The discretized path integral can be calculated numerically.

In lattice QCD, we have access to path-integral expectation value, but not to the Hamiltonian.

Problem: Assuming that we know only thermal expectation values of time-ordered products of field operators, how do we extract the energy levels?

1) $T \to \infty$ limit of thermal expectation values = vacuum expectation values

2) Energy levels can be extracted from 2pt functions

$T \to \infty$ limit and vacuum expectation values

$\hat{H} = \hat{K} + \hat{V}$ $\qquad$ $\hat{T}(\tau) = e^{-\frac{\tau}{2}\hat{V}} e^{-\hat{K}} e^{-\frac{\tau}{2}\hat{V}} = e^{-\tau\hat{H} + O(\tau^2)}$

Define the effective Hamiltonian $\qquad$ $\hat{H}_{eff}(\tau) = -\frac{1}{\tau} \log \hat{T}(\tau)$

$\hat{H}_{eff}(\tau)$ depends on τ, $\hat{H}$ does not $\qquad$ $\lim_{\tau \to 0} \hat{H}_{eff}(\tau) = \hat{H}$

Ground state of $\hat{H}$ $\equiv$ Vacuum $|\Omega\rangle$

Ground state of $\hat{H}_{eff}$ $\equiv$ $|\Omega_{eff}\rangle$: approximation of $|\Omega\rangle$

$\lim_{\tau \to 0} |\Omega_{eff}(\tau)\rangle = |\Omega\rangle$

at some point I will drop "eff"

	Continuous time	Discrete time
Simplifying assumption: discrete spectrum (not essential)	$\hat{H}\,\lvert E_n\rangle = E_n \lvert E_n\rangle$	$\hat{H}_{eff}\,\lvert E_n^{eff}\rangle = E_n^{eff}\lvert E_n^{eff}\rangle$
	$E_0 < E_1 \leq E_2 \leq \dots \; ; \; \lvert E_0\rangle \equiv \lvert\Omega\rangle$	$E_0^{eff} < E_1^{eff} \leq E_2^{eff} \leq \dots \; ; \; \lvert E_0^{eff}\rangle \equiv \lvert\Omega_{eff}\rangle$
Partition function	$Z = \mathrm{tr}\, e^{-T\hat{H}} = \sum_{n=0}^{\infty} e^{-TE_n}$	$Z = \mathrm{tr}\, \hat{T}^{T/\varepsilon} = \mathrm{tr}\, e^{-T\hat{H}_{eff}} = \sum_{n=0}^{\infty} e^{-TE_n^{eff}}$
Thermal expectation values	$\frac{1}{Z}\mathrm{tr}\{e^{-T\hat{H}}\hat{A}\} = \frac{1}{Z}\sum_n \langle E_n\rvert e^{-T\hat{H}}\hat{A}\lvert E_n\rangle = \dfrac{\sum_n e^{-TE_n}\langle E_n\rvert\hat{A}\lvert E_n\rangle}{\sum_n e^{-TE_n}}$	$\frac{1}{Z}\mathrm{tr}\{\hat{T}^{T/\varepsilon}\hat{A}\} = \frac{1}{Z}\mathrm{tr}\{e^{-T\hat{H}_{eff}}\hat{A}\} = \dfrac{\sum_n e^{-TE_n^{eff}}\langle E_n^{eff}\rvert\hat{A}\lvert E_n^{eff}\rangle}{\sum_n e^{-TE_n^{eff}}}$
Vacuum expectation values	$\lim_{T\to\infty}\frac{1}{Z}\mathrm{tr}\{e^{-T\hat{H}}\hat{A}\} = \dfrac{e^{-TE_0}\langle E_0\rvert\hat{A}\lvert E_0\rangle}{e^{-TE_0}} = \langle\Omega\rvert\hat{A}\lvert\Omega\rangle$	$\lim_{T\to\infty}\frac{1}{Z}\mathrm{tr}\{\hat{T}^{T/\varepsilon}\hat{A}\} = \langle\Omega_{eff}\rvert\hat{A}\lvert\Omega_{eff}\rangle$
$T\to\infty$: $e^{-TE_0} \gg e^{-TE_{n\neq 0}}$		

Vacuum 2pt functions and energy levels

$$C_T(t) = \frac{1}{Z}\,\mathrm{tr}\{e^{-TH}\,\hat{A}(t)\,\hat{B}(0)\} = \langle A(t)B(0)\rangle_{\substack{\text{path integral}\\ \text{with p.b.c. in time}}} \qquad t>0$$

$$C_\infty(t) \equiv \lim_{T\to\infty} C_T(t) \overset{(1)}{=} \langle\Omega_{eff}|\hat{A}(t)\,\hat{B}(0)\,|\Omega_{eff}\rangle$$

$$\overset{(2)}{=} \langle\Omega_{eff}|\,e^{t\hat{H}_{eff}}\,\hat{A}\,e^{-t\hat{H}_{eff}}\,\hat{B}\,|\Omega_{eff}\rangle$$

$$\overset{(3)}{=} \langle\Omega_{eff}|\,\hat{A}\,e^{-t(H_{eff}-E_0^{eff})}\,\hat{B}\,|\Omega_{eff}\rangle$$

$$\overset{(4)}{=} \sum_{n=0}^{\infty} \underbrace{e^{-t(E_n-E_0)}}_{} \underbrace{\langle\Omega|\hat{A}|E_n\rangle\langle E_n|\hat{B}|\Omega\rangle}_{\equiv c_n}$$

(1) see previous slide

(2) def of $\hat{A}(t)$

(3) $\hat{H}_{eff}|\Omega_{eff}\rangle = E_0^{eff}|\Omega_{eff}\rangle$

(4) drop "eff" – laziness
completeness rel. $I=\sum_{n=0}^{\infty}|E_n\rangle\langle E_n|$
in between the ops

spectral decomposition
of vacuum 2pt function

read off $E_n - E_0$ from the
t-dependence of vacuum
2pt function

notice that energies
are always defined
up to an arbitrary
constant. Only
energy differences
have physical meaning

$$= \underbrace{\langle\Omega|\hat{A}|\Omega\rangle\langle\Omega|\hat{B}|\Omega\rangle}_{\lim_{T\to\infty}\langle A\rangle\langle B\rangle} + \sum_{n=1}^{\infty} c_n\, e^{-t(E_n-E_0)}$$

$$c_n \equiv \langle\Omega|\hat{A}|E_n\rangle\langle E_n|\hat{B}|\Omega\rangle$$

$$C_\infty(t) \equiv \lim_{T\to\infty} C_T(t) = \underbrace{\lim_{T\to\infty} \langle A\rangle\langle B\rangle}_{\text{this term has no information on energy levels: subtract it away!}} + \sum_{n=1}^{\infty} c_n e^{-t(E_n-E_0)}$$

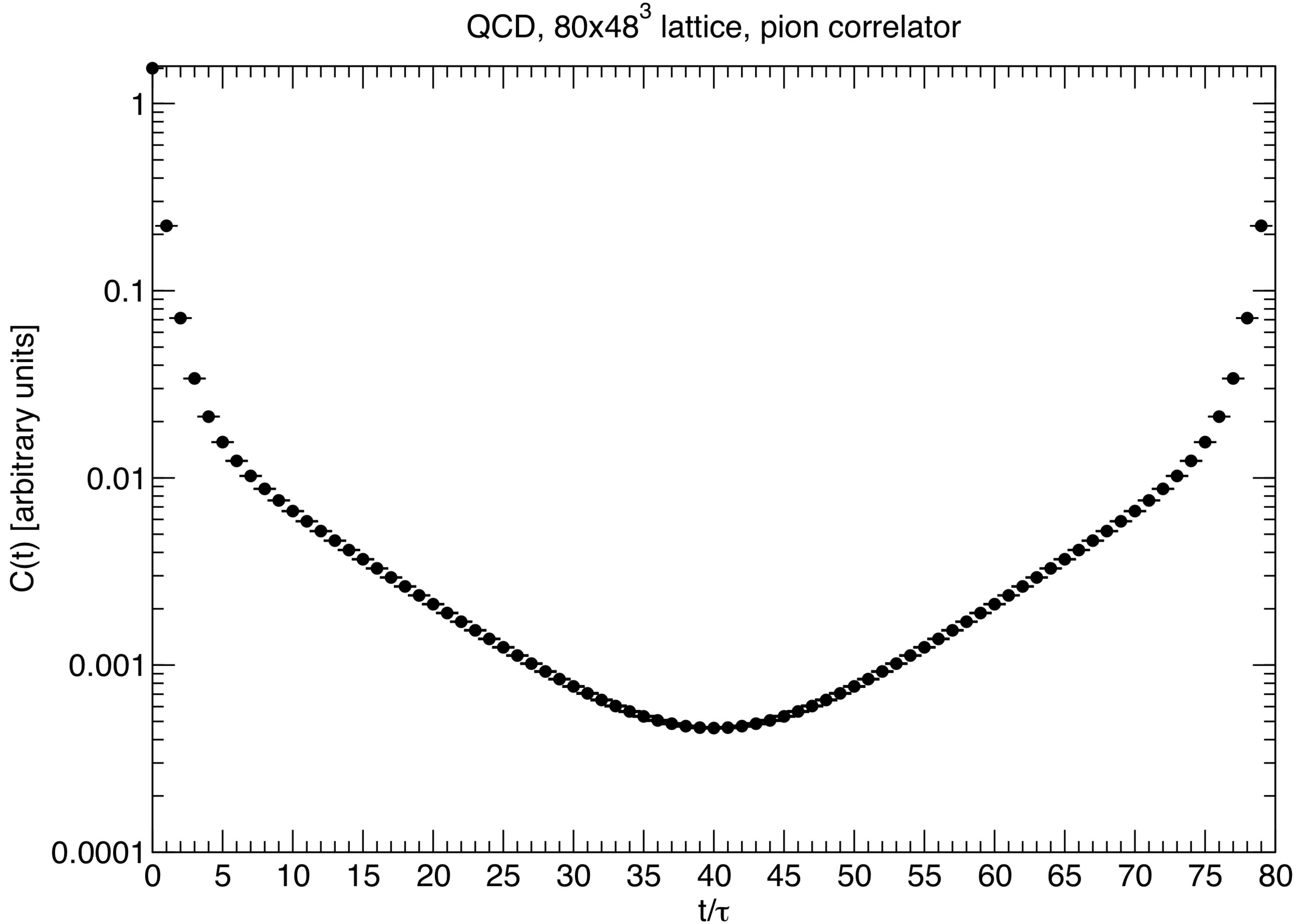
$$C_T^{conn}(t) \equiv \langle A(t)B(0)\rangle - \langle A\rangle\langle B\rangle$$ connected 2pt function [aka correlator]

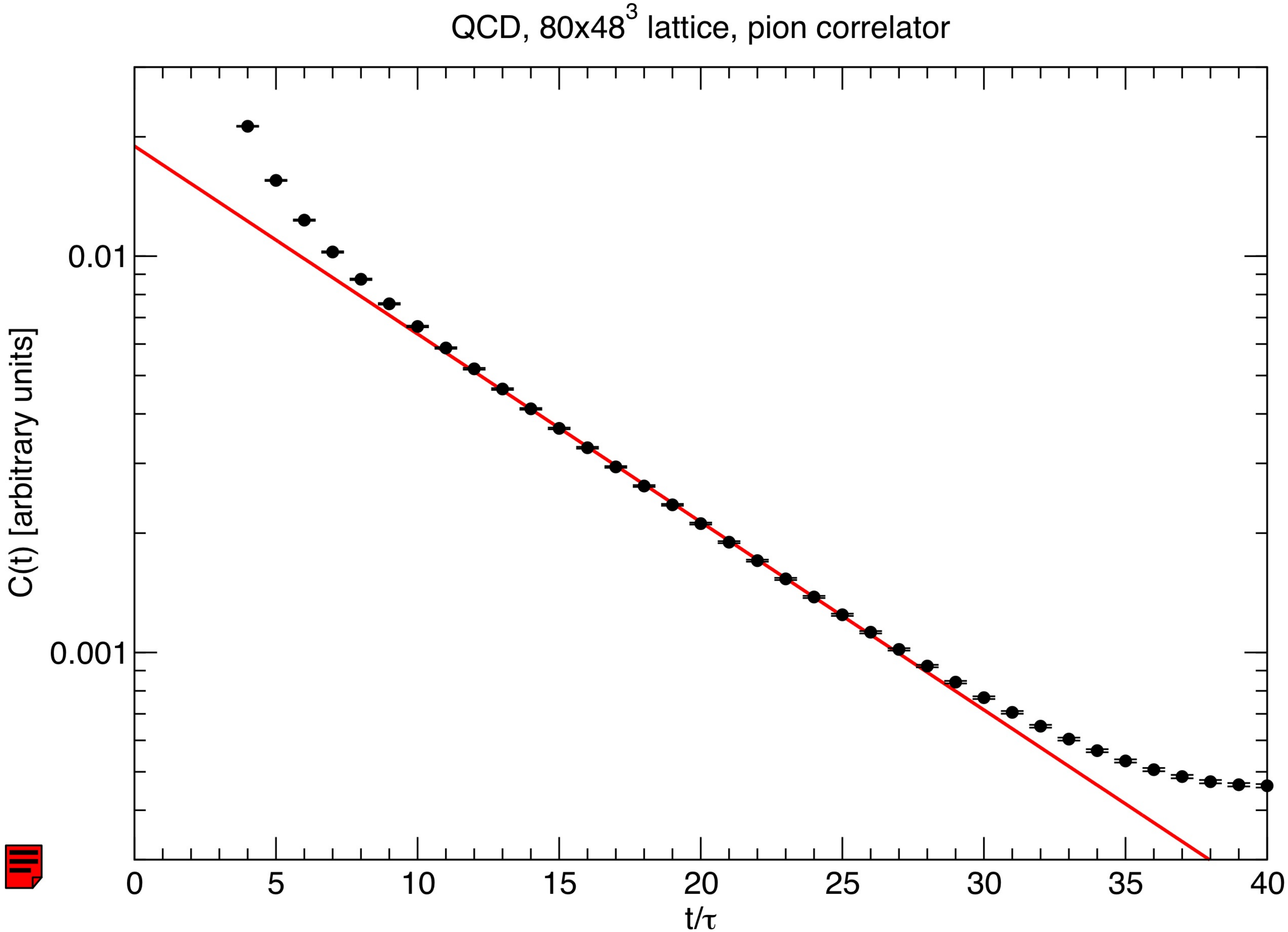
$$C_\infty^{conn}(t) \equiv \lim_{T\to\infty} C_T^{conn}(t) = \sum_{n=1}^{\infty} c_n e^{-t(E_n-E_0)}$$

The low energy levels can be extracted from the large t behaviour of $C_\infty^{conn}(t)$:

$$C_\infty^{conn}(t) \overset{t\to 0}{=} c_1 e^{-t(E_1-E_0)} + c_2 e^{-t(E_2-E_0)} + O\left(e^{-t(E_3-E_0)}\right)$$

This is how it is done in practice in lattice simulations


QCD, 80x48^3 lattice, pion correlator
C(t) [arbitrary units]
t/τ
1
0.1
0.01
0.001
0.0001
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80



QCD, 80x48^3 lattice, pion correlator
C(t) [arbitrary units]
0.01
0.001
0
5
10
15
20
25
30
35
40
t/τ

Energy levels and poles of the 2pt function

$$C_\infty(t) = \langle\Omega|\, \text{time-ordered } A(t)A(0)|\Omega\rangle = \lim_{T\to\infty} \langle A(t)\,A(0)\rangle$$

Spectral decomposition:

$$C_\infty(t) = \begin{cases} \langle\Omega|\,\hat{A}(t)\hat{A}(0)|\Omega\rangle = \langle\Omega|e^{t\hat{H}}\,\hat{A}\,e^{-t\hat{H}}\,\hat{A}\,|\Omega\rangle = \langle\Omega|\,\hat{A}\,e^{-t(H-E_0)}\,\hat{A}\,|\Omega\rangle & t>0 \\ \langle\Omega|\,\hat{A}(0)\hat{A}(t)|\Omega\rangle = \langle\Omega|\,\hat{A}\,e^{tH}\,\hat{A}\,e^{-t\hat{H}}|\Omega\rangle = \langle\Omega|\,\hat{A}\,e^{t(H-E_0)}\,\hat{A}\,|\Omega\rangle & t<0 \end{cases}$$

$$C_\infty(t) = [\ldots] = \sum_{n=0}^{\infty} c_n e^{-|t|(E_n-E_0)} = \left(\langle\Omega|\hat{A}|\Omega\rangle\right)^2 + \sum_{n=1}^{\infty} c_n e^{-|t|(E_n-E_0)} \qquad c_n = \langle\Omega|\hat{A}|E_n\rangle\langle E_n|\hat{A}|\Omega\rangle$$

$$C_\infty^{conn}(t) = \sum_{n=1}^{\infty} c_n\, e^{-|t|(E_n-E_0)}$$

we want to look at the Fourier transform

$$\tilde{C}^{conn}_{\infty}(p_0) = \int_{-\infty}^{\infty} dt\; e^{ip_0 t}\, C^{conn}_{\infty}(t)$$

$$C^{conn}_{\infty}(t) = \sum_{n=1}^{\infty} c_n\, e^{-|t|\Delta E_n} \quad , \quad \Delta E_n = E_n - E_0$$

E_n eigenvalues of $\hat{H}$

$$\int_{-\infty}^{\infty} dt\; e^{ip_0 t} e^{-|t|\omega} = \left.\frac{e^{ip_0 t - t\omega}}{ip_0 - \omega}\right|_{t=0}^{\infty} + \left.\frac{e^{ip_0 t + t\omega}}{ip_0 + \omega}\right|_{t=-\infty}^{0}$$

$$= \frac{1}{\omega - ip_0} + \frac{1}{\omega + ip_0} = \frac{2\omega}{p_0^2 + \omega^2}$$

[Assumption:
discrete spectrum
-valid for finite
volume QFT]

$$\tilde{C}^{conn}_{\infty}(p_0) = \sum_{t \in \tau\mathbb{Z}} e^{ip_0 t}\, C^{conn}_{\infty}(t)$$

$$C^{conn}_{\infty}(t) = \sum_{n=1}^{\infty} c_n\, e^{-|t|\Delta E_n} \quad , \quad \Delta E_n = E_n - E_0$$

E_n eigenvalues of $\hat{H}_{eff} = -\frac{1}{\tau}\log \hat{T}$

$$\sum_{t \in \tau\mathbb{Z}} e^{ip_0 t} e^{-|t|\omega} =$$

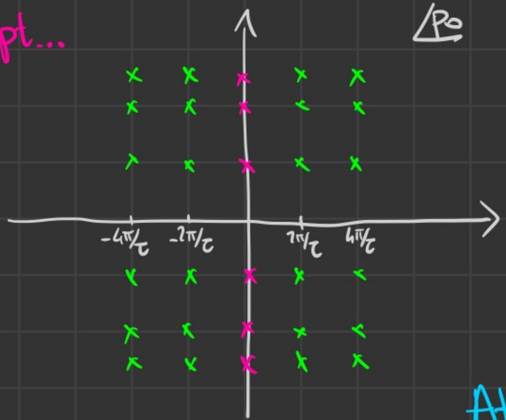
$$= \sum_{k=0}^{\infty} e^{(ip_0 - \omega)\tau k} + \sum_{k=0}^{\infty} e^{(-ip_0 - \omega)\tau k} - 1$$

$$= \frac{1}{1 - e^{(ip_0 - \omega)\tau}} + \frac{1}{1 - e^{(-ip_0 - \omega)\tau}} - 1$$

$$\tilde{C}^{conn}_{\infty}(p_0) = \sum_{n=1}^{\infty} \frac{c_n}{p_0^2 + (E_n - E_0)^2}$$

- analitically continued to $p_0 \in \mathbb{C}$ except...
- poles at $p_0 = \pm i\Delta E_n$

In both cases, you read the energy differences ΔE_n from the poles of the 2-pt function!



$$\tilde{C}^{conn}_{\infty}(p_0) = \sum_{n=1}^{\infty} c_n \left\{ \frac{1}{1 - e^{(ip_0 - \Delta E_n)}} + \frac{1}{1 - e^{(-ip_0 - \Delta E_n)}} - 1 \right\}$$

- periodic $\tilde{C}^{conn}_{\infty}\left(p_0 + \frac{2\pi}{\tau}\right) = \tilde{C}^{conn}_{\infty}(p_0)$
- analytically continued to $p_0 \in \mathbb{C}$ except...
- poles at $e^{(\pm ip_0 - \Delta E_n)} = 1 \iff p_0 = \pm i\Delta E_n + \frac{2\pi}{\tau} k$ with $k \in \mathbb{Z}$

At $L = \infty$ one has poles and cuts...

The simplest 2-pt function: free scalar theory

$$S = \sum_x \tau a^3 \left\{ \frac{1}{2} (\partial^f_\mu \varphi)^2 + \frac{m^2}{2} \varphi^2 \right\}$$

$x_0 = 0, \tau, \dots, T-\tau$

$x_k = 0, a, \dots, L-a \qquad k=1,2,3$

periodic b.c. in space and time:

$$\varphi(x_0+T, \underline{x}) = \varphi(x_0, \underline{x})$$

$$\varphi(x_0, \underline{x} + L\underline{e}_k) = \varphi(x_0, \underline{x})$$

$\underline{e}_1 = (1,0,0) \quad \underline{e}_2 = (0,1,0) \quad \underline{e}_3 = (0,0,1)$

forward derivatives $\quad \partial^f_0 \varphi(x_0, \underline{x}) = \dfrac{\varphi(x_0+\tau, \underline{x}) - \varphi(x_0)}{\tau} \quad , \quad \partial^f_k \varphi(x_0, \underline{x}) = \dfrac{\varphi(x_0, \underline{x} + a\underline{e}_k) - \varphi(x_0, \underline{x})}{a}$

We want to calculate

$$\langle \varphi(x) \varphi(y) \rangle = \frac{\int [d\varphi]\, e^{-S} \varphi(x) \varphi(y)}{\int [d\varphi]\, e^{-S}}$$

- φ can be thought as a vector (where x is the index)
- The action has the following form

  $$S = \frac{1}{2} \varphi^t M \varphi = \frac{1}{2} \sum_{xy} \varphi_x M_{xy} \varphi_y$$

  for a certain symmetric, real, positive-definite matrix M.
- We want to calculate the ratio of Gaussian integrals

  $$\frac{\int [d\varphi]\, e^{-\frac{1}{2}\varphi^t M \varphi} \varphi_x \varphi_y}{\int [d\varphi]\, e^{-\frac{1}{2}\varphi^t M \varphi}} = (M^{-1})_{xy}$$

1. Define the scalar product $\quad (\varphi_1, \varphi_2) \equiv \sum_x \varphi_1(x)\,\varphi_2(x) = \varphi^t \varphi$

2. Prove that $\quad (\partial_\mu^f)^t = -\partial_\mu^b$

$$\left[\begin{array}{l} t = \text{transposed} \\ \partial_0^b \varphi(x_0, \underline{x}) = \dfrac{\varphi(x_0,\underline{x}) - \varphi(x_0-\tau,\underline{x})}{\tau} \quad , \quad \partial_k^b \varphi(x) = \dfrac{\varphi(x_0,\underline{x}) - \varphi(x_0, \underline{x} - a\underline{e}_k)}{a} \\ \hookrightarrow \text{backwards derivatives} \end{array}\right]$$

$$\begin{aligned}
(\varphi_2, (\partial_0^f)^t \varphi_1) &\overset{①}{=} (\partial_0^f \varphi_2, \varphi_1) = \\
&\overset{②}{=} \sum_x \frac{\varphi_2(x_0+\tau, \underline{x}) - \varphi_2(x)}{\tau}\, \varphi_1(x) \\
&= \sum_x \frac{1}{\tau} \varphi_2(x_0+\tau, \underline{x})\, \varphi_1(x_0, \underline{x}) - \sum_x \frac{1}{\tau} \varphi_2(x) \varphi_1(x) \\
&\overset{③}{=} \sum_x \frac{1}{\tau} \varphi_2(x_0, \underline{x})\, \varphi_1(x_0-\tau, \underline{x}) - \sum_x \frac{1}{\tau} \varphi_2(x) \varphi_1(x) \\
&= \sum_x \varphi_2(x) \frac{-\varphi_1(x) + \varphi_1(x_0-\tau, \underline{x})}{\tau} \\
&= (\varphi_2, -\partial_0^b \varphi_1)
\end{aligned}$$

① Definition of transposition

② Explicit formulae for ∂_0^f and scalar product.

③ Replace $x_0 \to x_0 - \tau$ in first sum (this can be done because of periodic b.c.)

Since this is valid for every $\varphi_1, \varphi_2 \Rightarrow (\partial_0^f)^T = \partial_0^b$

same for $(\partial_k^f)^T = -\partial_k^f \ldots$

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3. $$S = \frac{\tau a^3}{2} \sum_\mu \left(\partial^f_\mu \varphi, \partial^f_\mu \varphi\right) + \frac{\tau a^3 m^2}{2} (\varphi, \varphi)$$

$$\overset{1}{=} -\frac{\tau a^3}{2} \sum_\mu \left(\varphi, \partial^b_\mu \partial^f_\mu \varphi\right) + \frac{\tau a^3 m^2}{2} (\varphi, \varphi)$$

$$\overset{2}{=} \frac{\tau a^3}{2} \left(\varphi, \left[-\sum_\mu \partial^b_\mu \partial^f_\mu + m^2\right] \varphi\right)$$

$$\overset{3}{\equiv} \frac{1}{2} (\varphi, A\varphi)$$

1. $(\partial^f_\mu)^T = \partial^b_\mu$

2. Bilinearity of scalar product

3. $A \equiv \tau a^3 \left[-\sum_\mu \partial^b_\mu \partial^f_\mu + m^2\right]$

1. Define the scalar product $\quad (\varphi_1, \varphi_2) \equiv \sum_x \varphi_1(x)\,\varphi_2(x) = \varphi^t \varphi$

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3. $$S = \frac{\tau a^3}{2} \sum_\mu (\partial^f_\mu \varphi, \partial^f_\mu \varphi) + \frac{\tau a^3 m^2}{2} (\varphi, \varphi) = \frac{1}{2} (\varphi, A\varphi) \qquad \text{with } A \equiv \tau a^3 \left[-\sum_\mu \partial^b_\mu \partial^f_\mu + m^2 \right]$$

Exercise: A is real, symmetric and strictly positive-definite

4. $$0 = \int [d\varphi] \frac{\partial}{\partial \varphi(x)} \left\{ \varphi(y)\, e^{-\frac{1}{2}(\varphi, A\varphi)} \right\} = \int [d\varphi] \left\{ \delta_{xy} - \varphi(y) (A\varphi)(x) \right\} e^{-S}$$

$$= \left\{ \delta_{xy} - \sum_z A_{xz} \langle \varphi(z) \varphi(y) \rangle \right\} \int [d\varphi]\, e^{-S}$$

i.e. $\displaystyle\sum_z A_{xz} \langle \varphi(z)\varphi(y) \rangle = \delta_{xy} \quad \Leftrightarrow \quad \langle \varphi(x)\varphi(y)\rangle = (A^{-1})_{xy}$

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3. $S = \dfrac{\tau a^3}{2} \sum_\mu \left(\partial^f_\mu \varphi, \partial^f_\mu \varphi\right) + \dfrac{\tau a^3 m^2}{2} (\varphi, \varphi) = \dfrac{1}{2}(\varphi, A\varphi) \quad$ with $\quad A \equiv \tau a^3 \left[-\sum_\mu \partial^b_\mu \partial^f_\mu + m^2\right]$

Exercise: A is real, symmetric and strictly positive-definite

4. $\langle \varphi(x)\varphi(y) \rangle = \dfrac{\int [d\varphi]\, \varphi(x)\varphi(y)\, e^{-S}}{\int [d\varphi]\, e^{-S}} = (A^{-1})_{xy}$

5. Calculate A^{-1} by diagonalizing A ...

$$A \equiv \tau a^3 \left[- \sum_\mu \partial^b_\mu \partial^f_\mu + m^2 \right]$$

In the continuum $A \propto (-\partial^2 + m^2)$ is diagonalized by plane waves e^{ipx}. Does this work on the lattice as well?

$$v_p(x) = e^{ipx}$$

Impose periodic b.c.

$$e^{ip_0(x_0+T) + i\underline{p}\underline{x}} = e^{ipx} \iff e^{ip_0T} = 1 \iff p_0 \in \frac{2\pi}{T}\mathbb{Z}$$

$$e^{ip_0x_0 + i\underline{p}(\underline{x} + L\underline{e}_k)} = e^{ipx} \iff e^{ip_kL} = 1 \iff p_k \in \frac{2\pi}{L}\mathbb{Z}$$

momentum is discrete!

$$v_{p_0 + \frac{2\pi}{\tau}, \underline{p}}(x) = e^{ipx} e^{i2\pi\frac{x_0}{\tau}} = e^{ipx} = v_p(x) \quad \text{because } \frac{x_0}{\tau} \in \mathbb{Z}$$

$$v_{p, \underline{p} + \frac{2\pi}{a}\underline{e}_k}(x) = e^{ipx} e^{i2\pi\frac{x_k}{a}} = e^{ipx} = v_p(x) \quad \text{because } \frac{x_k}{a} \in \mathbb{Z}$$

In order to take each v_p exactly once, one can restrict p to

- either $\quad \Pi = \left\{ p \in \frac{2\pi}{T}\mathbb{Z} \times \frac{2\pi}{L}\mathbb{Z}^3 \;\middle|\; 0 \le p_0 < \frac{2\pi}{\tau},\ 0 \le p_k < \frac{2\pi}{a} \right\}$
- or $\quad \Pi = \left\{ p \in \frac{2\pi}{T}\mathbb{Z} \times \frac{2\pi}{L}\mathbb{Z}^3 \;\middle|\; -\frac{\pi}{\tau} < p_0 \le \frac{\pi}{\tau},\ -\frac{\pi}{a} < p_k \le \frac{\pi}{a} \right\}$

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$\Big[$ t = transposed

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$\hookrightarrow$ backwards derivatives $\Big]$

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$$= \sum_x a^3 \varphi_2(x_0+\tau, \underline{x})\varphi_1(x_0, \underline{x}) - \sum_x a^3 \varphi_2(x)\varphi_1(x)$$
$$\overset{③}{=} \sum_x a^3 \varphi_2(x_0, \underline{x})\varphi_1(x_0-\tau, \underline{x}) - \sum_x a^3 \varphi_2(x)\varphi_1(x)$$
$$= \sum_x \tau a^3 \varphi_2(x) \frac{-\varphi_1(x) + \varphi_1(x_0-\tau, \underline{x})}{\tau}$$
$$= (\varphi_2, -\partial_0^b \varphi_1)$$

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same for $(\partial_k^f)^T = -\partial_k^f \ldots$

1. Define the scalar product $(\varphi_1, \varphi_2) \equiv \sum_x \tau a^3 \varphi_1(x)\, \varphi_2(x)$

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3. $$S = \frac{1}{2}\sum_\mu (\partial^f_\mu \varphi, \partial^f_\mu \varphi) + \frac{m^2}{2}(\varphi, \varphi)$$

$$\overset{①}{=} -\frac{1}{2}\sum_\mu (\varphi, \partial^b_\mu \partial^f_\mu \varphi) + \frac{m^2}{2}(\varphi,\varphi)$$

$$\overset{②}{=} \frac{1}{2}\left(\varphi, \left[-\sum_\mu \partial^b_\mu \partial^f_\mu + m^2\right]\varphi\right)$$

$$\equiv \frac{1}{2}(\varphi, A\varphi) \quad = \frac{1}{2}\tau a^3 \varphi^T A \varphi$$

① $(\partial^f_\mu)^T = \partial^b_\mu$

② Bilinearity of scalar product