Temporal correlators and energy spectrum by Monte-Carlo simulations of the path-integral

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Discretization of the path integral and the continuum limit

- To handle the problem numerically, we need to parameterize the generic path in terms of a finite number of stochastic variables $\Longrightarrow$ in place of the original time interval, $[0, \beta\hbar]$, take a lattice of N points separated by a lattice spacing $a = \beta\hbar/N$.

- It is necessary to describe the whole system in terms of dimensionless variables: rescale everything in lattice spacing (or some other typical scale) units

- We are interested in results valid in the continuum limit of our system: discretization implies systematic effects, which should be kept under control by studying the dependence of our results on the lattice spacing a.
  In general this is realized as $a \ll$ typical temporal scale of our system.

A simple example: the harmonic potential

$$S_E[x(\tau)] = \int_0^{\beta\hbar} d\tau \left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 + \frac{m\omega^2 x(\tau)^2}{2} \right]$$

$$y(n) \equiv \left(\sqrt{\hbar/m\omega}\right)^{-1} x(na)\,; \qquad n = 0, 1, \ldots N-1\,; \qquad \int_0^{\beta\hbar} d\tau \;\to\; \sum_{n=0}^{N-1} a$$

$$\frac{dx}{d\tau} \;\to\; \left(\sqrt{\frac{\hbar}{m\omega}}\right)^{-1} \frac{y(n+1) - y(n)}{a} \;\; \text{forward derivative} \qquad \eta \equiv a\omega$$

$$\frac{S_E^L}{\hbar} = \frac{m\hbar}{2\hbar m\omega} \sum_{n=0}^{N-1} a \left[\frac{(y(n+1)-y(n))^2}{a^2} + \omega^2 y(n)^2 \right] = \sum_{n=0}^{N-1} \left[y(n)^2 \left(\frac{\eta}{2} + \frac{1}{\eta}\right) - \frac{1}{\eta} y(n) y(n+1) \right]$$

The MC algorithm samples N stochastic variables $y(n)$ according to $\exp(-S_E^L/\hbar)$

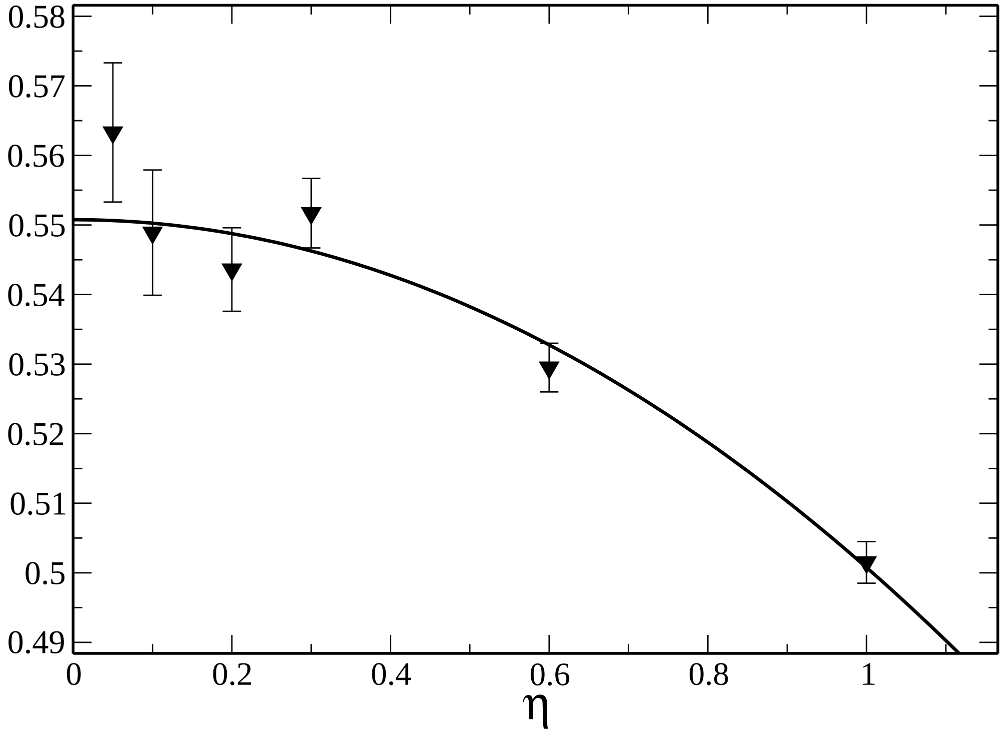
The lattice system is described in terms of two adimensional parameters, η and N

Continuum limit: $\eta = a\,\omega \to 0$ (life will be less simple in lattice gauge theories ...)

Different discretization are possible, continuum results should be independent of that

The temperature is given by the relation: $T/(\hbar\omega) = 1/(N\eta)$

An example: computation of the average squared displacement for $T = \hbar\omega/3$



Exact continuum value: $\langle y^2 \rangle = 0.5523957$ **(would have been 0.5 at zero T)**

Numerical estimates at finite lattice spacing fitted according to $\langle y^2 \rangle_\eta = \langle y^2 \rangle + A\eta^2$

Results (from a few minutes run on a laptop ...)

$$\langle y^2 \rangle = 0.551(3)\,; \quad A = -0.050(5)\,; \quad \chi^2/\mathrm{d.o.f.} = 1.12$$

Temporal correlators and energy gaps

Consider the connected two-point function of a generic function $O(q)$ of the coordinate operator q, we can expand it over a basis of energy eigenstates:

(we set again $\hbar = 1$)

$$
\begin{aligned}
C_O(\tau) &\equiv \langle 0|O(q(\tau))O(q(0))|0\rangle - |\langle 0|O(q)|0\rangle|^2 \\
&= \langle 0|e^{H\tau}O(q)e^{-H\tau}O(q)|0\rangle - |\langle 0|O(q)|0\rangle|^2 \\
&= \sum_n \langle O(q)|e^{H\tau}Oe^{-H\tau}|n\rangle\langle n|O(q)|0\rangle - |\langle 0|O(q)|0\rangle|^2 \\
&= \sum_{n\neq 0} e^{-(E_n-E_0)\tau}|\langle n|O(q)|0\rangle|^2 \rightarrow_{\tau\rightarrow\infty} e^{-(E_{n_{min}}-E_0)\tau}|\langle n_{min}|O(q)|0\rangle|^2
\end{aligned}
$$

for large Euclidean times τ it is dominated by the lowest energy state coupled to vacuum by O, hence it gives a measure of the gap (in the "O-channel"):

$\Delta_O E \equiv E_{n_{min}} - E_0$

Can we determine $C_O(\tau)$ in the path integral formulation?

$$\langle 0|O(q(\tau))O(q(0))|0\rangle = \lim_{\beta\to\infty}\frac{\mathrm{Tr}\left(e^{-\beta H}O(q(\tau))O(q(0))\right)}{\mathrm{Tr}\left(e^{-\beta H}\right)} = \lim_{\beta\to\infty}\frac{\mathrm{Tr}\left(e^{-(\beta-\tau)H}O(q)e^{-H\tau}O(q)\right)}{\mathrm{Tr}\left(e^{-\beta H}\right)}$$

$$= \lim_{\beta\to\infty}\frac{\int \mathcal{D}x(\tau)\exp\left(-S_E[x(\tau)]\right)O(x(\tau))O(x(0))}{\int \mathcal{D}x(\tau)\exp\left(-S_E[x(\tau)]\right)}$$

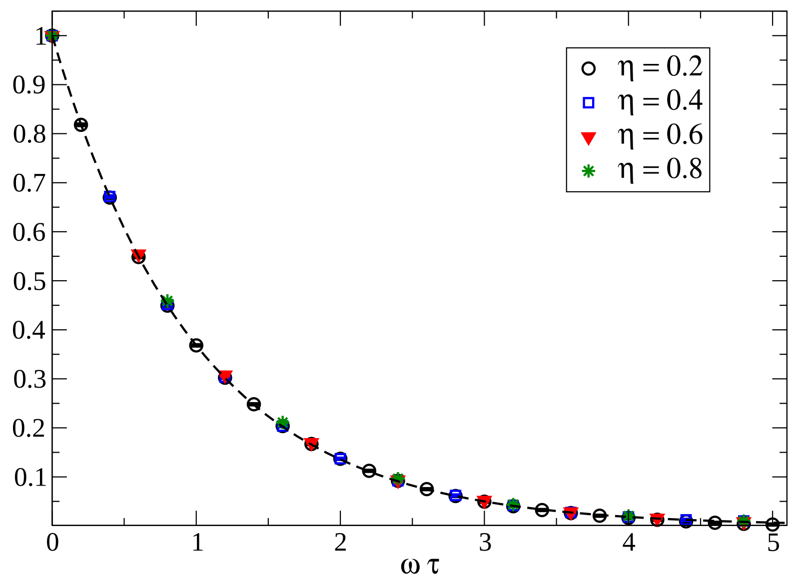
YES, we just need to measure the connected temporal correlator of the function $O(x)$ over the paths, in the limit of infinite temporal extent (in practice $1/\beta \gg \Delta E$):

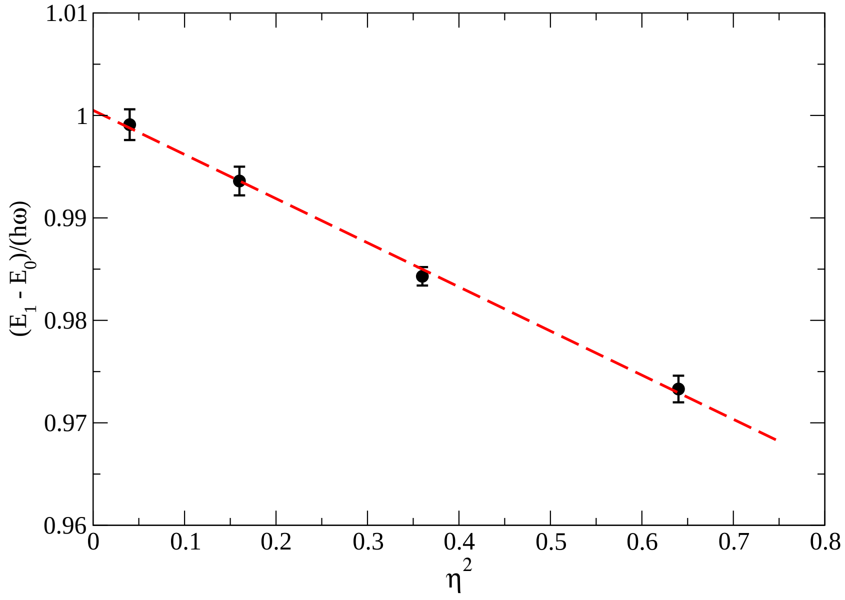
$$C_O(\tau) = \langle O(x(\tau))O(x(0))\rangle - \langle O(x(0))\rangle^2$$

Let us take $O(q) = q$ as a first example, for the harmonic oscillator $\langle n|q|0\rangle \propto \delta_{1n}$ hence the correlator is a single exponential for every τ, giving $E_1 - E_0$:

$$C_q(\tau) = |\langle n|q|0\rangle|^2 e^{-\omega\tau}$$

Extraction of $E_1 - E_0$ and continuum limit





- We show (left) results for the correlator $\langle x(\tau)x(0)\rangle$, obtained for different values of $\eta = a\omega$ and at fixed total temporal extension $\beta\omega = 20$.
- Fitting with a single exponential $\langle x(\tau)x(0)\rangle = A\exp(-(E_1 - E_0)\tau)$ we get $\Delta E = E_1 - E_0$
- Discretization effects are clearly visible in ΔE and can be parameterized as η^2 corrections. The value extrapolated to the continuum limit is $\Delta E = 1.003(6)\ \omega$, in agreement with expectations.
- Notice: in real spectrum computations working with $\beta\Delta E \gg 1$ is not achieavable, the leading correction is backward propagation: $\exp(-\Delta E\tau) \to \exp(-\Delta E\tau) + \exp(-\Delta E(\beta - \tau))$

QUESTION: **Can we choose $O(q)$ so as to compute higher energy levels? How to "select" contributions from other energy eigenstates?**

ANSWER: **Work first on the symmetries of the operator $O(q)$ to select the appropriate channel! In our simple case parity is the relevant symmetry:**

- **Choose for $O(q)$ an odd function of q to impose $\langle n|O(q)|0\rangle = 0$ when n is even and obtain information only about odd energy levels (odd channel)**
- **Choose for $O(q)$ an even function of q to impose $\langle n|O(q)|0\rangle = 0$ when n is odd and obtain information only about even energy levels (even channel)**

EXAMPLE: $O(q) = q^2 \propto {a^\dagger}^2 + a^2 + 2a^\dagger a + 1$ **only connects to** $n = 2$ **(remember** $q = (a + a^\dagger)/\sqrt{2m\omega}$ **and** $aa^\dagger - a^\dagger a = 1$**)**

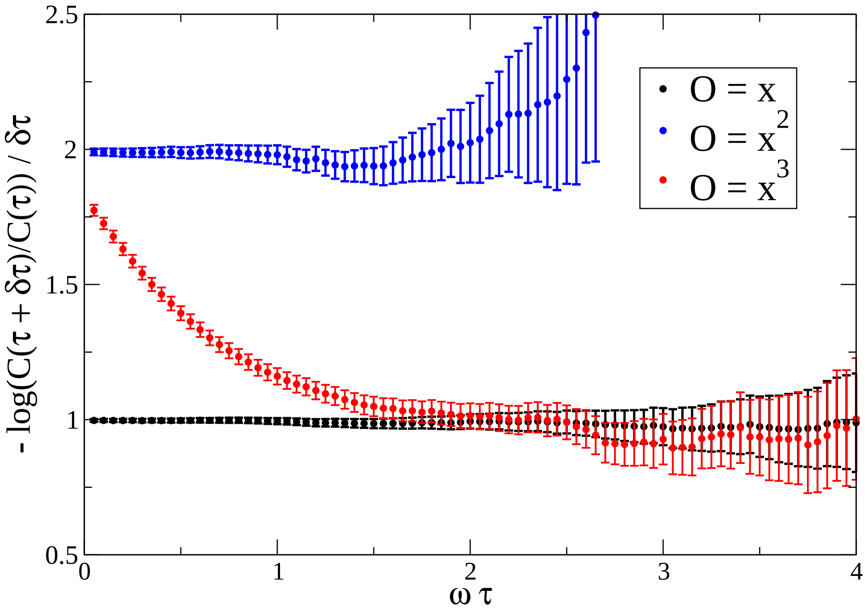
$$\langle x^2(\tau)x^2(0)\rangle - \langle x^2\rangle^2 = |\langle 2|q^2|0\rangle|^2 \exp\left(-(E_2 - E_0)\tau\right)$$

Enlarging the set of possible correlators: $q, q^2, q^3, \ldots$

Effective mass plots are a convenient way to fix the asymptotic behavior of the correlators

$$-\log(C_O(\tau+\delta\tau)/C_O(\tau))/\delta\tau$$

reaches a plateau as the single exponential regime sets in



- **For $C_x(\tau)$ and $C_{x^2}(\tau)$ the plateau starts soon since q and q^2 couple the vacuum to a single state. The plateaux give $\Delta E = \omega$ and 2ω respectively.**
- **For C_{x^3} the situation is less trivial since $\langle n|q^3|0\rangle \neq 0$ for $n = 1, 3.$.**

$$q^3 \propto a^{\dagger 3} + a^3 + 3a^{\dagger 2}a + 3a^{\dagger}a^2 + 3(a + a^{\dagger})$$

Asymptotic regime reached only when the contribution from $n = 3$ vanishes.

LESSON: overlap with lowest states can be enhanced by appropriate choices of the operator, leading to improved estimates of the lowest energy gaps in the given channel (important for lightest hadron masses).

BUT: contamination with higher energy states in a given channel contains essential information about excited spectrum (important for hadron excitations)

How to properly extract such information?

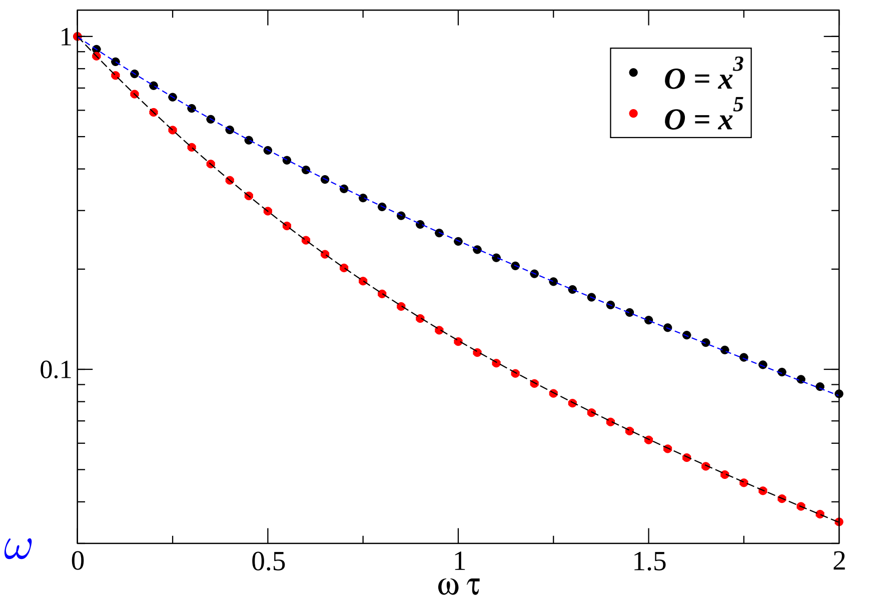
Multiexponential fits to correlators are usually not stable leading to wrong estimates

$$C_{x^3} = Ae^{-\Delta_{10}\tau} + Be^{-\Delta_{30}\tau}$$

$$\Delta_{10} \simeq 0.90(1)\,\omega\ ; \quad \Delta_{30} \simeq 2.5(1)\,\omega$$

$$C_{x^5} = Ae^{-\Delta_{10}\tau} + Be^{-\Delta_{30}\tau} + Ce^{-\Delta_{50}\tau}$$

$$\Delta_{10} \simeq 0.6(1)\,\omega\,;\ \Delta_{30} \simeq 1.5(2)\,\omega\,;\ \Delta_{50} \simeq 3.6(2)\,\omega$$



Can we find correlators which project out exactly a given state?

Consider the cubic operator, for which $\langle 3|q^3|0\rangle \neq 0$ and $\langle 1|q^3|0\rangle \neq 0$

$$q^3 \propto a^{\dagger 3} + a^3 + 3a^{\dagger 2}a + 3a^\dagger a^2 + 3(a + a^\dagger)$$

if we subtract the $(a + a^\dagger) \propto q$ term we eliminate the overlap with $n = 1$

$$q^3 - 3q/2 \propto a^{\dagger 3} + a^3 + 3a^{\dagger 2}a + 3a^\dagger a^2$$

hence we expect

$$C_{33}(\tau) \equiv \langle (x^3(\tau) - 3x(\tau)/2)(x^3(0) - 3x(0)/2)\rangle = A\, e^{-\Delta_{30}\tau}$$

and analogously for the mixed correlator ($\langle 0|(q^3 - 2q/3)|n\rangle\langle n|q|0\rangle = 0 \;\; \forall n$)

$$C_{31}(\tau) \equiv \langle (x^3(\tau) - 3x(\tau)/2)x(0)\rangle = 0$$

We have found a basis of orthogonal correlators resolving the spectrum for $n = 1, 3$

Can we generalize?

QUESTION: how to choose $O_{\bar{n}}(q)$ such that $\langle n|O_{\bar{n}}(q)|0\rangle \neq 0$ for a given $n = \bar{n}$ only?

$$\langle n|O(q)|0\rangle = \int dx \int dx' \langle n|x\rangle\langle x|O(q)|x'\rangle\langle x'|0\rangle = \int dx \psi_n^*(x) O(x)\psi_0(x)$$

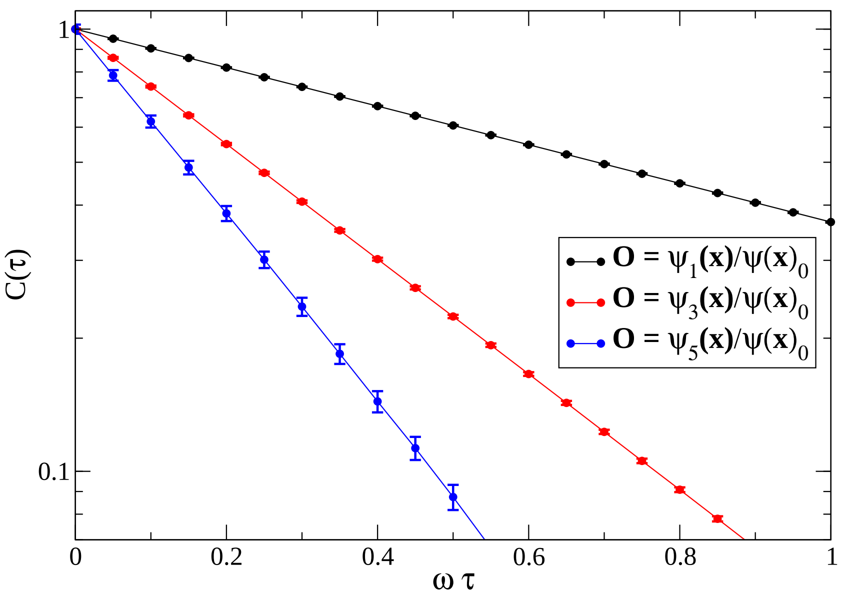
solution: $O(x)\psi_0(x) \propto \psi_n(x) \implies O_{\bar{n}}(q) = \psi_{\bar{n}}(q)/\psi_0(q)$

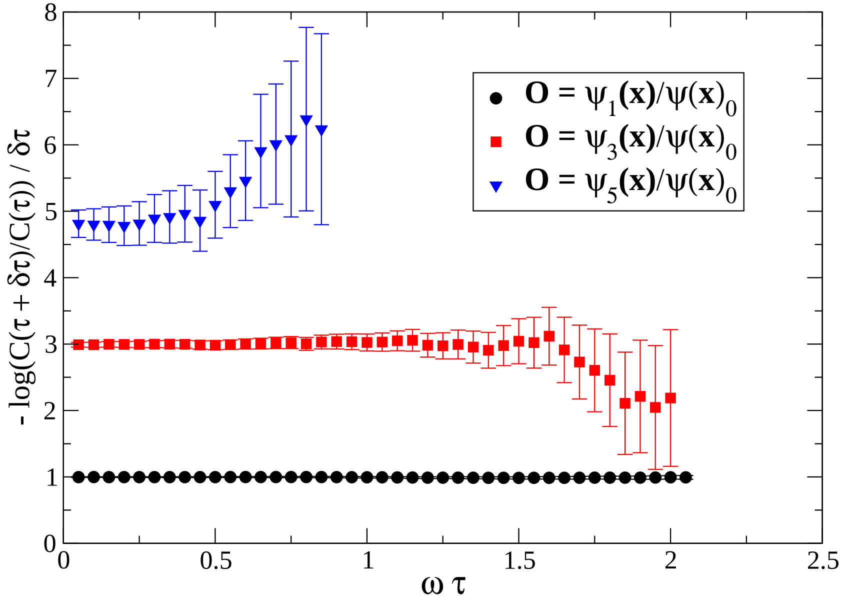
(remember $\psi_0(q)$ has no zeros hence it is invertible!)

General rule: to project out $E_{\bar{n}} - E_0$ exactly, you have to compute

$$\langle O_{\bar{n}}(x(\tau))O_{\bar{n}}(x(0))\rangle \propto \exp(-(E_{\bar{n}} - E_0)\tau)$$

(notice that it is already a connected correlator, i.e. $\langle O(x(\tau))\rangle = 0$, by construction)





The task is easy for the harmonic oscillator, $O_{\bar{n}}(q) = H_{\bar{n}}(q)$ **(Hermite polynomial)**

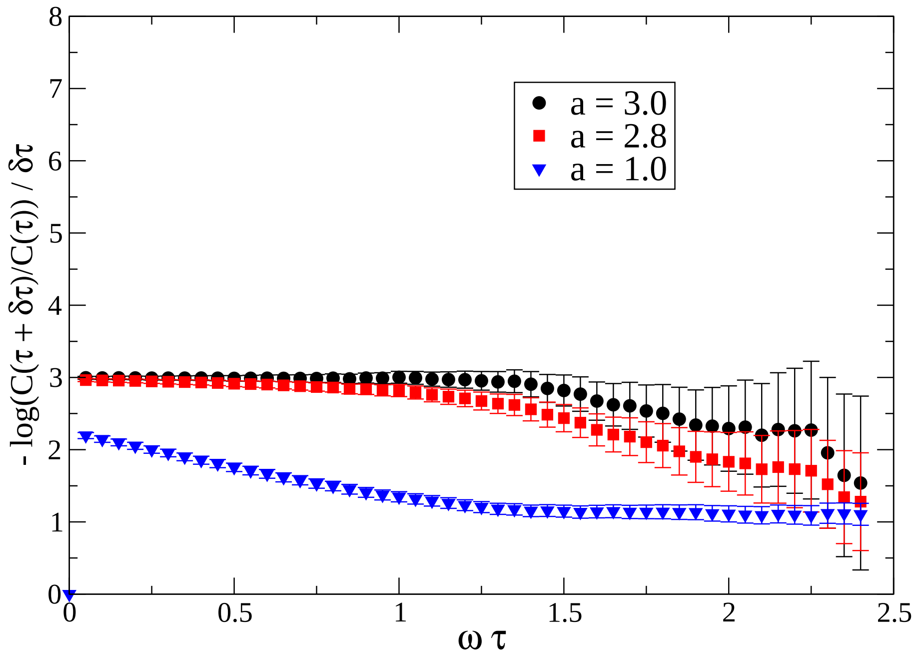
Improved correlators do their job, projecting onto the chosen energy level

This is useless for the general case!

We do not the exact solution hence we do not know wave functions!

However: **this is a useful guide for more general approaches.**

What happens if we miss the correct wave function?



Consider the case $O(q) = 2q^2 - aq$:

$a = 3$ **gives exactly ψ_3/ψ_0.**

- **for $a = 2.8$ we still get the correct result for $n = 3$: small overlap with $n = 1$**
- **for $a = 1.0$ the $n = 3$ energy level is lost**

if overlap is small, contamination is not harmful

A more general approach: The Variational Method

for first applications to lattice simulations see C. Michael, Nucl. Phys. B 259, 58 (1985); M. Luscher and U. Wolff, Nucl. Phys. B 339, 222 (1990)

- **Choose a basis of N operators $O_i(q)$ and look at the time evolution of the correlation matrix**

$$G_{ij}(\tau) \equiv \langle O_i(x(\tau)) O_j(x(0)) \rangle$$

- **Find the solution of the eigenvalue equation:**

$$G_{ij}(\tau + \delta\tau) u_j^\alpha = e^{-\Delta_\alpha \delta\tau} G_{ij}(\tau) u_j^\alpha$$

  which, for large enough τ, gives the energies of the N lowest eigenstates in the space spanned by the N operators $O_i(q)$.

- **A proper choice of the starting basis can optimize overlap with first excited levels**

- **Recent studies have shown that looking for the eigenvectors u_j^α ($\sim$ wave functions) instead that only for eigenvalues is more effective** (M. S. Mahbub *et al*, Phys. Lett. B 679, 418 (2009))

1 – From Quantum Mechanics to Lattice Field Theory

Many of the things learned in our exercise in Quantum Mechanics can be exported to Quantum Field Theory, with a bit of translation. But new things appear, of course

Let us first consider a free scalar neutral field at finite temperature in 3 spatial + 1 temporal dimensions.

coordinate operator $\hat{q} \longrightarrow$ **field operator** $\hat{\phi}(\vec{x})$

position eigenstate $|x\rangle \longrightarrow$ **field eigenstate** $|\varphi\rangle \qquad \hat{\phi}(\vec{x})|\varphi\rangle = \varphi(\vec{x})|\varphi\rangle$

completeness relation: $\int \mathcal{D}\varphi \, |\varphi\rangle\langle\varphi| = \mathrm{Id}$

functional integration is over all different spatial configurations of the field

Lagrangian $\longrightarrow$ **Lagrangian density** $\mathcal{L} = \frac{1}{2}\left[\left(\frac{\partial \phi}{\partial t}\right)^2 - \vec{\nabla}\phi \cdot \vec{\nabla}\phi - m^2\phi^2\right]$

The partition function can be written in the path integral formulation as

$$Z = \mathcal{N} \int_{p.b.c.} \mathcal{D}\varphi(\vec{x}, \tau) \exp\left(-S_E[\varphi]\right) \qquad S_E = \int_0^\beta d\tau \int d^3x \mathcal{L}_E$$

$$\mathcal{L}_E = \frac{1}{2}\left[\left(\frac{\partial\phi}{\partial t}\right)^2 + \vec{\nabla}\phi \cdot \vec{\nabla}\phi + m^2\phi^2\right] = \frac{1}{2}\left(\partial_\mu\phi\partial_\mu\phi + m^2\phi^2\right)$$

We set $\hbar = c = k_B = 1$. Again, $iS \to -S_E$ by rotating $t \to -i\tau$.

The functional integration is over all 4 dimensional field configurations defined on Euclidean space-time.

Periodic boundary conditions **in time direction $\Longrightarrow$ thermal theory with $\tau \in [0, 1/T]$.**

Thermal averages are expectation value of field operators over field configurations distributed proportionally to a positive weight $\exp(-S_E[\varphi])$:

$$\langle O\rangle_T = \int \mathcal{D}\varphi P[\varphi] O[\varphi] = \frac{\int \mathcal{D}\varphi \exp\left(-S_E[\varphi]\right) O[\varphi]}{\int \mathcal{D}\varphi \exp\left(-S_E[\varphi]\right)}$$

remember as usual that $\lim_{T\to 0}\langle O\rangle_T = \langle 0|O|0\rangle$**.**

To sample important configurations contributing the path integral, we need again to discretize the system (also in space!) The simplest possibility is to take an isotropic space-time cubic lattice with spacing a. A site on this lattice will be associated to four integer coordinates: $n \equiv (n_1, n_2, n_3, n_4)\ ,\qquad n + \hat{\mu} \equiv (n_1, \dots n_\mu + 1, \dots)$

$$x_\mu \to a n_\mu \qquad \varphi \to \tfrac{1}{a}\hat{\varphi} \qquad m \to \tfrac{1}{a}\hat{m} \qquad \textstyle\int d^4x \to \sum_n a^4$$

$$\partial_\mu \varphi \to \tfrac{1}{a^2}\hat{\partial}^F_\mu \hat{\varphi} = \tfrac{1}{a^2}\left(\hat{\varphi}(n+\hat{\mu}) - \hat{\varphi}(n)\right)$$

forward derivative, but infinitely many different discretizations are possible

A finite (but large enough!) spatial volume must be taken as well, in order to have a finite number of stochastic variables. Any kind of boundary conditions can be taken in spatial directions (e.g. periodic)

Finally, lattice field configurations are sampled according to

$$\int (\prod_n d\hat{\varphi}(n)) P_L[\hat{\varphi}] \qquad\qquad P_L[\hat{\varphi}] = \exp(-S_L[\hat{\varphi}])$$

$$S_L = \frac{1}{2} \sum_n \left(\sum_{\mu=1}^{4} (\hat{\varphi}(n+\hat{\mu}) - \hat{\varphi}(n))^2 + \hat{m}^2 \hat{\varphi}(n)^2 \right)$$

$T = \frac{1}{\beta} = \frac{1}{N_t a}$ **where N_t is the temporal extent in lattice units.**

Actually, a is not explicitly known: N_t and $\hat{m}$ are the only tunable parameters.

Indeed, since m is the only other scale of our system, the only sensible parameter is

$$\frac{T}{m} = \frac{1}{\hat{m} N_t}$$

Continuum limit? Easy! It is reached as $\hat{m} \to 0$ ($\hat{\xi} \to \infty$). But the answer may be much less trivial in interacting field theories ... Indeed, a finite lattice spacing a is a regulator, $a \to 0$ is like removing the UV cutoff. This operation is cost-free for a non-interacting theory, but otherwise strictly linked to renormalization.

Mass spectrum computation in Quantum Field Theories

Correlators in the Euclidean time can be defined and computed similarly to what we have done in QM

$$C_O(\tau) = \langle 0|\hat{O}[\varphi(\tau)]\hat{O}[\varphi(0)]\rangle - |\langle 0|\hat{O}[\varphi(0)]\rangle|^2$$

and

$$\langle 0|\hat{O}[\varphi(\tau)]\hat{O}[\varphi(0)]\rangle = \int \mathcal{D}\varphi P[\varphi] O[\varphi] = \frac{\int \mathcal{D}\varphi \exp\left(-S_E[\varphi]\right) O[\varphi(\tau)] O[\varphi(0)]\rangle}{\int \mathcal{D}\varphi \exp\left(-S_E[\varphi]\right)}$$

$C_O(\tau)$ **can expanded over a set of energy eigenstates and is dominated, for large** τ **by the lowest state:**

$$C_O(\tau) = \sum_{n\neq 0} e^{-(E_n - E_0)\tau} |\langle n|\hat{O}[\varphi]|0\rangle|^2 \rightarrow_{\tau\rightarrow\infty} e^{-(E_{n_{min}} - E_0)\tau} |\langle n_{min}|\hat{O}[\varphi]|0\rangle|^2$$

Facing a continuum of energy levels

A problem emerges in this case: the lowest energy state is in general the lower edge of a continuum of states! Consider the field-field correlator $\hat{O}[\varphi(0)] = \varphi(\vec{x}, 0)$ $\varphi(\vec{x})$ couples to all single particle state, i.e.

$$C_\varphi(\vec{x}, \tau; \vec{x}, 0) = \langle 0|\varphi(\vec{x}, \tau)\varphi(\vec{x}, 0)]\rangle \propto \int \frac{d^3\vec{p}}{2E(\vec{p})} |\langle\vec{p}|\varphi(\vec{x})|0\rangle|^2 e^{-\sqrt{m^2+|\vec{p}|^2}\,\tau}$$

that means that, while $|\vec{p} = \vec{0}\rangle$ is indeed the lowest energy state, whose energy is equal to the particle mass, we have energy levels arbitrarily close to it, so that the single exponential behavior $C_\varphi(\tau) \sim e^{-m\tau}$ will be visible at asymptotically large times.

ACTUALLY: in a finite volume momenta are discretized, $\vec{p} = 2\pi\vec{n}/L$ where L is the box size, hence energy levels are always discrete, but in practice this is a problem anyway, convergence is slower.

SOLUTION?

PROJECT ONTO ZERO MOMENTUM

$$\varphi(\vec{x}) \to \tilde{\varphi}(\vec{p}=0) \equiv \int d^3x\, \varphi(\vec{x})$$

this is done in practice by integrating the point-point correlator over one (or both) spatial slices at fixed times τ and 0 (point-point $\to$ wall-wall correlator).

Coupling to $\vec{p} \neq 0$ states disappears, $\langle \vec{p}|\tilde{\varphi}(\vec{q})|0\rangle \propto \delta^3(\vec{p}-\vec{q})$, hence

$$\int d^3x d^3y\, C_\varphi(\vec{x},\tau;\vec{y},0) \propto e^{-m\tau} \quad \forall\, \tau$$

Is projection onto zero momentum always a solution for eliminating continuum state contributions?

NO, unfortunately ...

Consider an operator bilinear in the field φ, which couples to two particle states. Even projecting over zero momentum, we cannot eliminate the contribution from two particle states $|\vec{p}, -\vec{p}\rangle$ with a continuum spectrum

$$E_{|\vec{p},-\vec{p}\rangle} = \sqrt{m^2 + |\vec{p}|^2} + \sqrt{m^2 + |\vec{p}|^2}$$