Note sul path integral per la particella sul cerchio: topologia, termine θ e problema nella simulazione numerica

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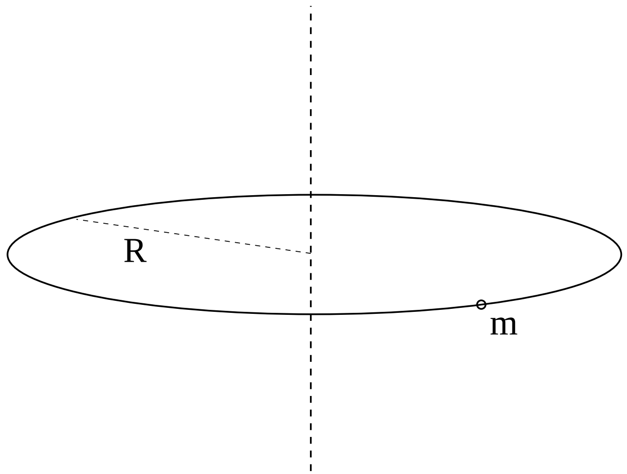
The free particle on a circle

alias: the simplest QM problem with non-trivial topological structure and numerical challenges



We will consider the path integral formulation for a free particle constrained on a circle of radius R

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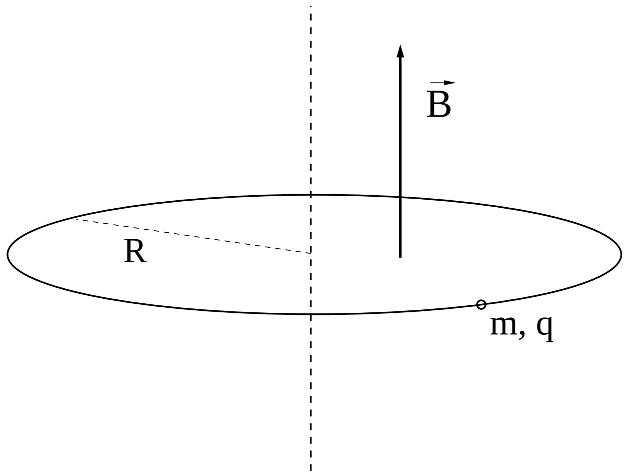

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with and without a uniform magnetic field orthogonal to the circle

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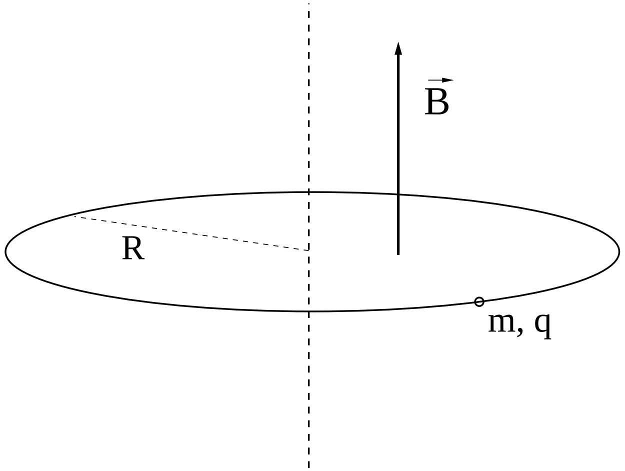

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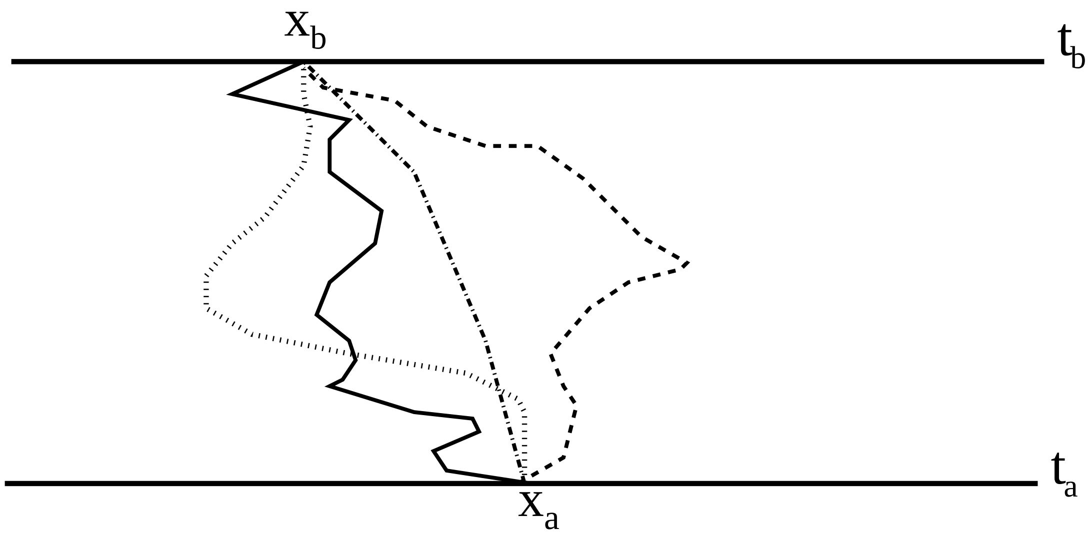
- This is a great example, where basic issues concerning topology and θ-dependence in gauge theories can be discussed in a simplified framework

- Even if everything is analitically computable here, as we try to study it by Monte-Carlo simulations, we face the same problems and failures as in QCD

Feynman path integral in a few words



The starting point is rewriting the probability amplitude for going from point x_a to point x_b in time $t_b - t_a$

$$\langle x_b | e^{-iH(t_b-t_a)/\hbar} | x_a \rangle = \mathcal{N} \int_{x(t_{a/b})=x_{a/b}} \mathcal{D}x(t) \exp\left(\frac{iS[x(t)]}{\hbar}\right)$$

All possible paths contribute,"weighted" by an oscillating phase factor $\exp\left(\frac{iS[x(t)]}{\hbar}\right)$, where S is the classical action associated with each path.

$$S[x(t)] = \int_{t_a}^{t_b} dt' \mathcal{L}(x(t'), \dot{x}(t'))$$

The thermal partition function can be given a path integral formulation as well

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right) = \sum_n e^{-\beta E_n} = \int dx \langle x | e^{-\frac{H}{k_B T}} | x \rangle$$

the trace can be taken over energy eigenstates, but also over position eigenstates

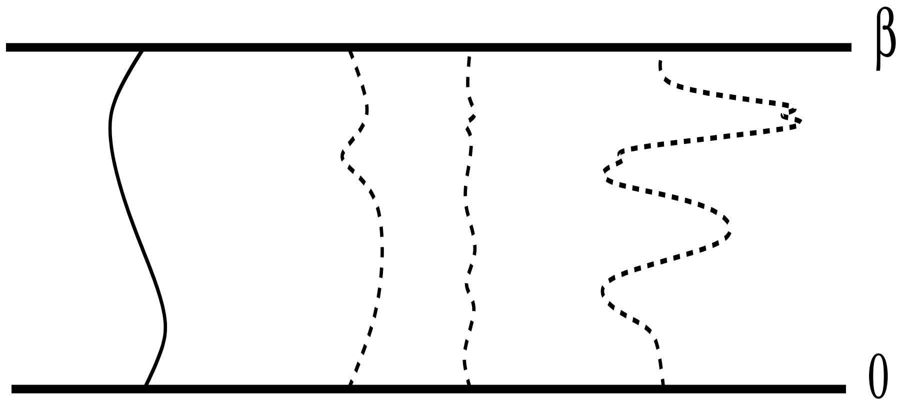
same amplitude as before if $|x_a\rangle = |x_b\rangle = |x\rangle$ **and** $\beta = \frac{1}{k_B T} = i(t_b - t_a)/\hbar$**.**

$$Z = \mathcal{N} \int_{x(0)=x(\beta\hbar)} \mathcal{D}x(\tau) \exp\left(\frac{-S_E[x(\tau)]}{\hbar}\right)$$

τ **is the Euclidean time,** $\tau \in [0, \hbar/(k_B T)]$**. Integration is over paths periodic in** τ**.**

S_E **is the Euclidean action, obtained from** S **after Wick rotation** $t \to -i\tau$

$F = -\frac{1}{\beta} \log Z$ **is the free energy of the system, which in the** $T \to 0$ **limit (**$\beta\hbar \to \infty$**) coincides with the ground state energy**



Z **is a sum over periodic paths, weighted by factor** $\exp(-\frac{S_E}{\hbar})$**.**

For well behaved potentials that can be given a probabilistic interpretation

Thermal averages are then expectation values of path functionals over a thermal path probability distribution function $P[x(\tau)]$

$$\langle O\rangle_T = \frac{\mathrm{Tr}\left(e^{-\beta H}O\right)}{\mathrm{Tr}\left(e^{-\beta H}\right)} = \frac{\int \mathcal{D}x(\tau)\exp\left(\frac{-S_E[x(\tau)]}{\hbar}\right)O[x(\tau)]}{\int \mathcal{D}x(\tau)\exp\left(\frac{-S_E[x(\tau)]}{\hbar}\right)} \equiv \int \mathcal{D}x(\tau)P[x(\tau)]O[x(\tau)]$$

as $\beta\to\infty$, one recovers vacuum expectation values

Monte-Carlo computation of the path integral

- **After discretization (continuum $\to$ lattice), the number of integration variables is finite, the problem is numerically affordable.**

- **Huge number of variables $\Longrightarrow$ Optimal strategy: Monte-Carlo extraction of a sample of paths $x_1(\tau), x_2(\tau), \ldots, x_M(\tau)$ distributed according to $P[x(\tau)]$.**

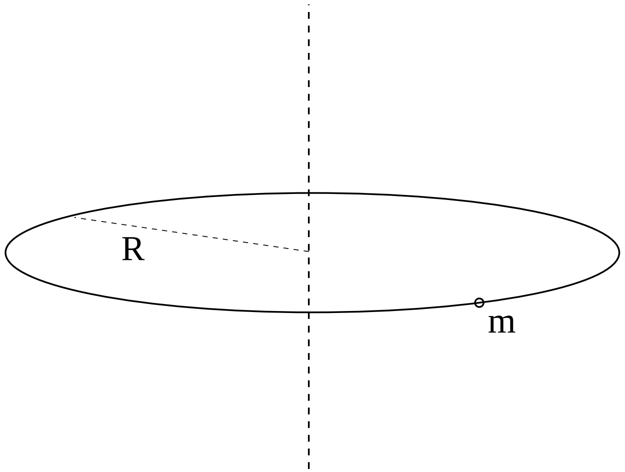
- **The sample average**

$$\bar{O} = \frac{1}{M} \sum_{i=1}^{M} O[x_i(\tau)]$$

is normally distributed around the true average $\langle O \rangle = \int \mathcal{D}x(\tau) P[x(\tau)] O[x(\tau)]$ with a statistical error of order $1/\sqrt{M}$ *(Central Limit Theorem)*

- **Of course, the discretization must be fine enough and one needs numerical results for several lattice spacings in order to extrapolate to the continuum limit**

Let us go back to the circle



In the standard approach Z is written a sum over energy/angular momentum eigenstates

$$Z = \sum_{n=-\infty}^{\infty} \exp\left(-\beta \frac{\hbar^2 n^2}{2mR^2}\right)$$

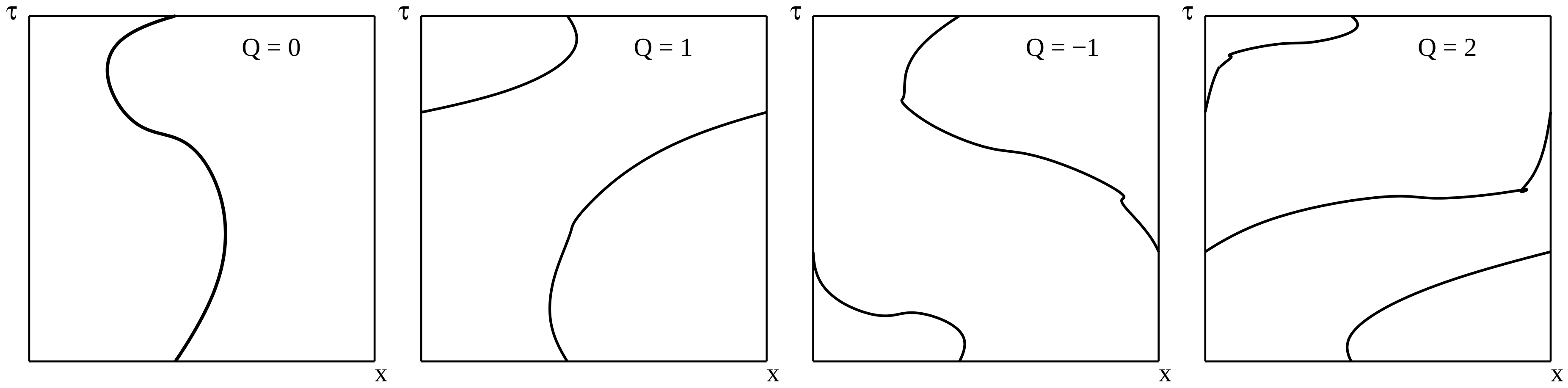
in the path integral approach

$$Z = \mathcal{N} \int_{x(0)=x(\beta\hbar)} \mathcal{D}x(\tau) \exp\left(\frac{-S_E[x(\tau)]}{\hbar}\right) \quad ; \quad S_E[x(\tau)] = \int_0^{\beta\hbar} d\tau \, \frac{1}{2} m \left(\frac{dx}{d\tau}\right)^2$$

New feature: paths divide in topological classes

Boundary conditions in space $\Longrightarrow$ each path $x(\tau)$ contributing to Z is a continuous application from the temporal circle to the spatial circle.

how many times does the path wind around the circle before closing in eucl. time?



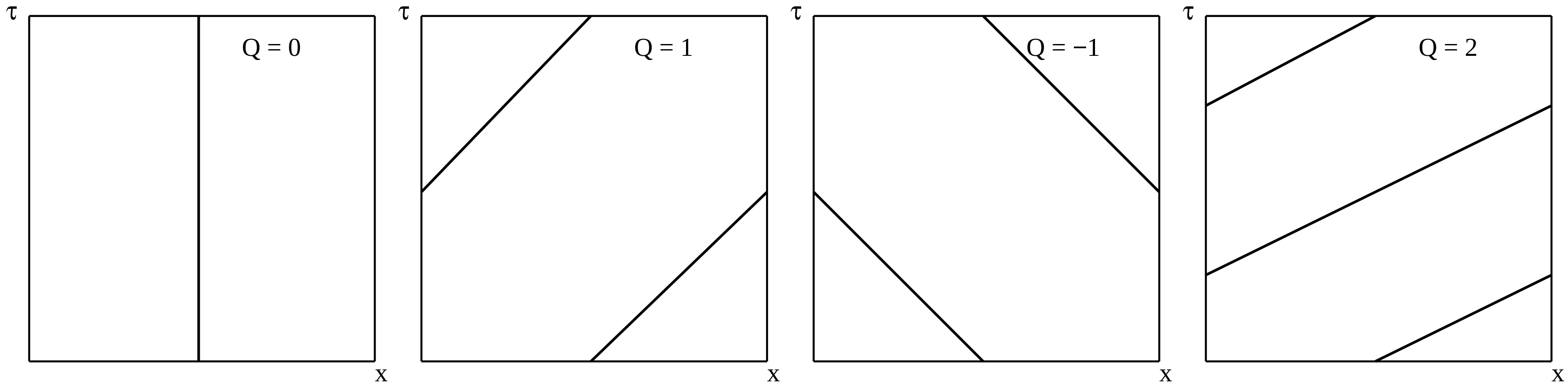
Paths are divided in homotopy classes according to their winding number Q which cannot be changed without cutting the path.

On the other hand, discontinuous paths have zero measure in the path integral

Wiener measure: first derivative divergent, but continuity is guaranteeed

The homotopy group is $\pi_1(S^1) = \mathbb{Z}$

Can we compute the contribution of each topological sector to the path integral? YES



- **The path integral over each sector can be done by integrating over classical solutions, which are minima of the Euclidean action**

- **In this simple case the integration can be done exactly, yielding a result proportional to $\exp(-S_Q/\hbar)$ where S_Q is the action of the classical path**

$$S_Q = \frac{1}{2} m \frac{(2\pi R Q)^2}{\beta\hbar}$$

- **We have therefore an expression for the weight of each sector, which is nothing but the probability distribution $P(Q)$ over the winding number Q**

$$P(Q) \propto \exp\left(-\frac{Q^2}{2\beta\hbar\chi}\right) \quad ; \quad \chi \equiv \frac{\hbar}{4\pi^2 m R^2}$$

Low and high T limits

$$Z = \sum_{n=-\infty}^{\infty} \exp\left(-\beta \frac{\hbar^2 n^2}{2mR^2}\right) = \frac{1}{\sqrt{2\pi\beta\hbar\chi}} \sum_{Q=-\infty}^{\infty} \exp\left(-\frac{1}{\beta}\frac{Q^2}{2\hbar\chi}\right)$$

the partition function can be written in terms of two different series, which are sort of dual to each other (β vs $1/\beta$ in the exponential)

- **low T (ground state physics)** ($\beta\hbar^2/(mR^2) \sim \hbar\beta\chi \gg 1$)

  - only lowest energy levels (lowest $|n|$) contribute

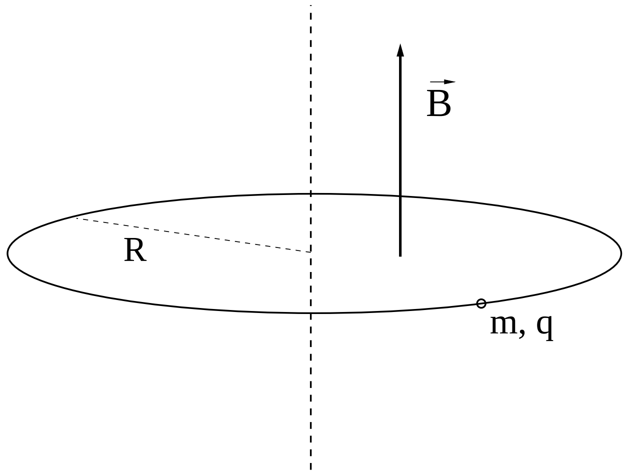
  - all Q values contribute and they are $\sim$ Gaussian distributed with variance $\sigma = \hbar\beta\chi$

- **high T:** ($\beta\hbar^2/(mR^2) \sim \hbar\beta\chi \ll 1$)

  - all energy levels n contribute, they are $\sim$ Gaussian distributed with variance $\sigma = 1/(4\pi^2\beta\hbar\chi)$

  - only lowest winding numbers contribute

And now the magnetic field, alias the θ-term



A magnetic flux Φ_B across the circle has a possible tangential gauge potential $A = \Phi_B/(2\pi R)$, hence

$$L = \frac{1}{2}mv^2 + qAv = \frac{1}{2}mv^2 + \frac{q\Phi_B}{2\pi R}v$$

while the energy levels change into

$$E_n = \frac{\hbar^2(n - \theta/(2\pi))^2}{2mR^2} \qquad \theta \equiv \frac{q\Phi_B}{\hbar}$$

In the Euclidean path integral formalism ($t \to -i\tau$) that amounts to adding the following term to the Euclidean action S_E:

$$i\frac{qBR}{2\hbar}\int_0^{\beta\hbar} d\tau \frac{dx}{d\tau} = i\frac{qBR}{2\hbar}\, 2\pi R Q = i\theta Q\,.$$

Notice: a total derivative in the Lagrangian, does not change the classical equations, but leads to a global contribution which is constant in each topological sector

How the partition function changes

$$Z = \sum_{n=-\infty}^{\infty} e^{-\beta E_n} = \sum_{n=-\infty}^{\infty} e^{-\frac{\beta\hbar\chi}{2}(2\pi n-\theta)^2} \propto \mathcal{N}\int \mathcal{D}x(\tau) e^{-S_E[x(\tau)]/\hbar} e^{i\theta Q} \propto \sum_{Q=-\infty}^{\infty} e^{-\frac{1}{2\hbar\chi\beta}Q^2} e^{i\theta Q}$$

- **θ-dependence of the free energy $F(\theta) = -\log Z(\theta)/\beta$ here is related to the magnetic properties of the system. General features:**

  - $F(\theta + 2\pi) = F(\theta)$ **(θ is an angular variable) ;** $F(-\theta) = F(\theta)$

  - $Z(\theta) \le Z(0) \implies F(\theta) \ge F(0) \implies$ **diamagnetism**

- **in the path integral formalism, a complex weight appears, which hinders the application of Monte-Carlo simulations. This is usually known as the sign problem.**

- **It afflicts other theories with a topological term. Here, it disappears when resumming Z in terms of other variables (n): such a rewriting is still a mirage in other cases**

  Then, how to investigate θ-dependence in the path-integral approach?

Taylor expansion approach

$$F(\theta) - F(0) = \frac{1}{2}F^{(2)}\theta^2 + \frac{1}{4!}F^{(4)}\theta^4 + \ldots \quad ; \qquad F^{(2n)} = \left.\frac{d^{2n}F}{d\theta^{2n}}\right|_{\theta=0}$$

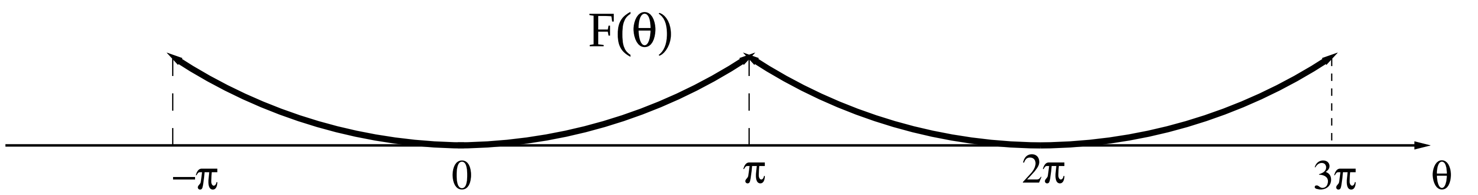
Taylor coefficients: cumulants of the Q distribution $P(Q) \propto e^{-Q^2/(2\hbar\beta\chi)}$ at $\theta = 0$

$$F^{(2)} = \frac{\langle Q^2\rangle_c}{\beta\hbar} = \frac{\langle Q^2\rangle - \langle Q\rangle^2}{\beta\hbar} \; ; \quad F^{(4)} = -\frac{\langle Q^4\rangle_c}{\beta\hbar} = -\frac{\langle Q^4\rangle - 3\langle Q^2\rangle^2}{\beta\hbar} \; ; \quad F^{(2n)} = -(-1)^n\frac{\langle Q^{2n}\rangle_c}{\beta\hbar}$$

as $\hbar\beta\chi \to \infty$ (vacuum), Q is purely Gaussian, only $F^{(2)} \neq 0$ (topological susceptibility)

$$F(\theta) - F(0) = \frac{\chi}{2}\theta^2$$

that, when combined with the expected periodicity and symmetries, gives rise to a multibranched function with quantum phase transitions at $\theta = \pi$ or odd multiples of it



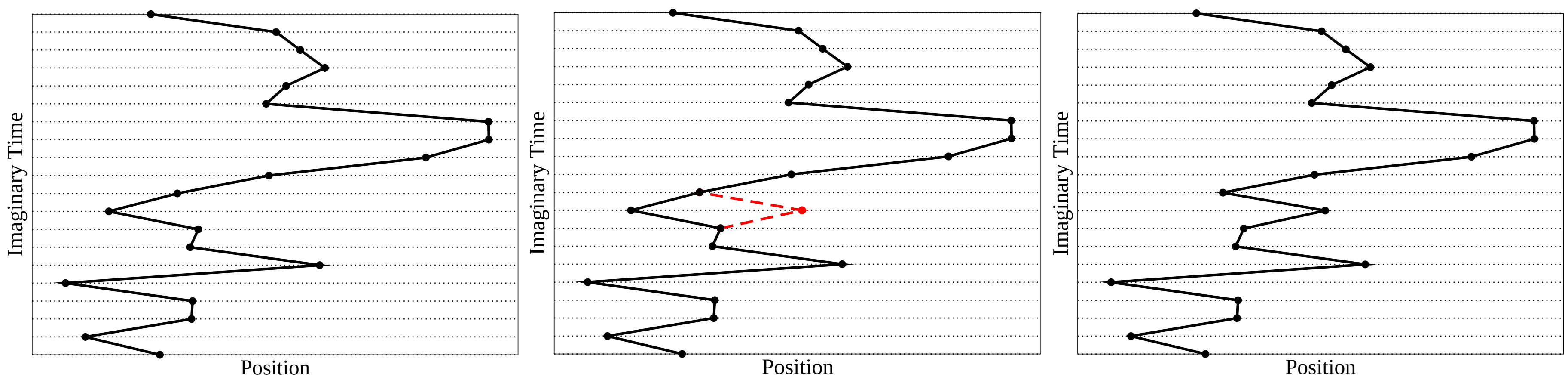
In terms of energy levels, at π we have a level crossing associated with the quantum phase transition, which disappears as soon as $T \neq 0$

In the opposite, hight T limit, $\hbar\beta\chi \ll 1$, only the lowest topological sectors contribute, taking just $Q = 0, 1, -1$:

$$Z(\theta) \propto 1 + 2e^{-1/(2\hbar\beta\chi)} \cos\theta \implies F(\theta) - F(0) \simeq -\frac{2}{\beta} e^{-1/(2\hbar\beta\chi)} \cos\theta$$

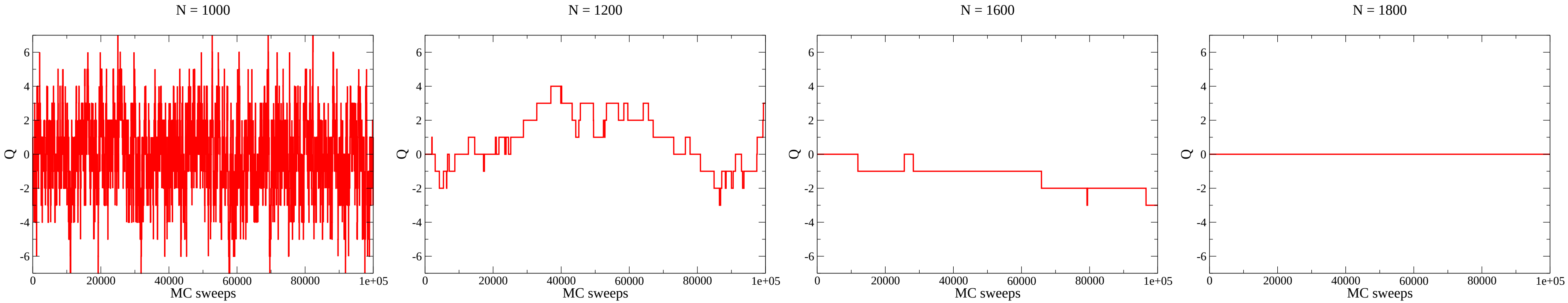
i.e. a smooth, periodic behavior in θ

Problems in numerical sampling of topological modes



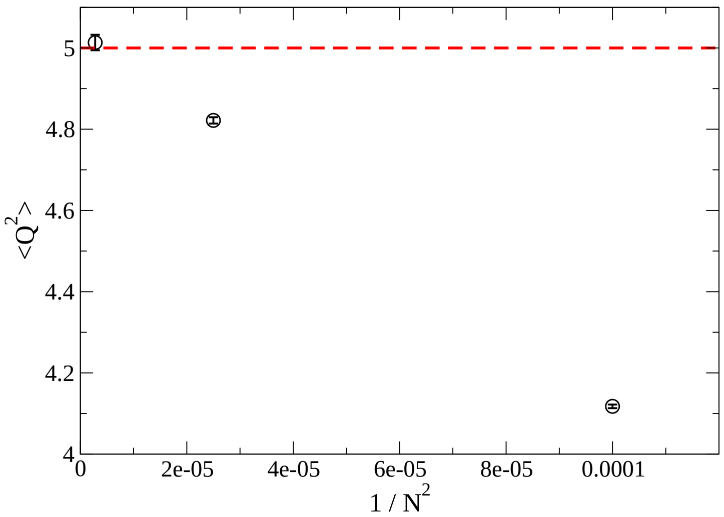
Apart from the sign problem, the study of θ-dependence faces other numerical challenges:

- **standard algorithms update the path configuration by small local steps**
- **in the continuum limit, paths evolve *almost continuously* in configuration space**
- **how is it possible, in this limit, to change topological sector? One should move across unlikely "discontinuous paths", which in the continuum limit have zero measure.**
- **standard algorithms become slower and slower in moving from one topological sector to the other, until they become completely non-ergodic.**



Set of MC histories (100K sweeps, Metropolis algorithm), obtained at fixed $\hbar\beta\chi = 5$ varying the number of temporal slices N

Critical slowing down proceeds fast towards complete freezing of topological modes



Luckily enough, in this case numerical results approach the continuum limit quite earlier (finest point $N = 600$)