt{\frac{\varepsilon\hbar}{m}} \qquad \kappa = \frac{1}{4}\varepsilon^2\omega^2$$

$$\frac{S}{\hbar} = \frac{1}{2}\sum_{j=0}^{N-1}\left[(d_{j+1}-d_j)^2 + \kappa(d_{j+1}+d_j)^2\right]$$

Discretization of action (continued)

- a few more manipulations produce

$$\frac{S}{\hbar} = \frac{1}{2}(1+\kappa)(d_0^2+d_N^2)+(1+\kappa)\left[\sum_{j=1}^{N-1} d_j^2\right]-(1-\kappa)\left[\sum_{j=0}^{N-1} d_j d_{j+1}\right]$$

- first constant is irrelevant (can be set to zero), then one last rescaling

$$u_j = d_j\sqrt{1+\kappa} \quad g = \frac{1-\kappa}{1+\kappa} \quad d_0 = d_N = 0$$

- final result for action

$$\frac{S}{\hbar} = \left[\sum_{j=1}^{N-1} u_j^2\right] - g\left[\sum_{j=0}^{N-1} u_j u_{j+1}\right]$$

Metropolis updating of path

- **to update location u_j (at a single time)**
  - propose random shift $-\Delta \leq \delta \leq \Delta$ with uniform prob.
  - calculate change to the action

$$\delta S/\hbar = \delta \left(\delta + 2u_j - g(u_{j-1} + u_{j+1})\right)$$

  - accept $u_j^{\text{new}} = u_j + \delta$ with probability $\min\left(1, e^{-\delta S/\hbar}\right)$
  - rule of thumb: fix Δ for about 50% acceptance rate
    - lower rate = wasting too much time with rejections
    - higher rate = moving through phase space too slowly

- **repeat for each u_j for $j = 1 \ldots N-1$ (this is called one sweep)**
- **repeat for certain number of sweeps**
  - until autocorrelations sufficiently small

Actual C++ code

- **Here is the actual C++ code which does the updating**

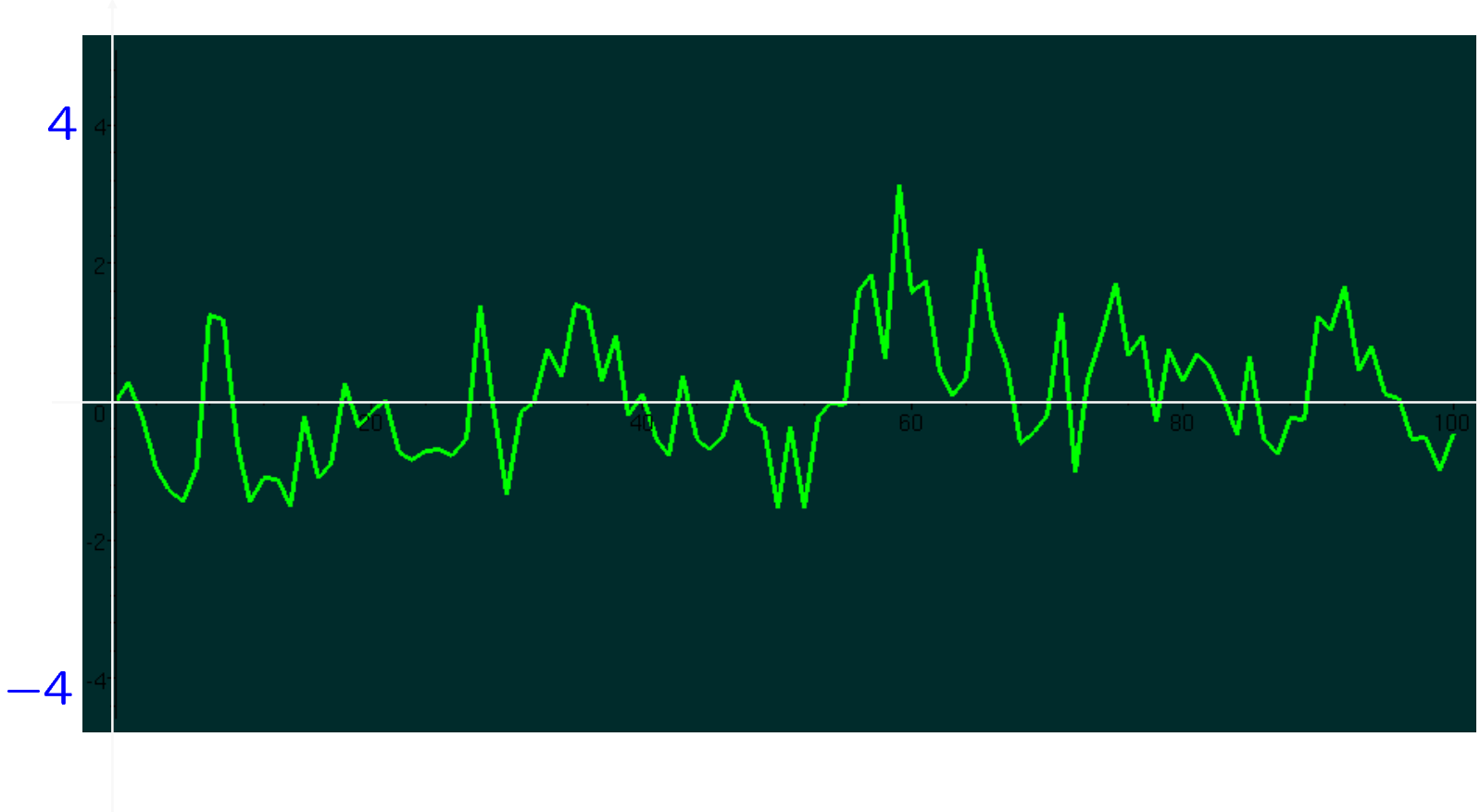
```
void markov::update()
{
 double shift,deltaS;

 for (int i=1;i<=Nsweeps;i++)

    for (int t=1;t<Ntimesteps;t++){

            // propose shift in location[t]
       shift=2.0*max_shift_per_instance*(rng.generate()-0.5);

            // compute change in action
       deltaS=shift*(shift+2.0*locations[t]
                  -hop_param*(locations[t-1]+locations[t+1]));

            // Metropolis accept or reject
       if (deltaS<0.0) accept=1;
       else accept=(rng.generate()<=exp(-deltaS));
       if (accept) locations[t]+=shift;

       }

}
```

Simulation guidelines

- **to start Markov chain**
  - choose a random path (hot start)
  - or choose $u_j = 0$ for all j (cold start)
  - update N_{therm} times until fixed point of chain achieved (thermalization) → check some simple observable
- **once thermalized, begin "measurements"**
- **must choose**
  - ε so discretization errors sufficiently small
  - Δ for adequate acceptance rate
  - N_{sweeps} for sufficiently small autocorrelations
  - N_{meas} for desired precision of results

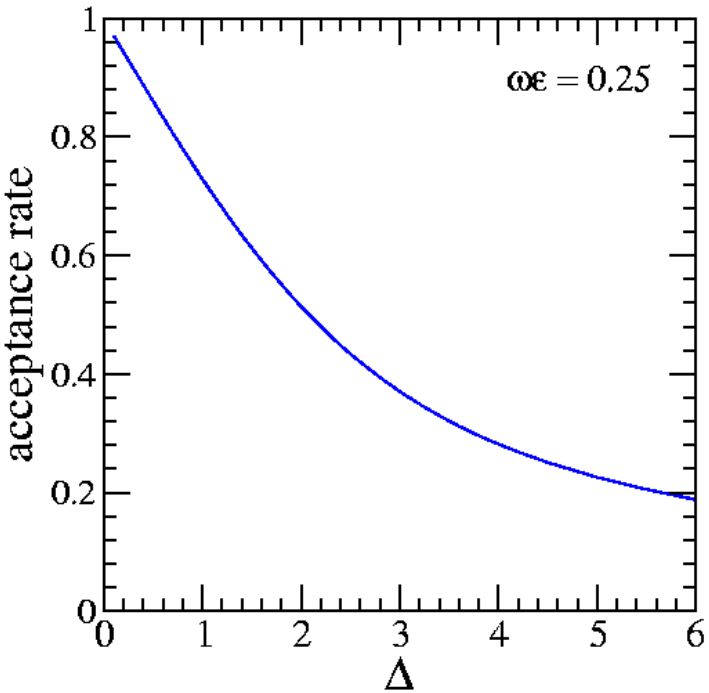
Path animation

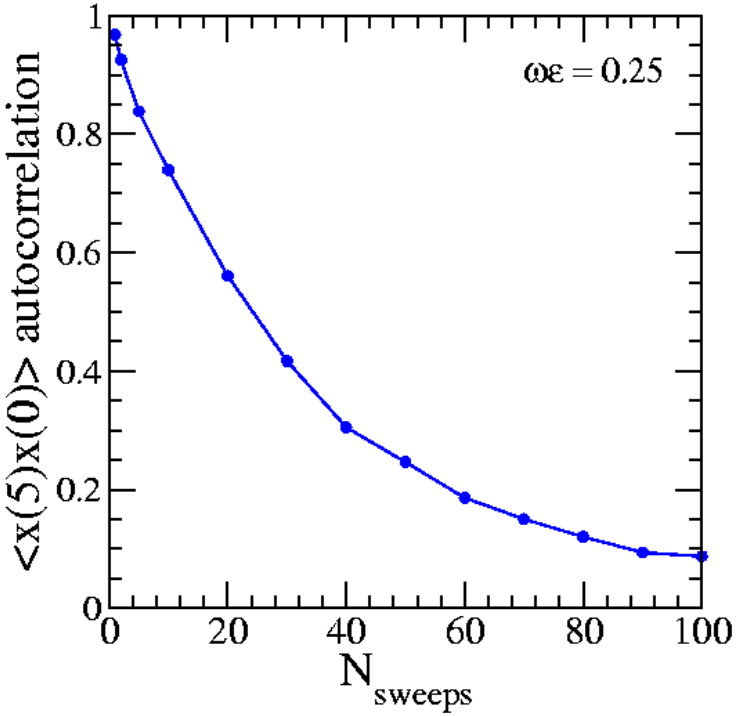
- animation of first 100 time slices of u_j path



Acceptance rate, autocorrelations

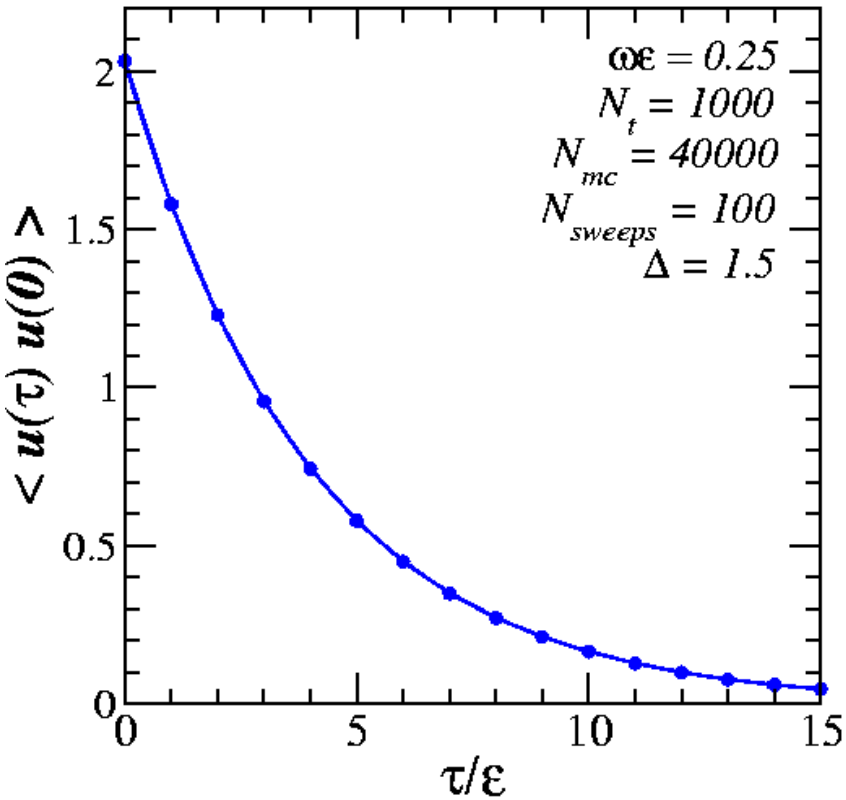
- choose Δ so acceptance rate near 0.5
- choose N_{sweeps} so autocorrelations near 0.1





Correlation function

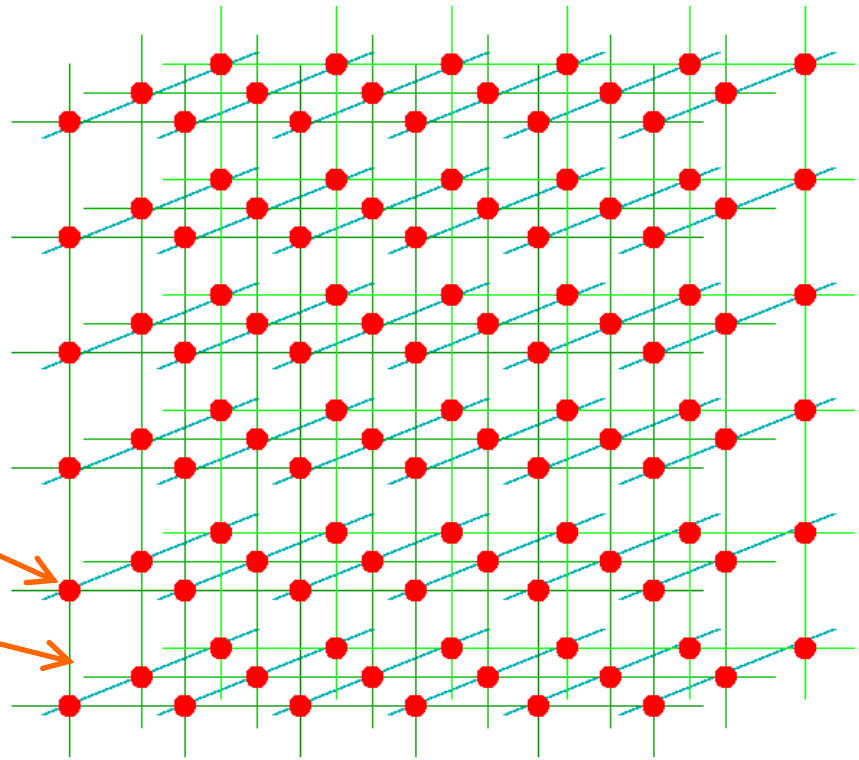
- **comparison of Monte Carlo estimates with exact results**



- exact result shown as curve
- Monte Carlo estimates shown by circles (statistical uncertainties too small to see)

Lattice Quantum ChromoDynamics

- **hypercubic space-time lattice**
- **quarks reside on sites, gluons on links between sites**
- **for gluons, 8 dimensional integral on *each link***
- **path integral has dimension** $32N_xN_yN_zN_t$
  - 10.6 million for 24^4
- **more sophisticated updating algorithms**
- **systematic errors**
  - discretization
  - finite volume

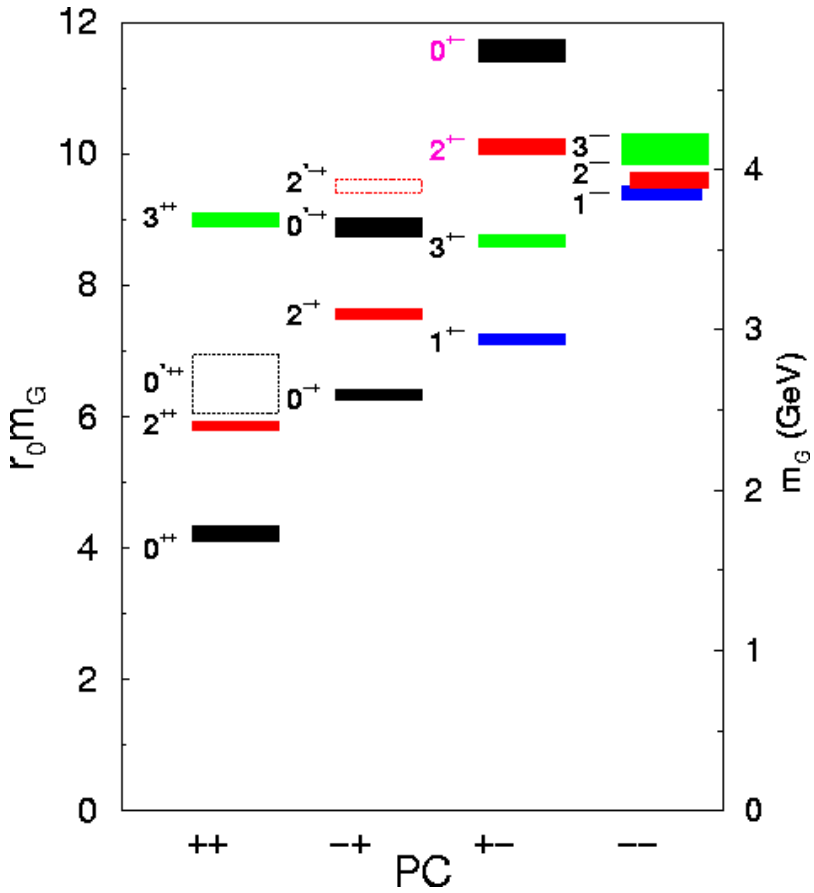


Yang-Mills SU(3) Glueball Spectrum

- **gluons can bind to form glueballs**
  - e.m. analogue: massive globules of pure light!
- **states labeled by** J^{PC}
- **scale set by**

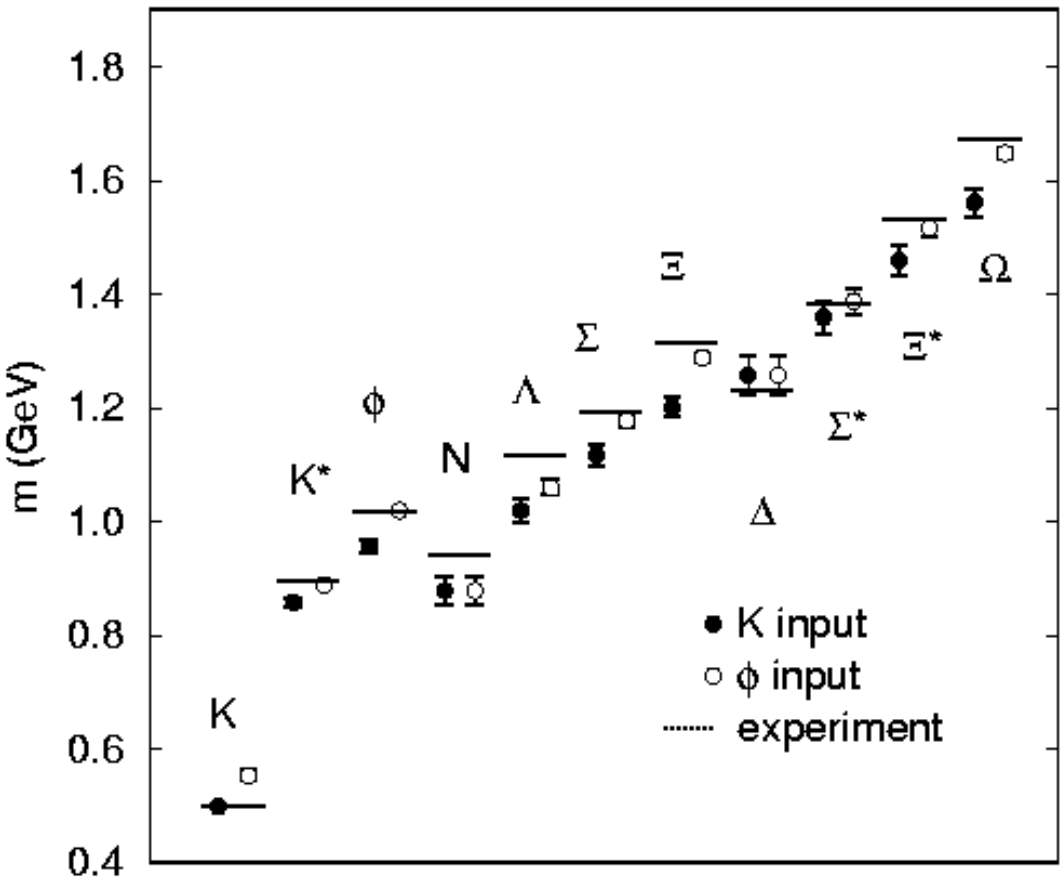
  $r_0^{-1} = 410(20)\ \mathrm{MeV}$
- **computed using same techniques as for SHO**
  - 24×24 correlation *matrices* in each symmetry channel
- **spin identification**

C. Morningstar and M. Peardon,
Phys. Rev. D 60, 034509 (1999)



Light hadron spectrum (without quark loops)

- **CP-PACS collab. (Japan) Phys Rev Lett 84, 238 (2000)**



Conclusion

- **observables in quantum mechanical systems can be extracted from the correlation functions of the theory**
- **correlation functions can be computed using path integrals**
- **path integrals in the imaginary time formalism can be evaluated using the Monte Carlo method**
  - importance sampling from Markov chains
- **the Metropolis method was applied to the 1-dimensional simple harmonic oscillator**