From Un-importance Sampling to Importance Sampling

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another possible (optimistic) title:

When the sign problem
turns into the sign blessing

- In this talk we mainly consider 2-flavor QCD with a baryon chemical potential (QCD_B), its phase quenched version (which is equivalent to QCD with a finite isospin chemical potential, QCD_I), and chiral random matrix theories (RMT_B and RMT_I).

- But the method can be applied to other theories — not necessarily QCD or even field theory — as well.

- Unless otherwise stated, we consider the massless limit.

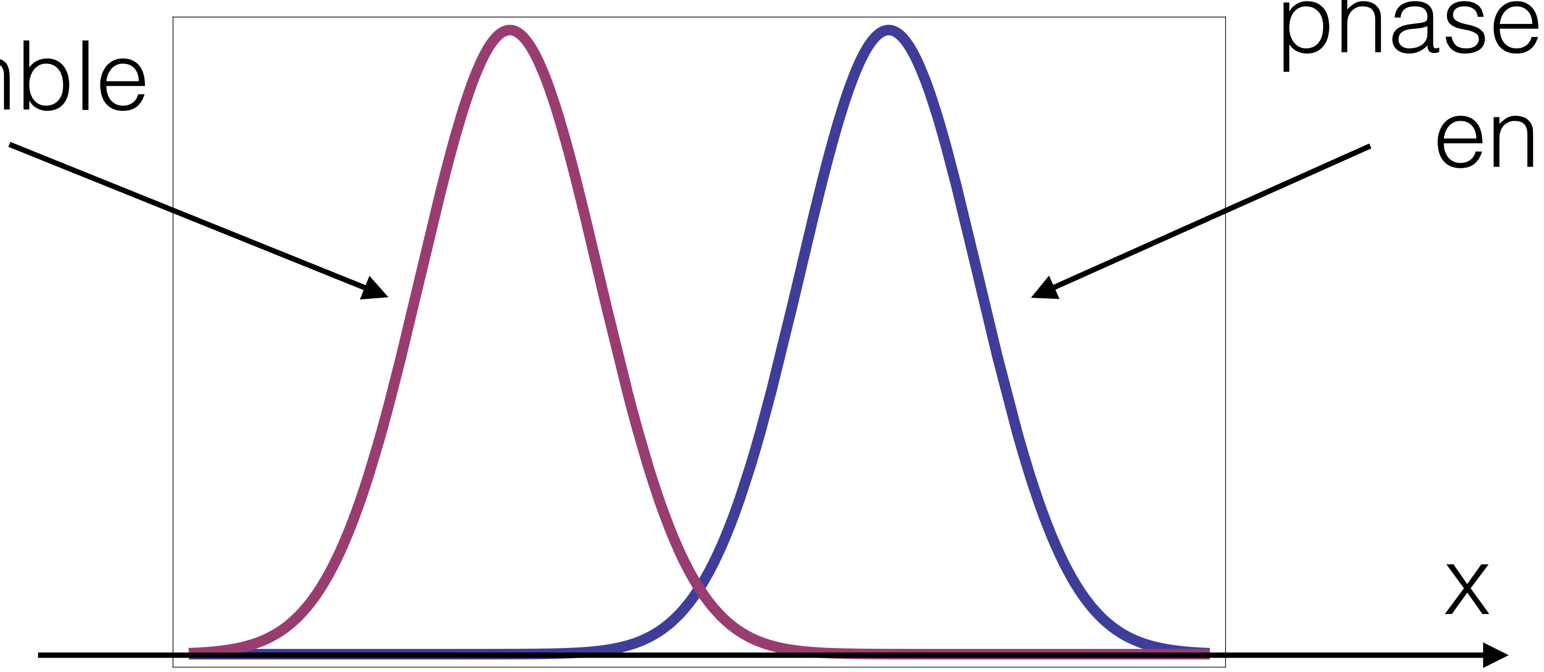
Sign problem is severe when the overlapping problem exists

real ensemble

$\rho_{real}(x)$

phase-quenched ensemble

$\rho_{p.q.}(x)$

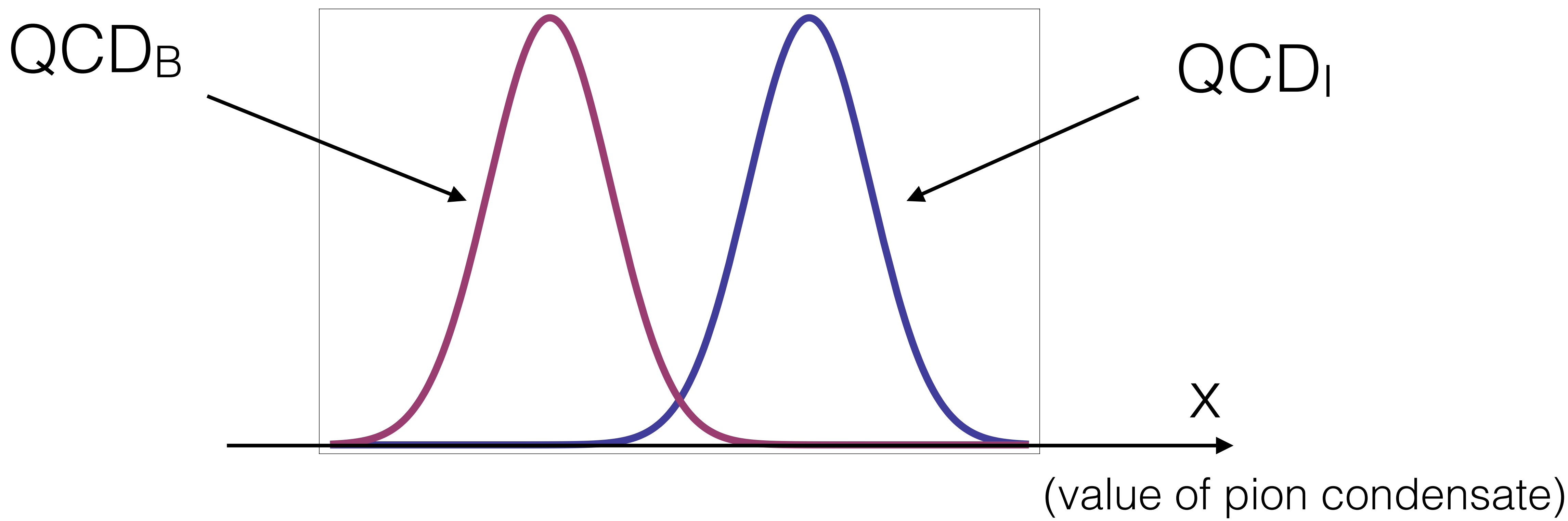


(some observable which characterizes the vacuum)

$$\langle e^{i\Theta} \rangle_x \sim \rho_{real}(x)/\rho_{p.q.}(x)$$

The role of the sign = erase the wrong vacuum

Sign problem is severe when the the pion condenses



$$\langle e^{i\Theta}\rangle_x \sim \rho_B(x)/\rho_I(x)$$

The role of the sign = erase the pion condensation

- Pion condensation → overlapping problem.
- Overlapping problem → only unimportant configurations are sampled.
- So, a naive phase reweighting method is UN-IMPORTANCE SAMPLING, when π^+ condenses. Unimportant samples are preferred!

What happens if the pion condensate is deleted by hand?

- The phase quench approximation becomes exact in the 't Hooft large-N limit. (Cherman-M.H.-Robles Llana 2010, M.H.-Yamamoto 2011; see also Toublan 2003, Cohen 2004)
- So, such configurations are 'important.'
- To calculate 1/N correction, we have to take sign into account. Still, we can expect the average sign is not so small when $\pi^+ \sim 0$.

$$\langle e^{i\Theta} \rangle_x \sim \rho_B(x)/\rho_I(x)$$

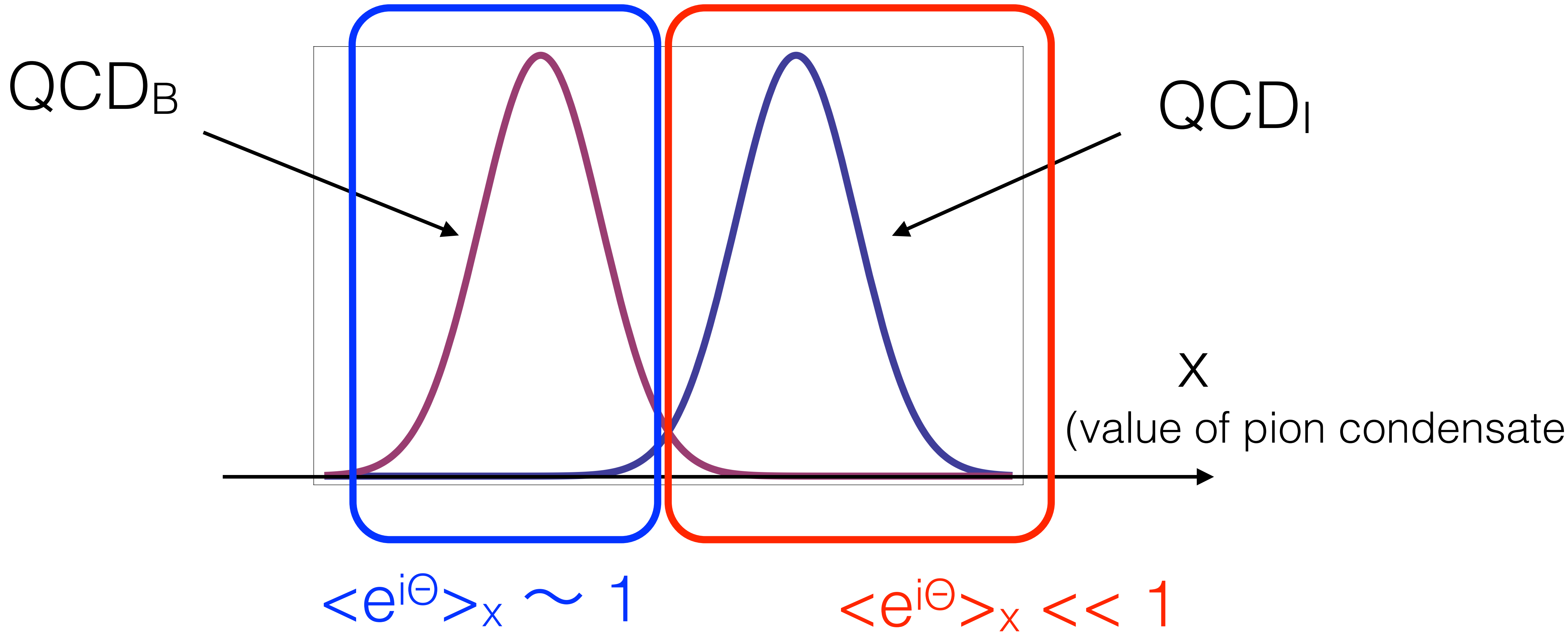
From Un-importance Sampling to Importance Sampling

- We should sample only IMPORTANT samples.

- At large-N, only $\pi^+=0$ contributes.
  → We MUST fix π^+ to be 0.

- At finite-N, why don't we sample ONLY around $\pi^+=0$?

- (A possible by-product: the zero mode could be lifted without introducing a source)



The role of the sign = erase the pion condensation

If the average sign is very small, we don't even have to measure it. SUCH CONFIGURATIONS ARE NOT IMPORTANT. Simply neglect them.

a common belief

When the average sign is small, one should invest more resource to measure them precisely.

our point of view

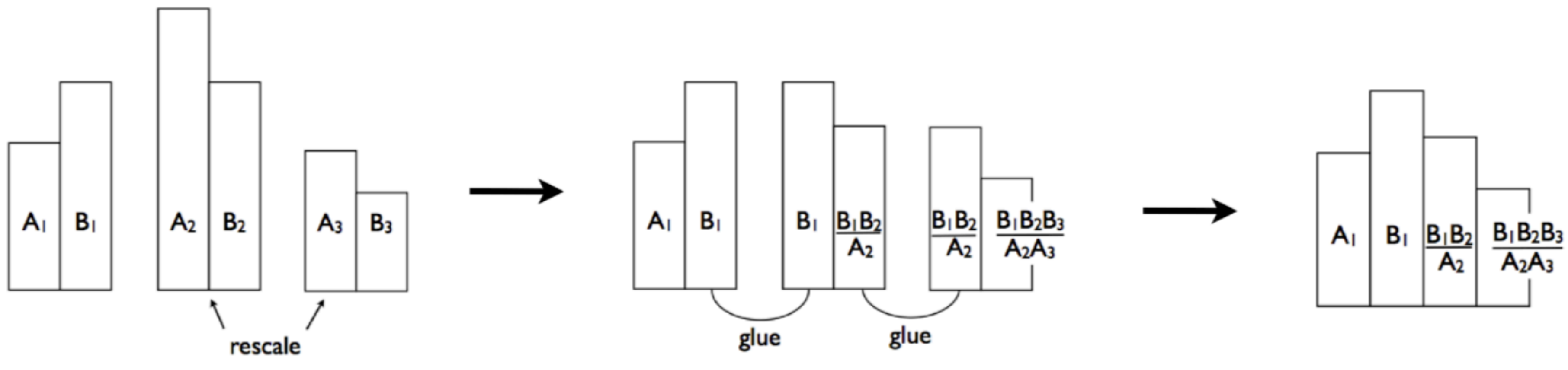
When the average sign is small, we do not have to measure them. It is telling us we can save the simulation cost — sign blessing.

Strategy

- Divide the path integral to I_1, I_2, I_3, …, which is labeled by the value of the pion condensate. I_1: $0 < \pi^+ < \varepsilon$, I_2: $\varepsilon < \pi^+ < 2\varepsilon$, I_3: $2\varepsilon < \pi^+ < 3\varepsilon$, ….

- Do constrained simulations at (I_1+I_2), (I_2+I_3), …..

- Make the relative path-integral weight ρ_k for I_k(histogram of the pion condensate) by gluing partial histograms.



$$\langle e^{iS_I} \rangle_{P.Q.} = \frac{\sum_i \langle e^{iS_I} \rangle_i \cdot \rho_i}{\sum_i \rho_i}$$

$<e^{i\Theta}>_k = <e^{iS\_I}>_k$

the average phase at I_k

(I am sorry that I use two different notations simultaneously.)

$$\langle e^{iS_I} \cdot \hat{O} \rangle_{P.Q.} = \frac{\sum_i \langle e^{iS_I} \cdot \hat{O} \rangle_i \cdot \rho_i}{\sum_i \rho_i}$$

$$\langle \hat{O} \rangle_{full} = \frac{\langle e^{iS_I} \cdot \hat{O} \rangle_{P.Q.}}{\langle e^{iS_I} \rangle_{P.Q.}} = \frac{\sum_i \langle e^{iS_I} \cdot \hat{O} \rangle_i \cdot \rho_i}{\sum_i \langle e^{iS_I} \rangle_i \cdot \rho_i}$$

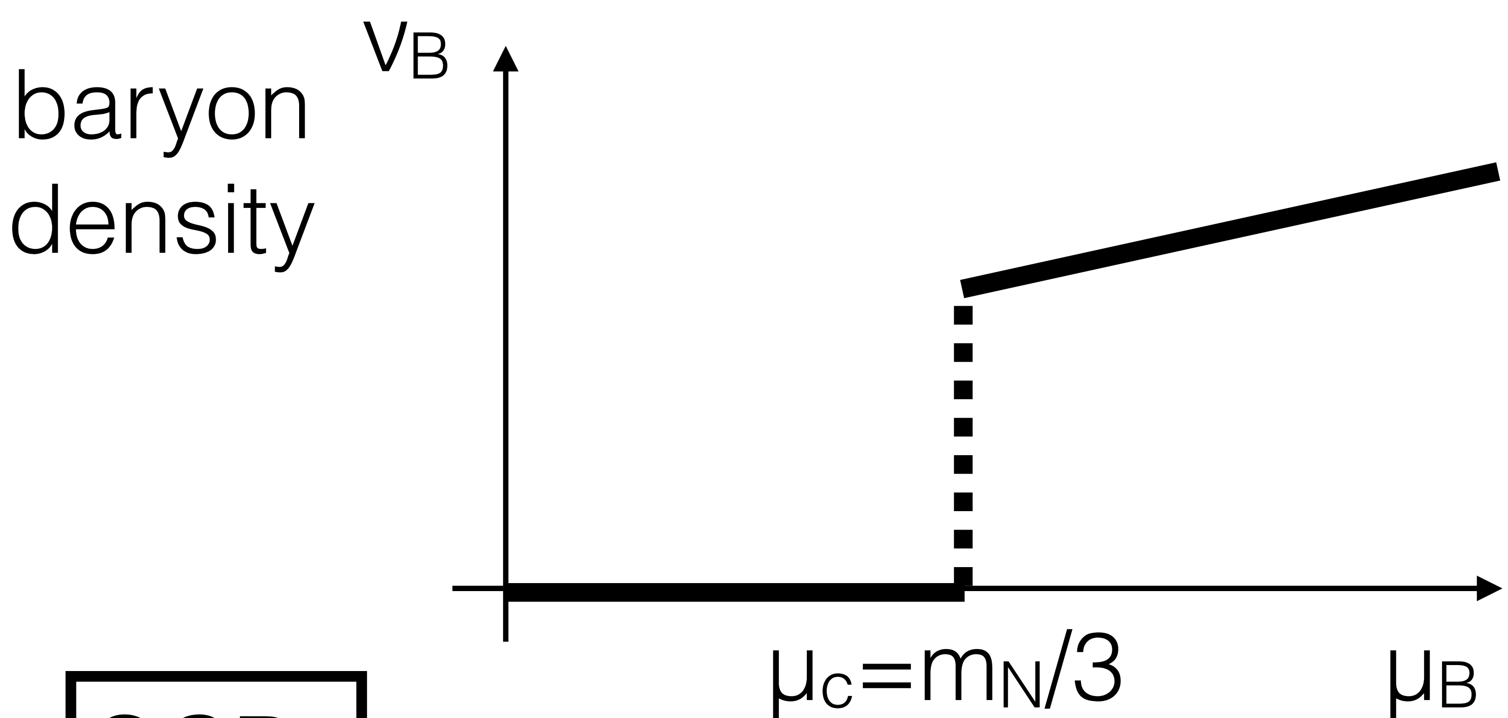
We need only ‘relative’ weight.
We do not even have to know ρ_i
when $<e^{i\Theta}>_i$ is close to zero.

Strategy (cont'd)

- Measure the average phase $<e^{i\Theta}>_k$ at I_k
- The weight in the full theory is $\rho_k \times <e^{i\Theta}>_k$.
- If $<e^{i\Theta}>_k$ is too small and hard to distinguish from 0, such I_k does not contribute . **Simply neglect them**.
- In the same way, if $<\hat{O} \times e^{i\Theta}>_k$ is too small and hard to distinguish from 0, **simply neglect them**.

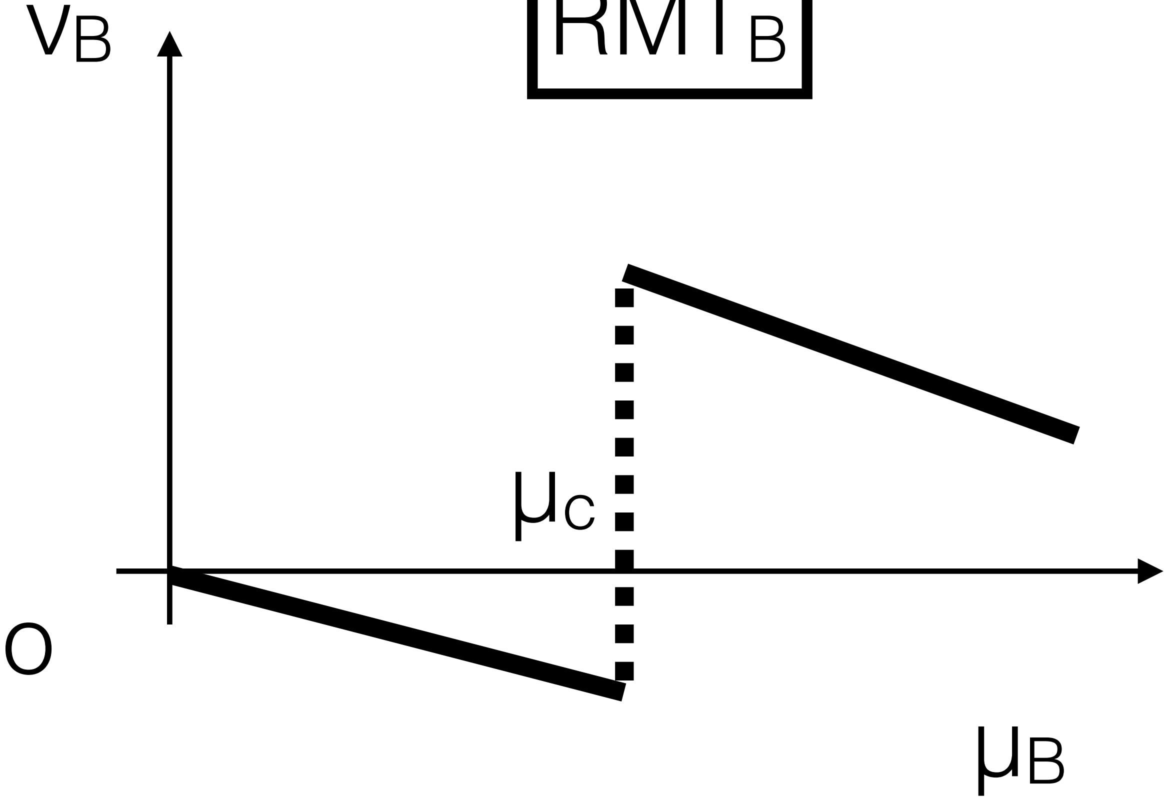
We do not even have to measure the sign when it is hard to measure.

Demonstration in RMT



QCD_B

RMT_B



negative v_B rather than $v_B=0$
→ artifact of the model.

Still there is a transition similar to the condensation of baryons.

$$Z = \int d\Phi d\Psi \ e^{-S}, \qquad S = S_B + S_F$$

$$S_B = N \,\mathrm{tr}\, \Phi\Phi^\dagger, \qquad S_F = \sum_{f=1}^{N_f} \bar{\Psi}_f \mathcal{D}_f \Psi_f$$

N×N complex

$$\mathcal{D} = \begin{pmatrix} m_f \mathbf{1}_N & \Phi + \mu_f \mathbf{1}_N \\ -\Phi^\dagger + \mu_f \mathbf{1}_N & m_f \mathbf{1}_N \end{pmatrix}$$

$N_f=2$, $m_f=0$, $\mu_1=\mu_2$

$S \to S + \Delta S$

$$\Delta S = \gamma|\pi^+ - x|^2 \quad \text{for} \quad |\pi^+ - x| \geq \epsilon$$

※ we introduce source only for ΔS (not for S).
→ no need for turning off the source.

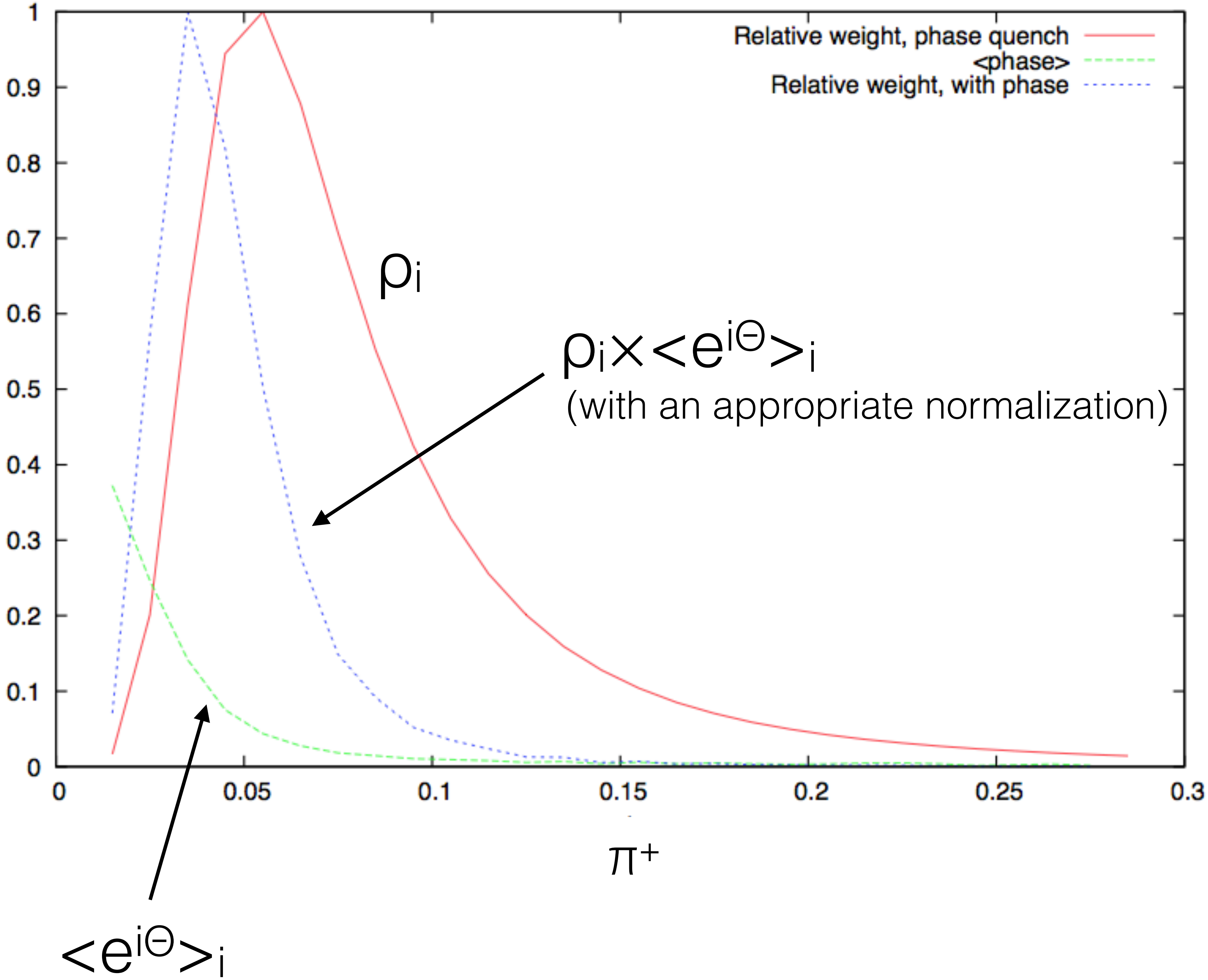
$$\mathcal{D} = \left(\begin{array}{cc|cc} 0 & \Phi + \mu \mathbf{1}_N & c\mathbf{1}_N & 0 \\ -\Phi^\dagger + \mu \mathbf{1}_N & 0 & 0 & -c\mathbf{1}_N \\ \hline -c\mathbf{1}_N & 0 & 0 & \Phi - \mu \mathbf{1}_N \\ 0 & c\mathbf{1}_N & -\Phi^\dagger - \mu \mathbf{1}_N & 0 \end{array}\right)$$

$$\pi^+ \equiv Tr[\gamma_5 \cdot (\mathcal{D}^{-1})_{21}]/N$$

$$\gamma_5 = \begin{pmatrix} \mathbf{1}_N & 0 \\ 0 & -\mathbf{1}_N \end{pmatrix}$$

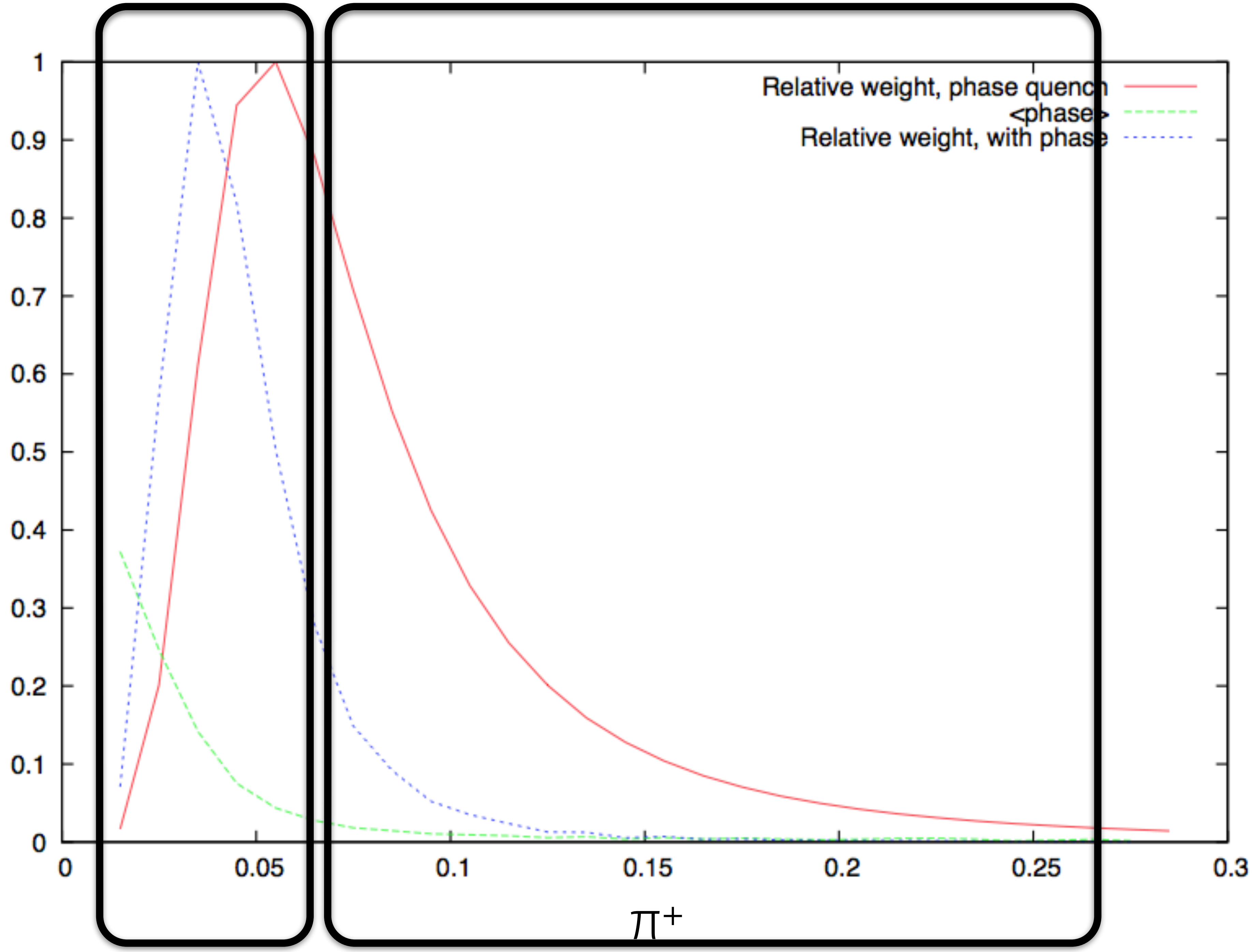
※ because RMT is numerically cheap, we use the Metropolis algorithm.
We will comment on HMC for QCD later.

N=4, μ=0.7, m=0, c=0.02



important

NOT important



baryon density ν_B

$$\langle \bar{u}\gamma^0 u\rangle_{\mathbf{B}} + \langle \bar{d}\gamma^0 d\rangle_{\mathbf{B}} = 2\langle \bar{u}\gamma^0 u\rangle_{\mathbf{B}}$$

$$\langle \bar{u}\gamma^0 u\rangle_{\mathbf{I}} - \langle \bar{d}\gamma^0 d\rangle_{\mathbf{I}} = 2\langle \bar{u}\gamma^0 u\rangle_{\mathbf{I}}$$

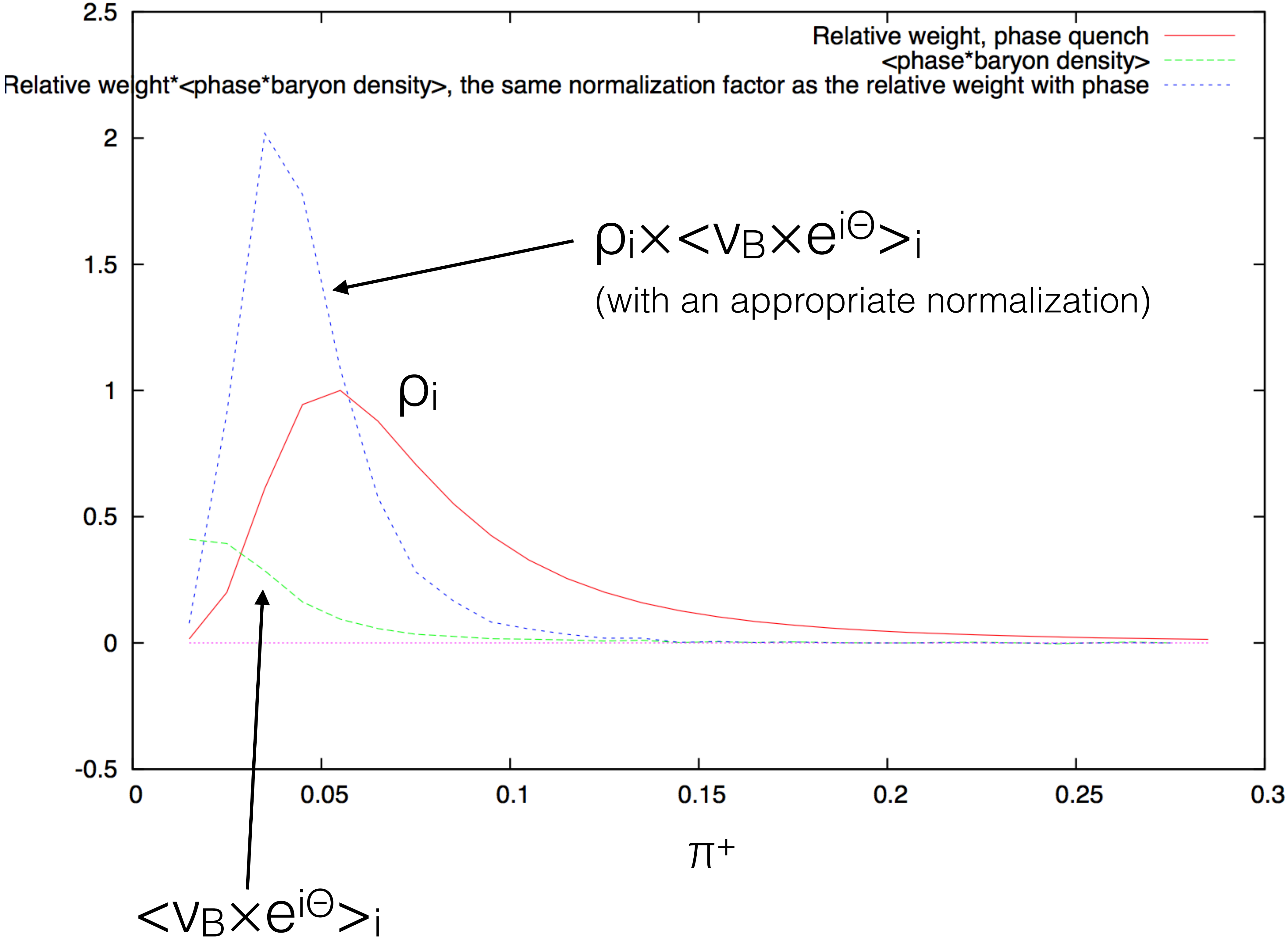
$$\langle \nu_B \rangle_{P.Q.} = \langle \nu_I \rangle_I$$

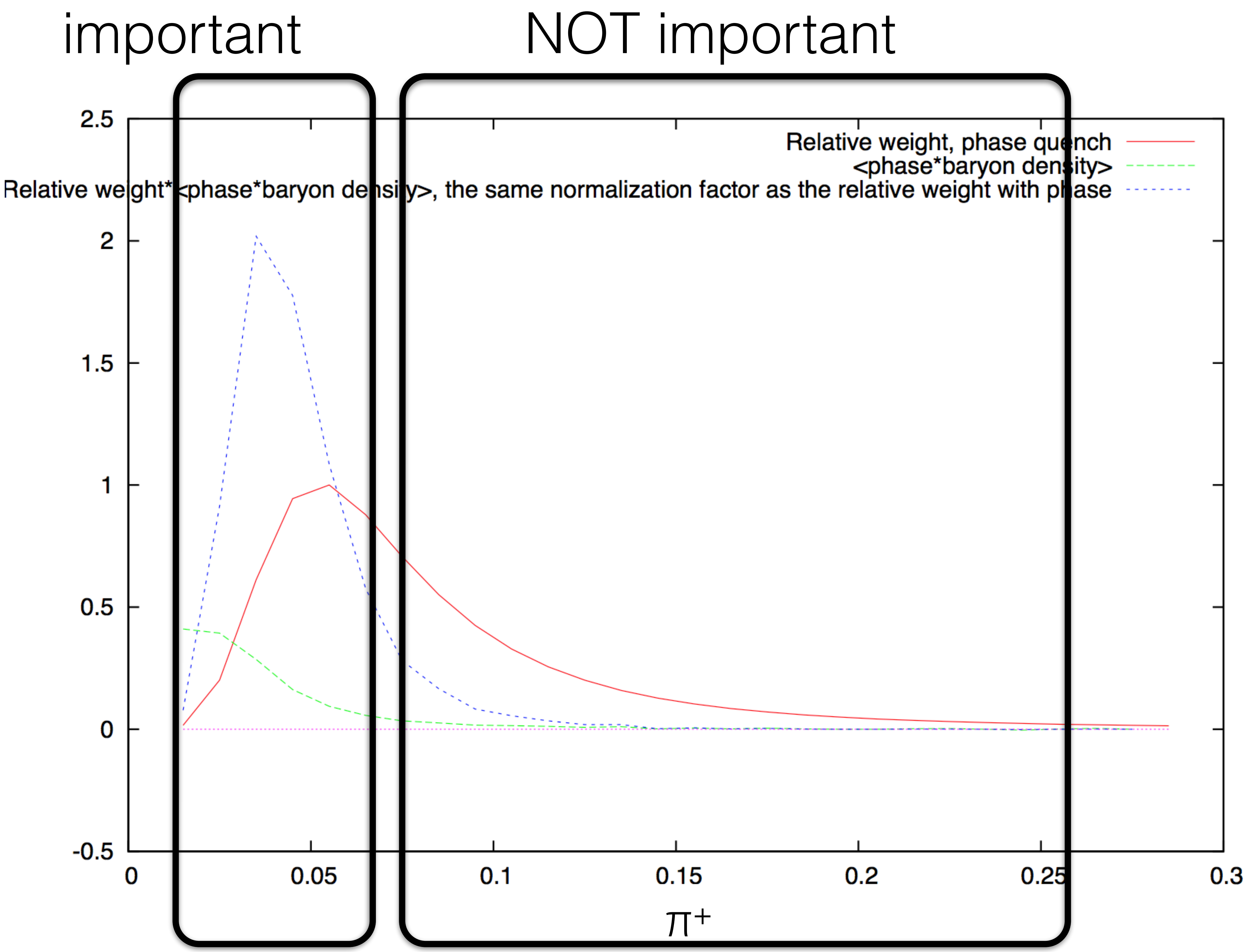
$$\gamma^0 = \begin{pmatrix} 0 & \mathbf{1}_N \\ \mathbf{1}_N & 0 \end{pmatrix}$$

$$\langle e^{iS_I} \cdot \nu_B \rangle_{P.Q.} = \langle e^{iS_I} \cdot \nu_I \rangle_I$$

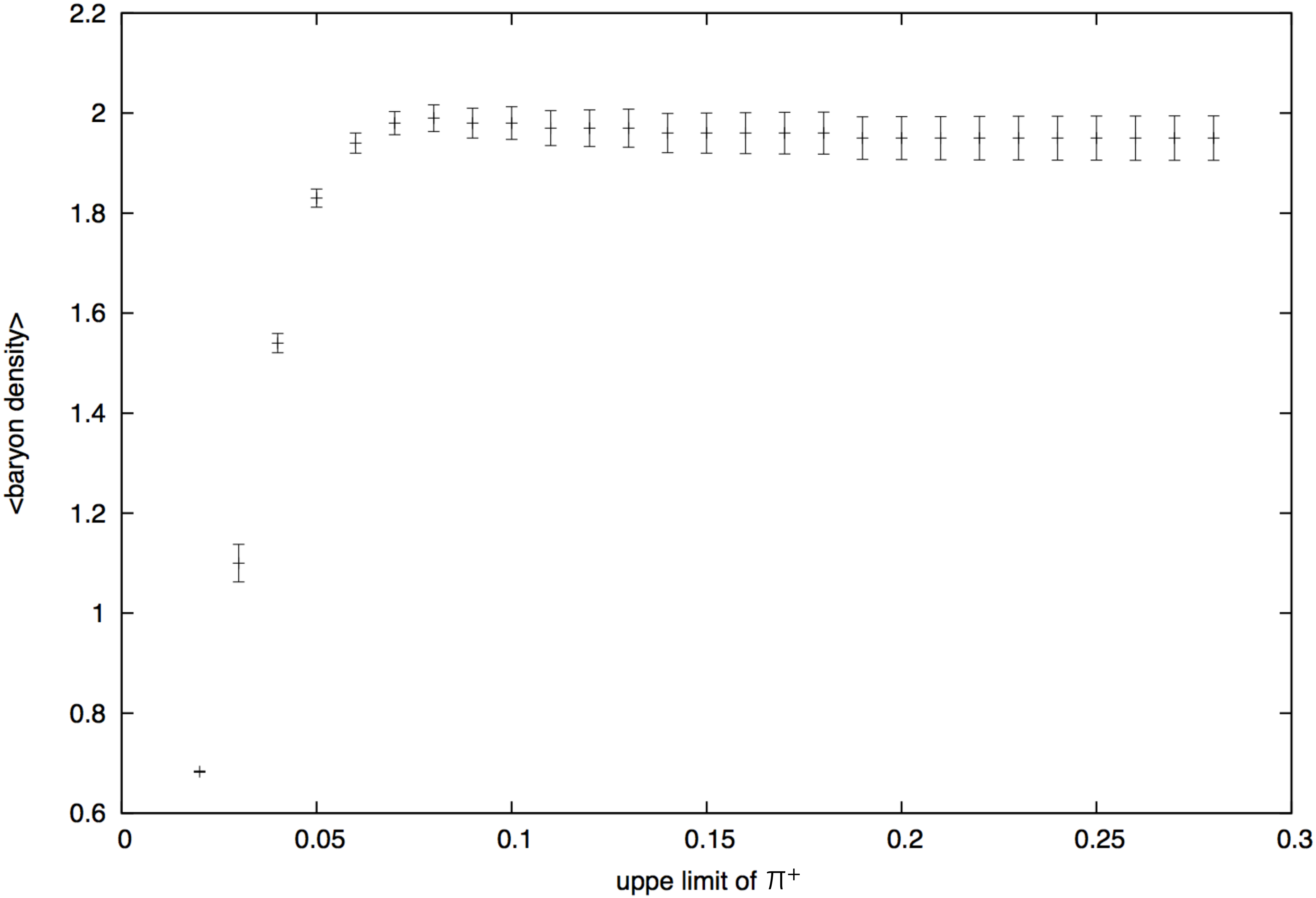
d in phase quenched theory = anti-d in QCD_I

N=4, μ=0.7, m=0, c=0.02





important
NOT important
Relative weight, phase quench
<phase*baryon density>
Relative weight*<phase*baryon density>, the same normalization factor as the relative weight with phase
2.5
2
1.5
1
0.5
0
-0.5
0
0.05
0.1
0.15
0.2
0.25
0.3
π^+

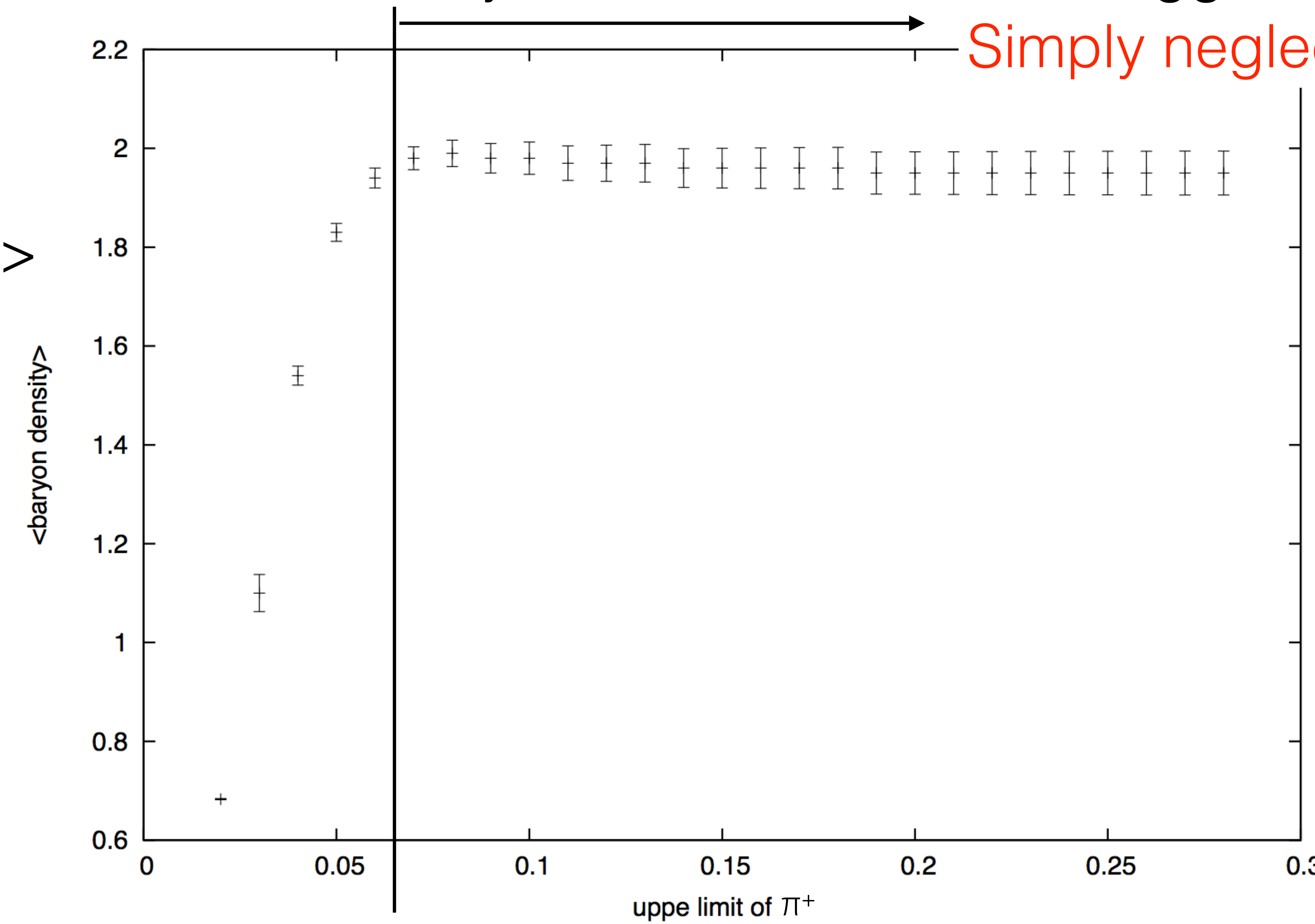


2.2
2
1.8
1.6
1.4
1.2
1
0.8
0.6
<baryon density>
0
0.05
0.1
0.15
0.2
0.25
0.3
uppe limit of π^+

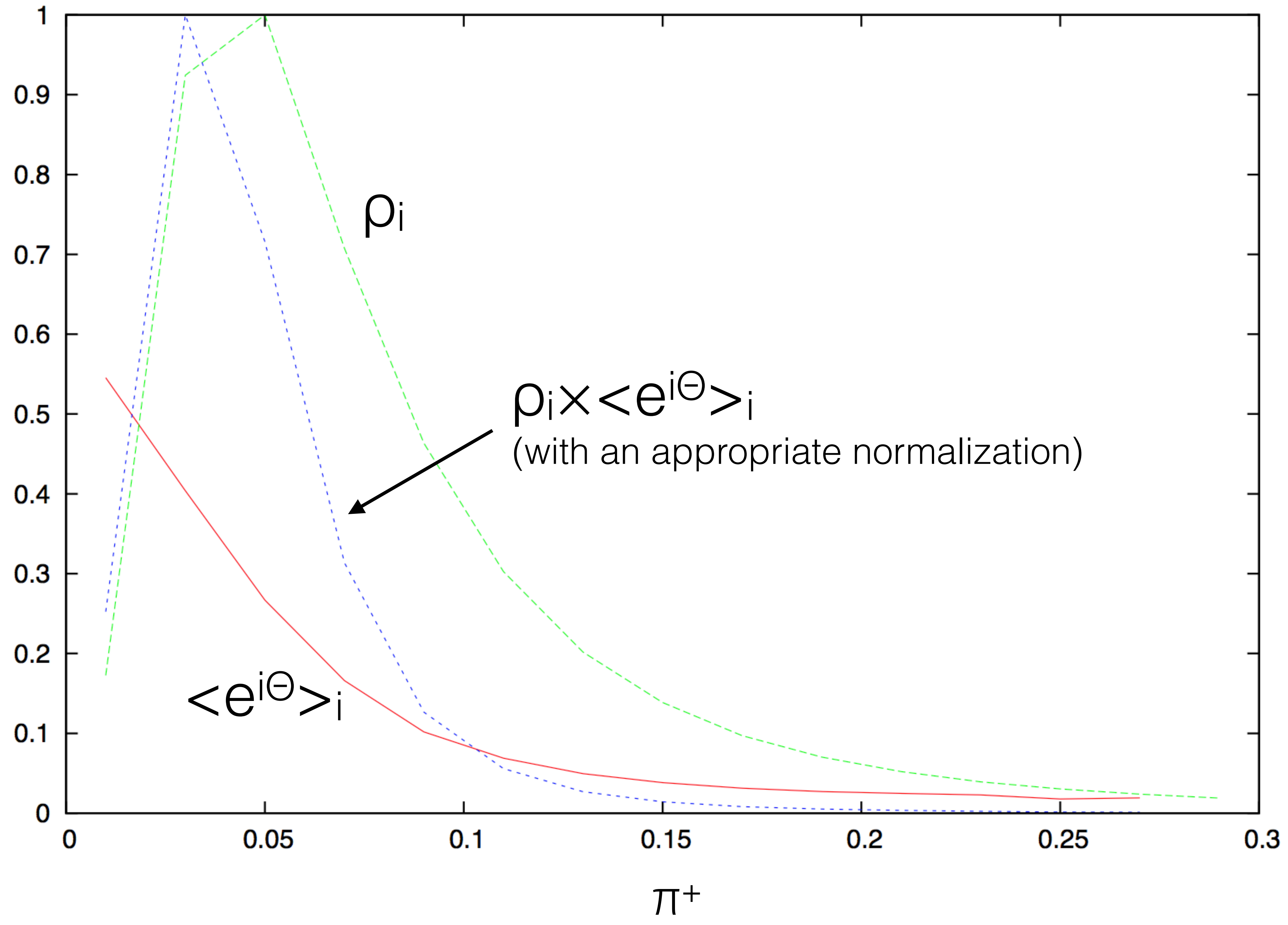
unimportant configurations
just make the error bar bigger.

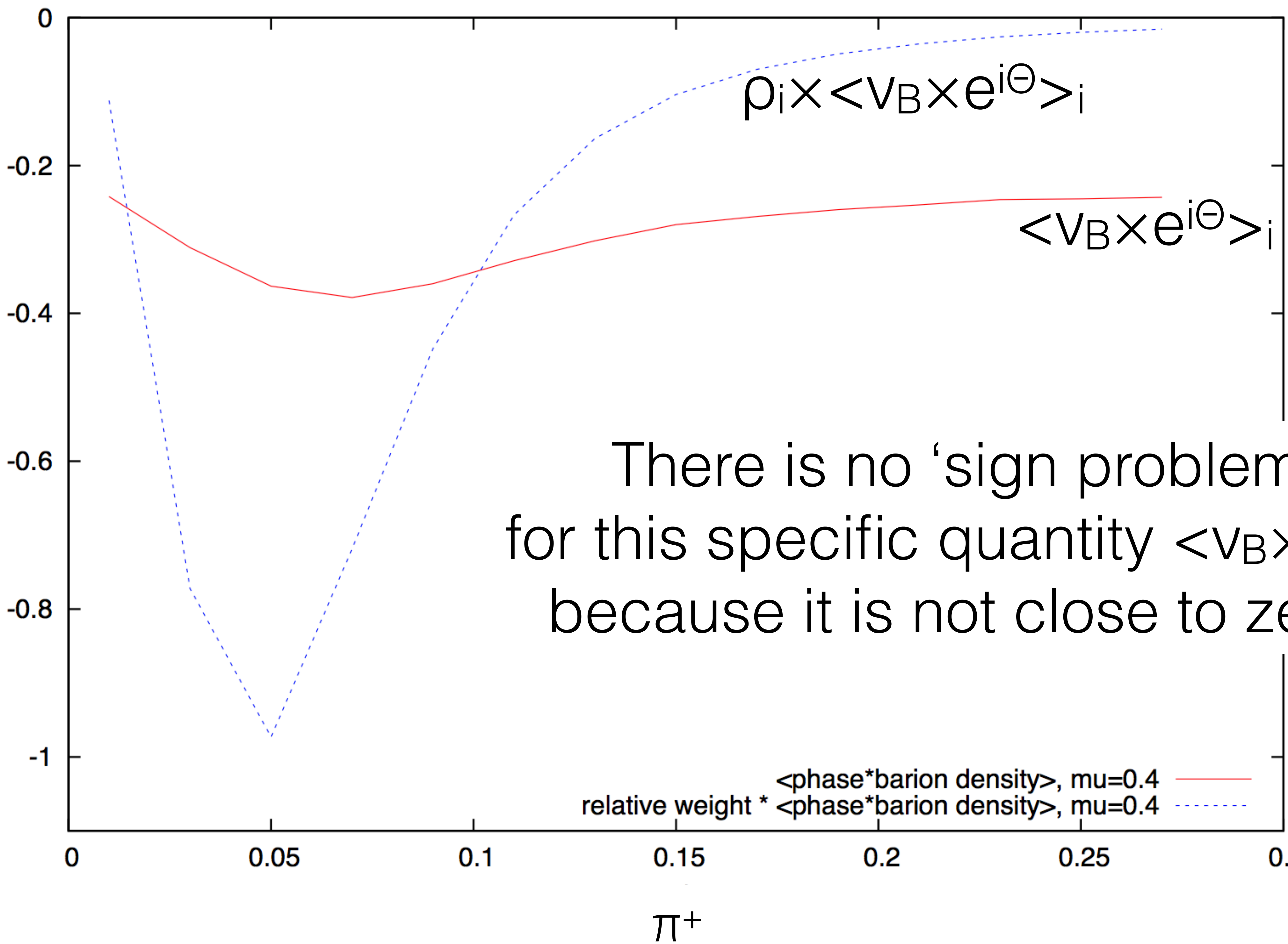
Simply neglect them.

$<V_B>$

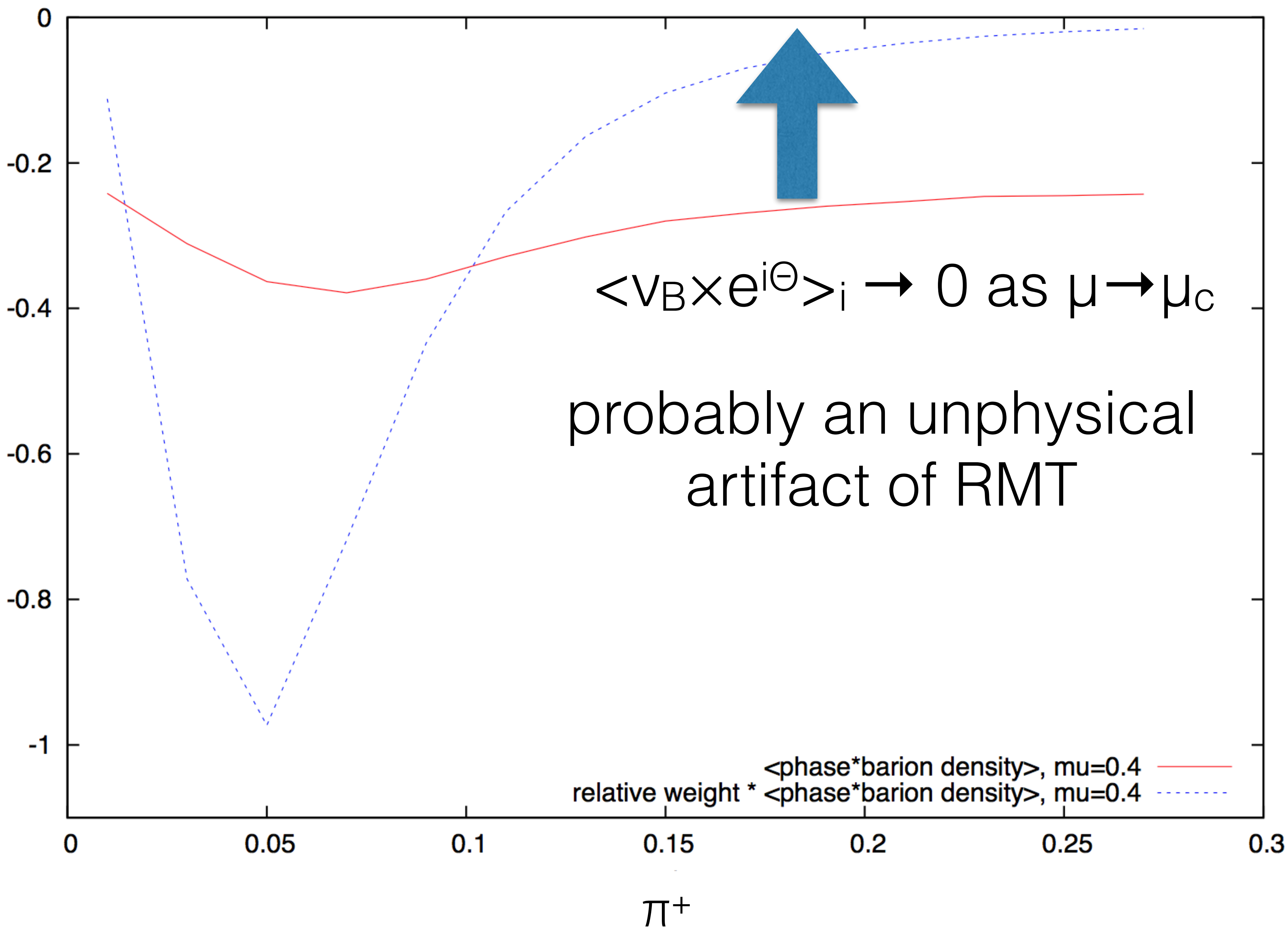


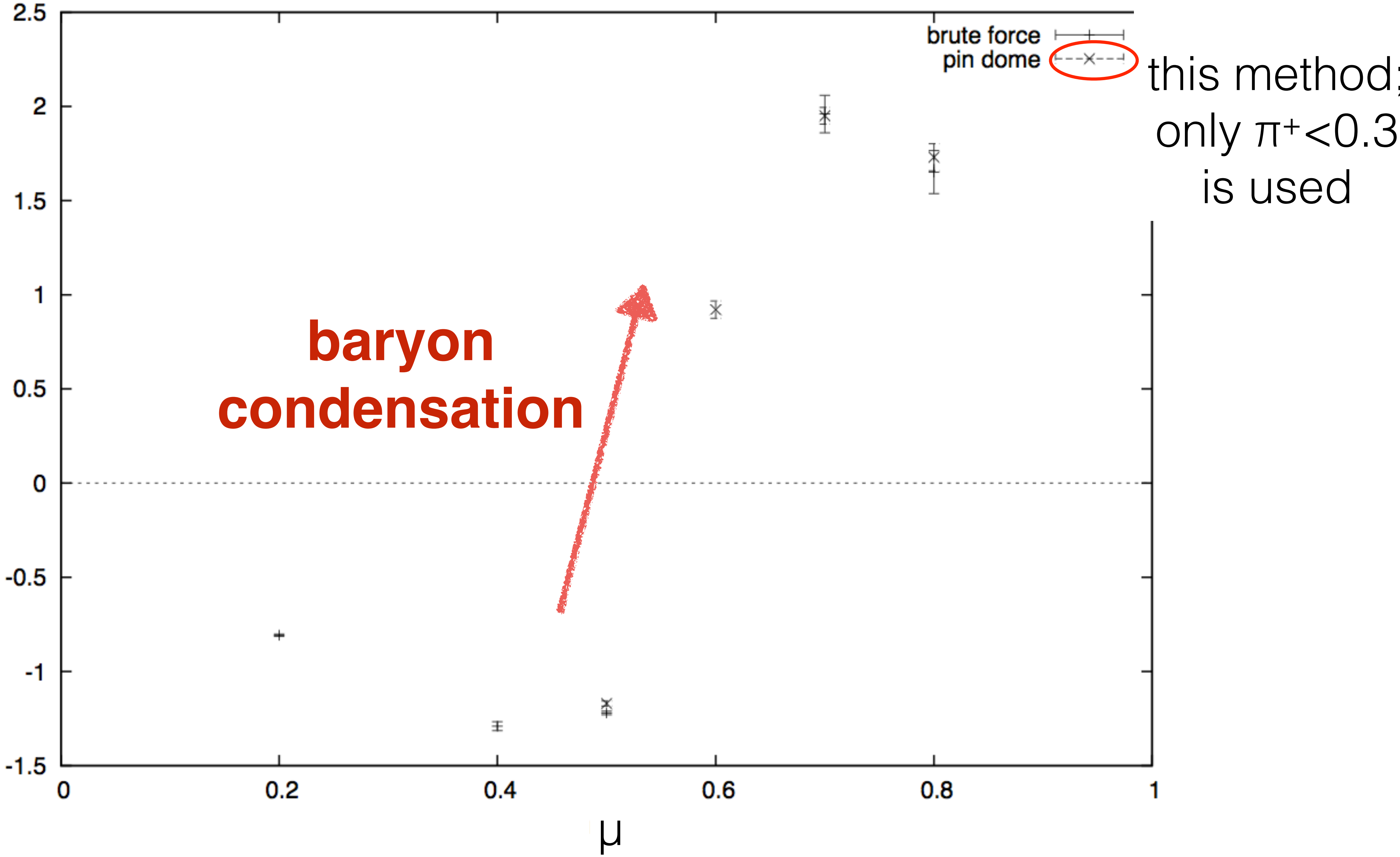
N=4, μ=0.4, m=0, c=0.02
(below μ_c)





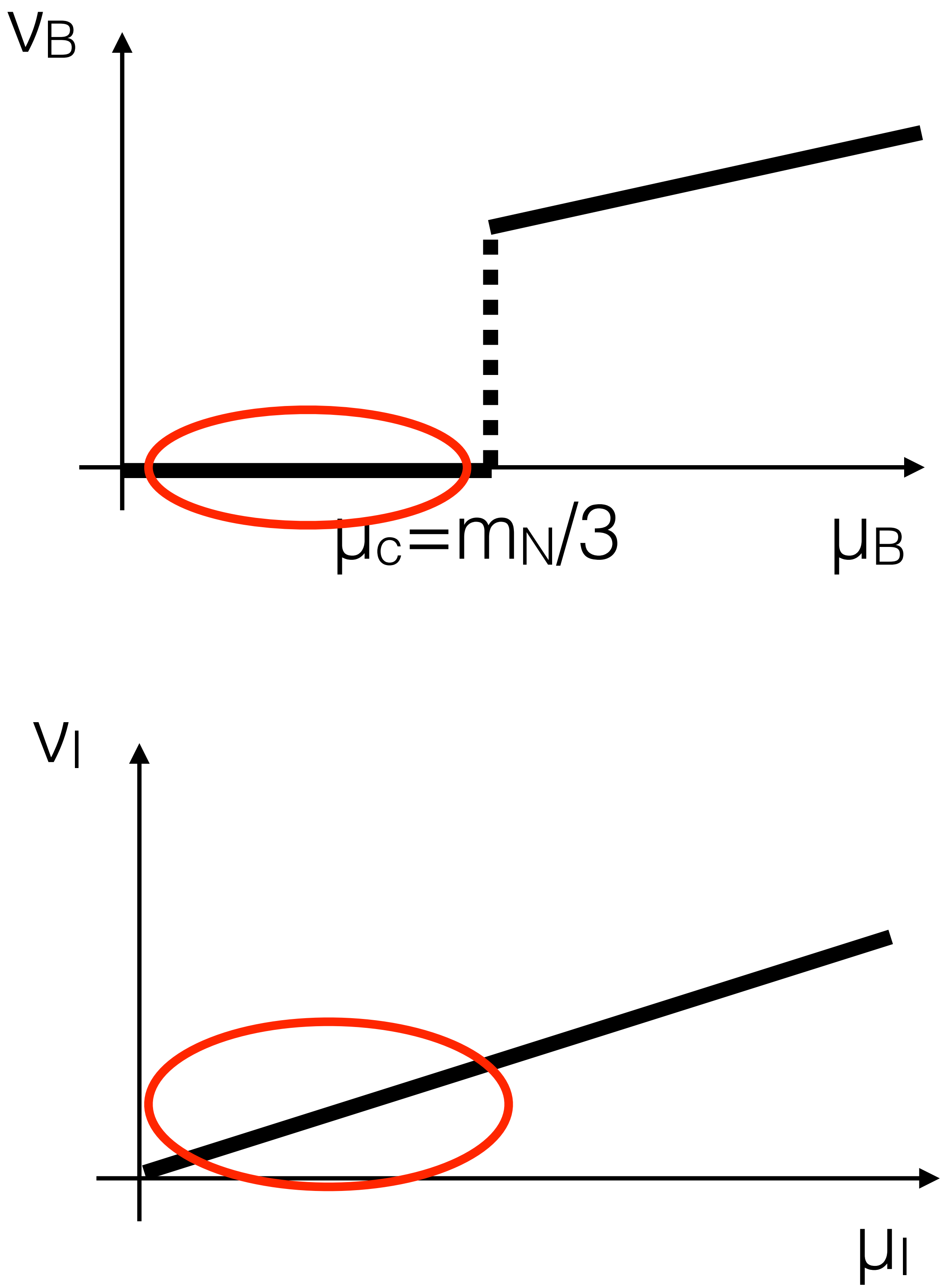
There is no ‘sign problem’ for this specific quantity $\langle v_B \times e^{i\Theta} \rangle$ because it is not close to zero.


$\langle v_B \times e^{i\Theta} \rangle_i \to 0$ as $\mu \to \mu_c$
probably an unphysical artifact of RMT
<phase*barion density>, mu=0.4
relative weight * <phase*barion density>, mu=0.4
0
-0.2
-0.4
-0.6
-0.8
-1
0
0.05
0.1
0.15
0.2
0.25
0.3
π^+



2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
0
0.2
0.4
0.6
0.8
1
μ
brute force
pin dome
baryon condensation
this method;
only π^+<0.3
is used

What happens
if we fix other observables,
e.g. baryon density?



$\mu_c = m_\pi/2 = 0$ (chiral limit)

QCD_B

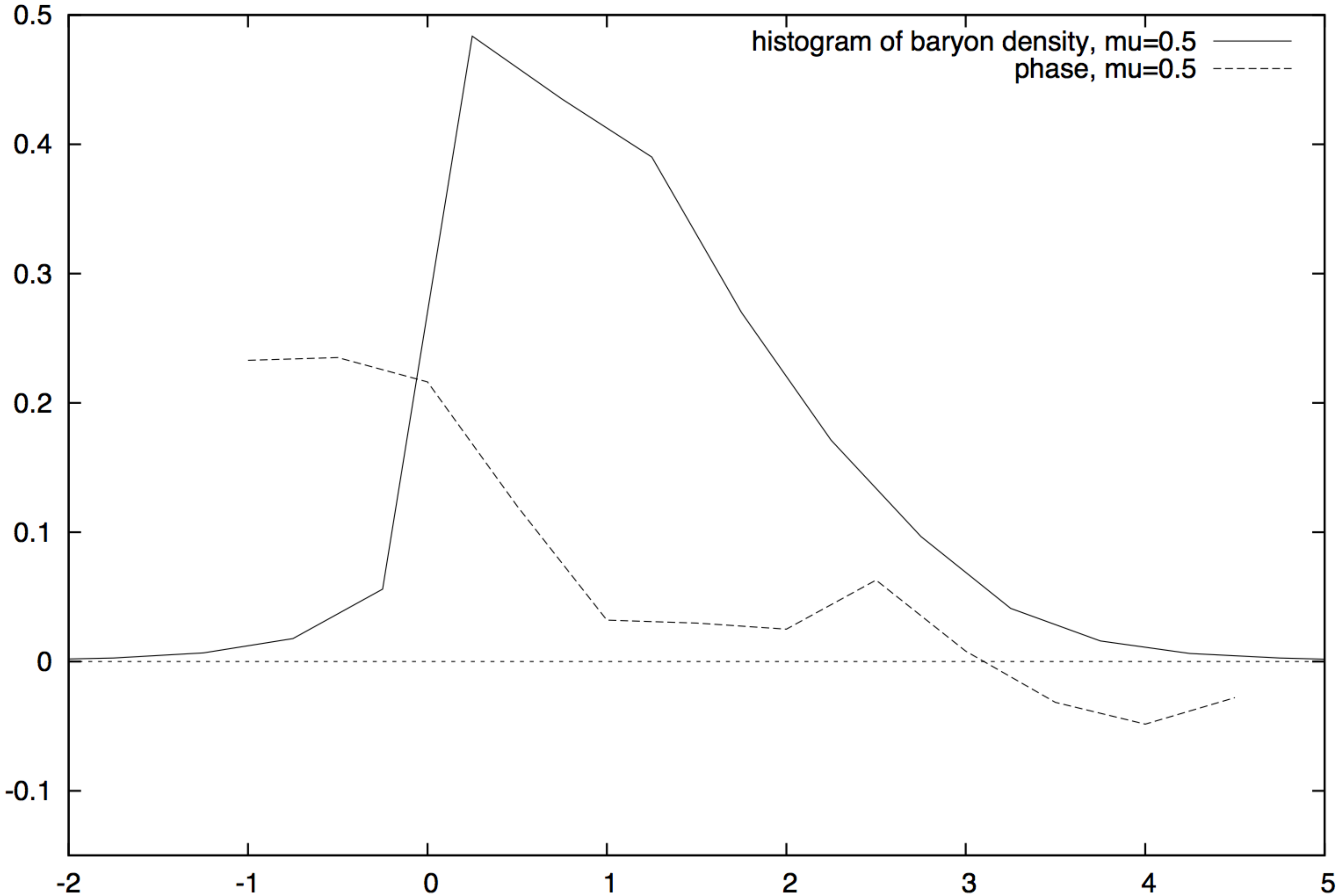
$v_B = 0$ at $\mu < \mu_c = m_N/3$

$v_I = 0$ might resemble the vacuum of QCD_B @ $\mu < m_N/3$

QCD_I

$v_I > 0$ at $\mu > 0$

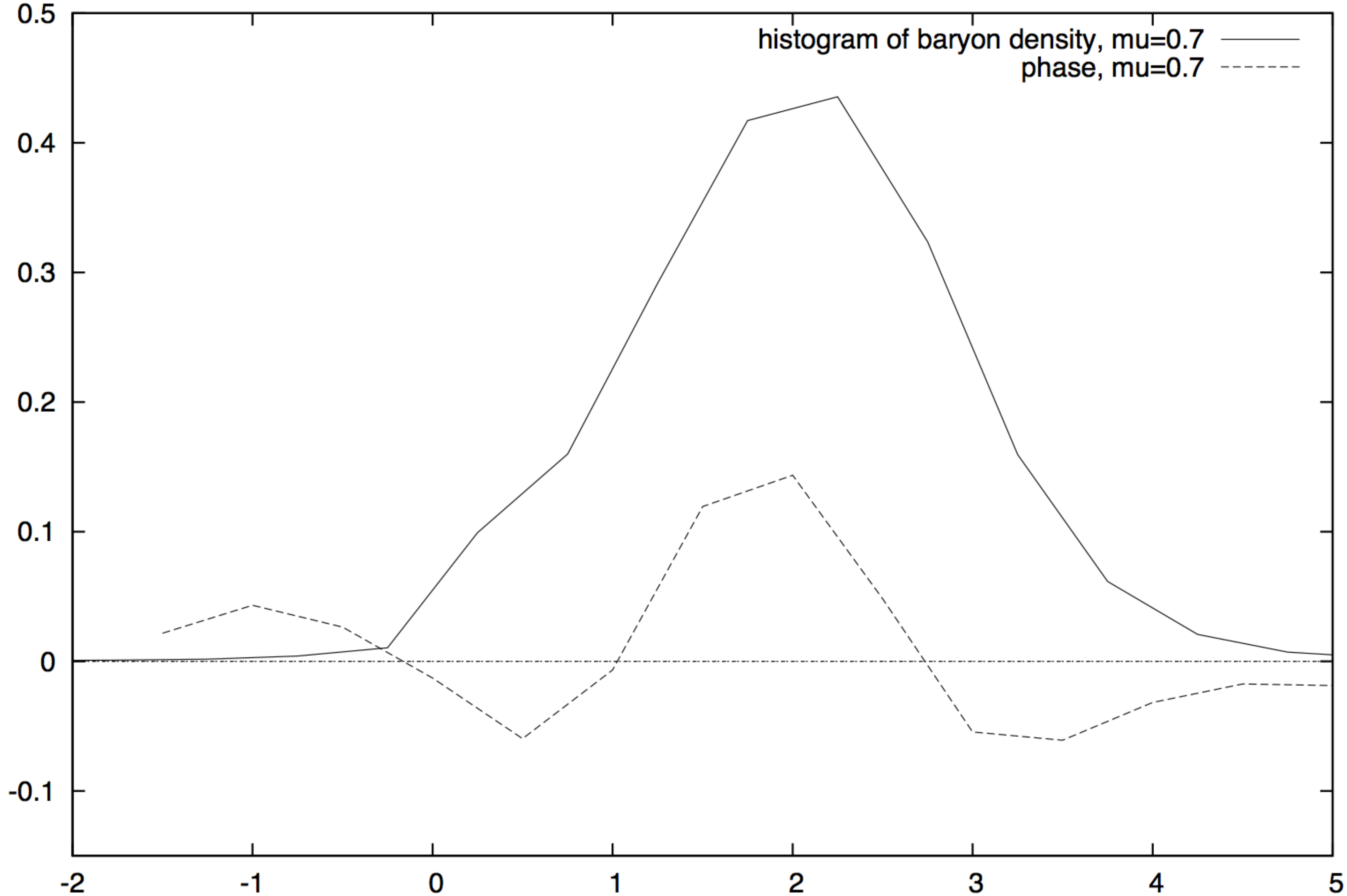
$\mu = 0.5 < \mu_c$



$v_B,\ v_I$

$v_I = 0$ resembles the vacuum of QCD_B

$\mu = 0.7 > \mu_c$



$v_B,\ v_I$

hard to mimic the vacuum of QCD_B by adjusting v_I

Toward application to QCD

Q. Can we use HMC?

A. well, Metropolis without a severe sign problem is by far better than HMC with it ;)

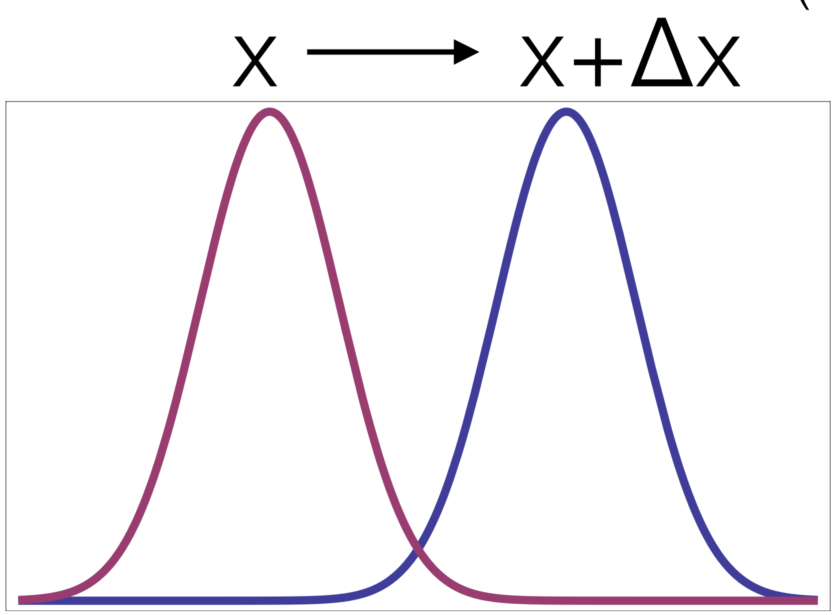
What pin-down potential ΔS allows us to use HMC?

- Simply Gaussian potential, $\Delta S=\gamma|\pi^{+}-x|^{2}$, which is nonzero everywhere.

- Then introduce an auxiliary field. Be careful not to introduce extra sign problem.

$d\rho_{P.Q.}/dx$ can be read off from Δx.

(Anagnostopoulos-Nishimura 2002)



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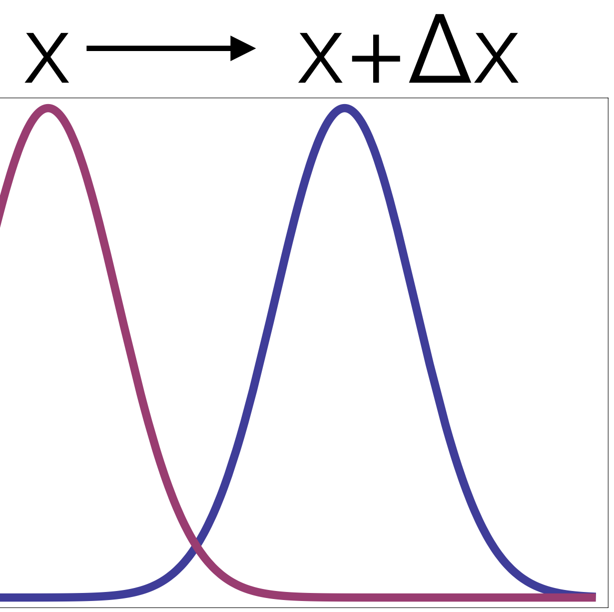


$$\rho_{S+\Delta S}(\pi) \sim \rho_S(\pi) \cdot e^{-\gamma(\pi - x)^2}$$

$$0 = [\rho_{S+\Delta S}(x+\Delta x)]' \rightarrow \sim [\log \rho_S(x+\Delta x)]' = 2\gamma\Delta x$$

$$\rightarrow \rho_S = \mathrm{const} \cdot \exp[\int^x dx\, 2\gamma\Delta x]$$

advantages

- $\langle e^{i\Theta} \rangle$ should be larger. Sign problem still exists, but hopefully it is manageable by using clever techniques e.g. cumulant expansion. (Analogous to $\mu < m_\pi/2$.)

- No need for introducing the source term. (needed only for ΔS) → no extrapolation needed. (Usually, without introducing the source term, simulation is hard in the pion condensation region because of the zero mode.)

- Phase quench should already be a good approximation. (Exact @ large-N)

(A possible) strategy for $\mu < m_\pi/2$ at finite-T

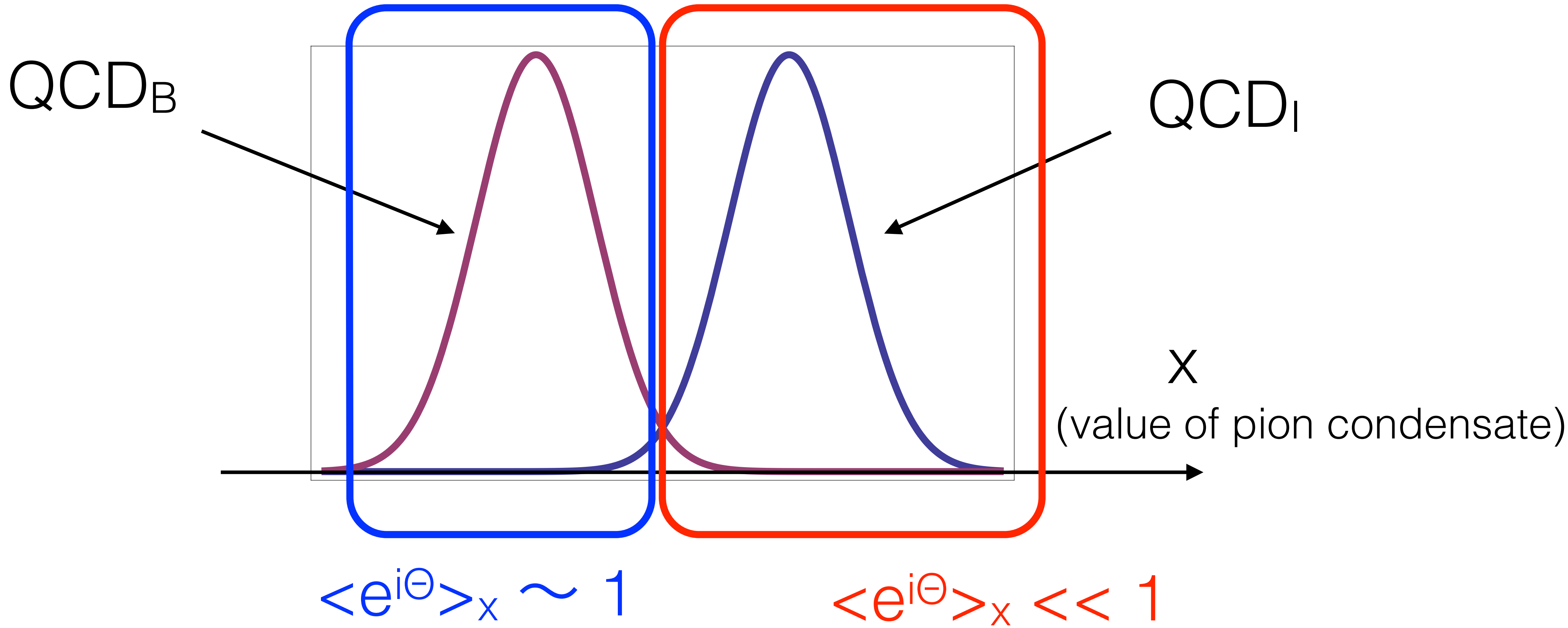
- Phase quench is exact at large-N. (Cherman-M.H.-Robles Llana 2010, M.H.-Yamamoto 2011.)

- 1/N-suppressed overlap problem:
pion gas ($\rightarrow$ larger v_I) vs. baryon gas ($\rightarrow$smaller v_B)

- So, start with the existing phase quenched ensemble, classify the configurations by the value of v_I, and then apply our method. Large v_I should not contribute because of the phase fluctuation. Just neglect them.

- Then the sign problem should become milder and it should be possible to study larger volume.

conclusion



The role of the sign = erase the pion condensation

If the average sign is very small, we don't even have to measure it. SUCH CONFIGURATIONS ARE NOT IMPORTANT. Simply neglect them.

Too severe sign problem can be a sign blessing.