The Sign Problem in QCD

Subtleties with the infinite volume limit

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Overview

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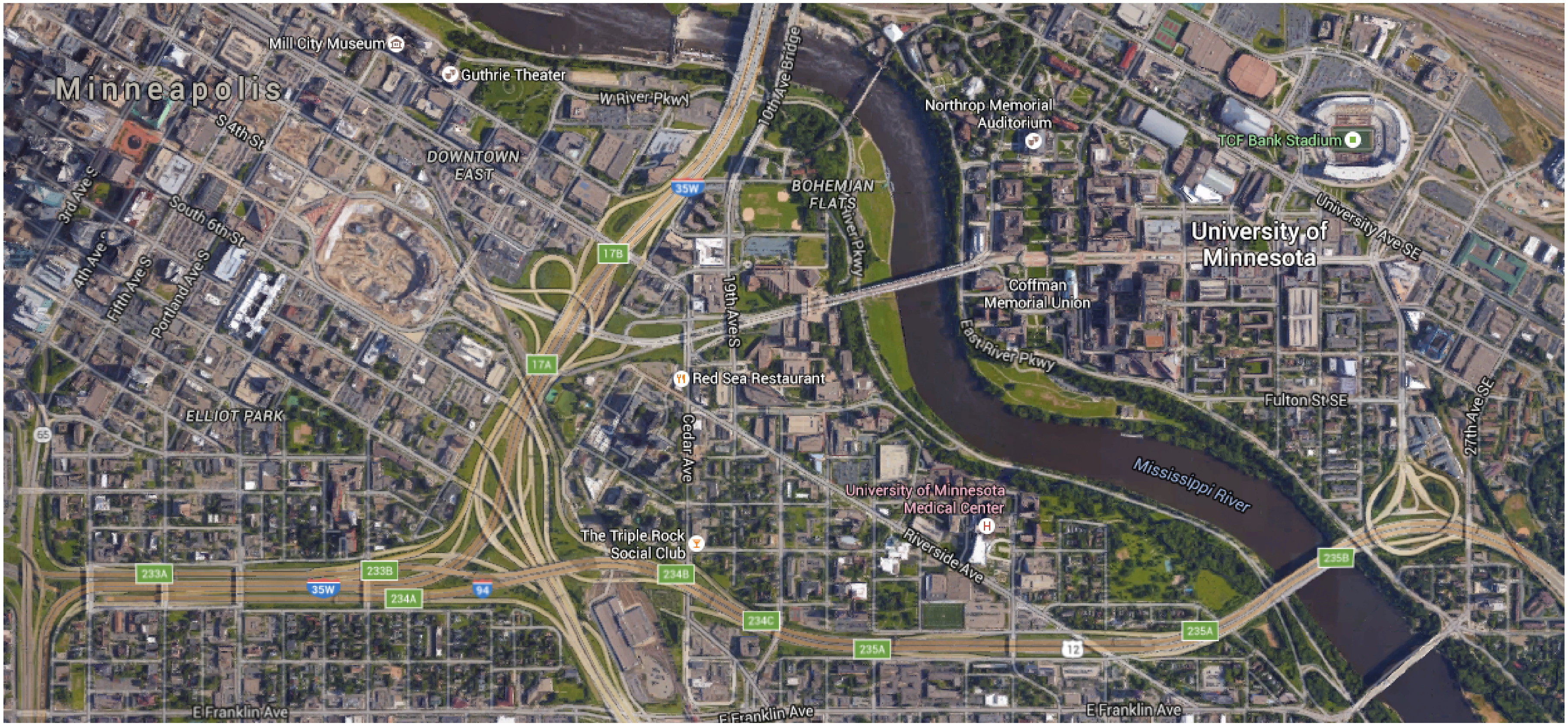

Minneapolis
Mill City Museum
Guthrie Theater
W River Pkwy
10th Ave Bridge
Northrop Memorial Auditorium
TCF Bank Stadium
S 4th St
DOWNTOWN EAST
BOHEMIAN FLATS
River Pkwy
3rd Ave S
South 6th St
University of Minnesota
University Ave SE
4th Ave S
Fifth Ave S
Portland Ave S
19th Ave S
Coffman Memorial Union
East River Pkwy
Red Sea Restaurant
Fulton St SE
ELLIOT PARK
Cedar Ave
27th Ave SE
Mississippi River
University of Minnesota Medical Center
The Triple Rock Social Club
Riverside Ave
35W
17B
17A
233A
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234A
94
234B
234C
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65
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Overview

- Introduction
  - What is the sign problem and why it matters
  - Why study the θ-term
- The sign problem for QCD with a θ-term
  - A surprise with the infinite volume limit: a puzzle emerges
  - A resolution via the saddle point approximation
  - Implications

The Fermion Sign Problem in Lattice QCD

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  - Finding a way to evade the fermion sign problem is the most important theoretical issue facing lattice QCD.

- The fermion sign problem is an example of a very general class of sign problems.

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  - Troyer and Wiese (PRL 2005) showed that there exists a system (a type of spin glass) known to be NP hard that suffers from a sign problem. Thus a generic solution implies that P=NP. It is strongly believed among complexity theorists that P≠NP. However this is unproved.

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All I ask is a 10% finders fee for pointing this out to you!!

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- It may be useful to get insight and experience from other sign problems that can emerge in QCD.
- A particularly interesting case is QCD and related gauge theories with a θ-term. Theories with θ-terms intrinsically have sign problems

$$\mathcal{L} = \mathcal{L}_{QCD} + \theta \frac{g^2}{32\pi^2} G\tilde{G}$$

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- Some interesting features
  - Theta term breaks P and CP.
    - Note that in strong sector CP violation is VERY small (as seen for example in the neutron electric dipole moment.) Why is an interesting question (the strong CP puzzle) which is beyond the scope of this talk.
  - The θ–term in Euclidean problem is imaginary. Thus there is a sign problem.
  - The problem is topological in Eucliden space: the theta term can be written as a total derivative (albeit of a gauge variant quantity) and hence depends on the boundary. Its volume integral is a winding number which is constrained to be an integer, we will denote the winding number as *Q*.

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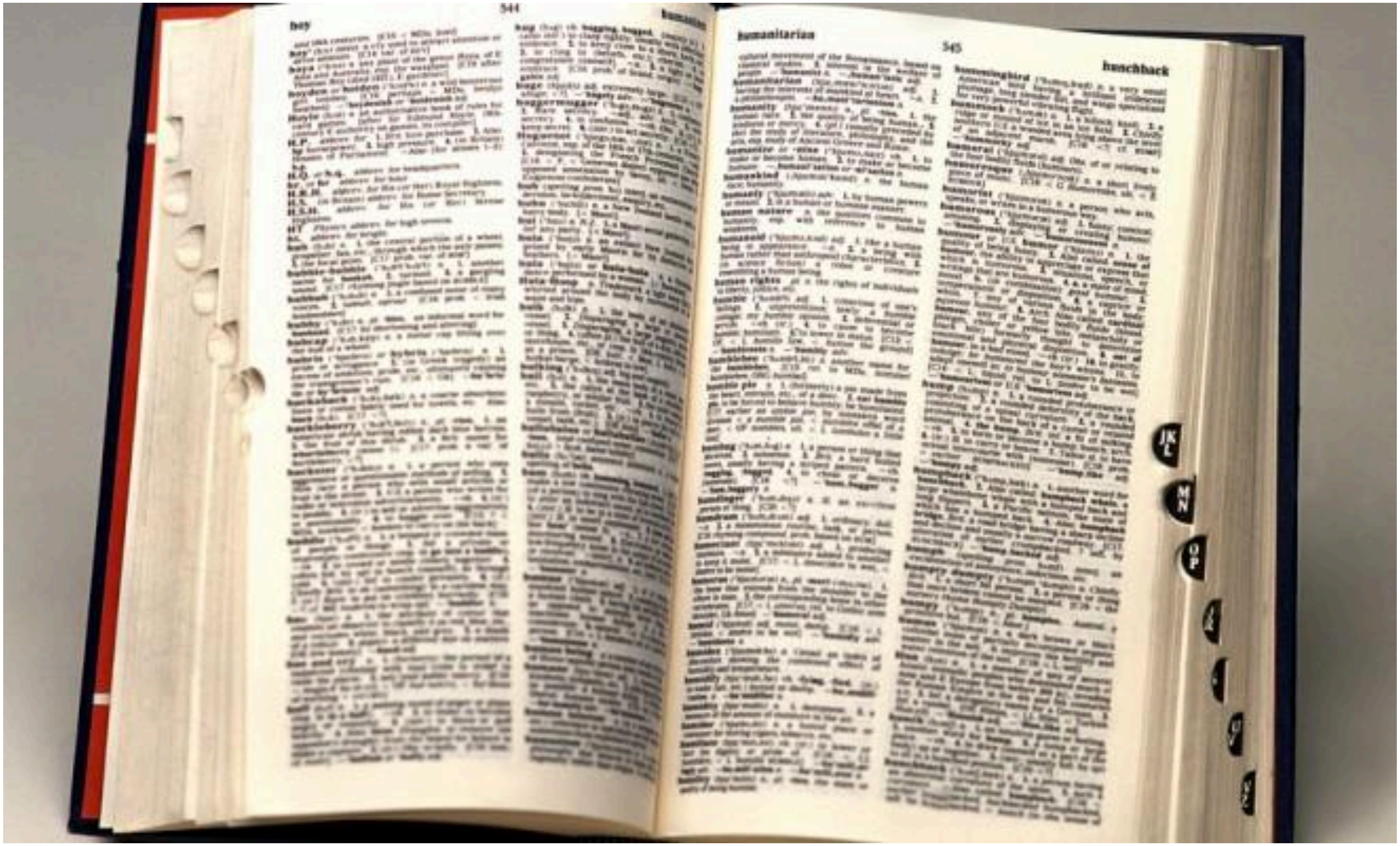
$$Q = \int_V \frac{g^2}{32\pi^2} \epsilon^{\alpha\beta\mu\nu} G_{\alpha\beta} G_{\mu\nu}$$

Some definitions



Definitions of key quantities

$$\varepsilon(\theta) = -\lim_{V\to\infty} \frac{1}{V} \log \mathcal{Z}(\theta, V)$$

Where V is the four dimensional volume of the box.

$$\mathcal{Z}(\theta, V) = \int [dA] \, \det[i \not{D}[A] - M] \, \exp(-S_{YM} - i\theta Q)$$

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$$\mathcal{Z}(\theta, V) = \sum_{Q\in\mathbb{Z}} \mathcal{Z}_Q(V)\, e^{i\theta Q}$$

Oscillates rapidly indicating a sign problem

$$\mathcal{Z}_Q(V) = \frac{1}{\pi}\int_0^\pi \mathcal{Z}(\theta)\, e^{-i\theta Q}\, \mathrm{d}\theta$$

Precise form uses the fact that the theta dependence is even and periodic.

Definitions of some key quantities

$$q \equiv \frac{Q}{V}$$

Defines the topological charge density

$$\tilde{\varepsilon}(q,V) = -\frac{1}{V}\log(\mathcal{Z}_{(qV)}(V))$$

Defines an energy density as a function of topological charge density

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Intuitively this limit ought to exist; the quantity is the intensive energy density as a function of the topological charge density which is also intensive. One expects this to be independent of volume.

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For simplicity
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Thus to capture the θ dependence in ε, *B* must cancel *A* to one part in $\exp(V(\varepsilon(\pi) - (0)))$. Thus one needs both *A* and *B* at this accuracy.

Kinky Behavior

$\varepsilon(\theta) = \varepsilon(\theta + 2\pi)$ Q is an integer:the generating function must be periodic in θ $\mathcal{Z}(\theta, V) = \sum_{Q\in\mathbb{Z}} \mathcal{Z}_Q(V)\, e^{i\theta Q}$

$\varepsilon(\theta) = \varepsilon(-\theta)$ since QCD is CP invariant except for θ term

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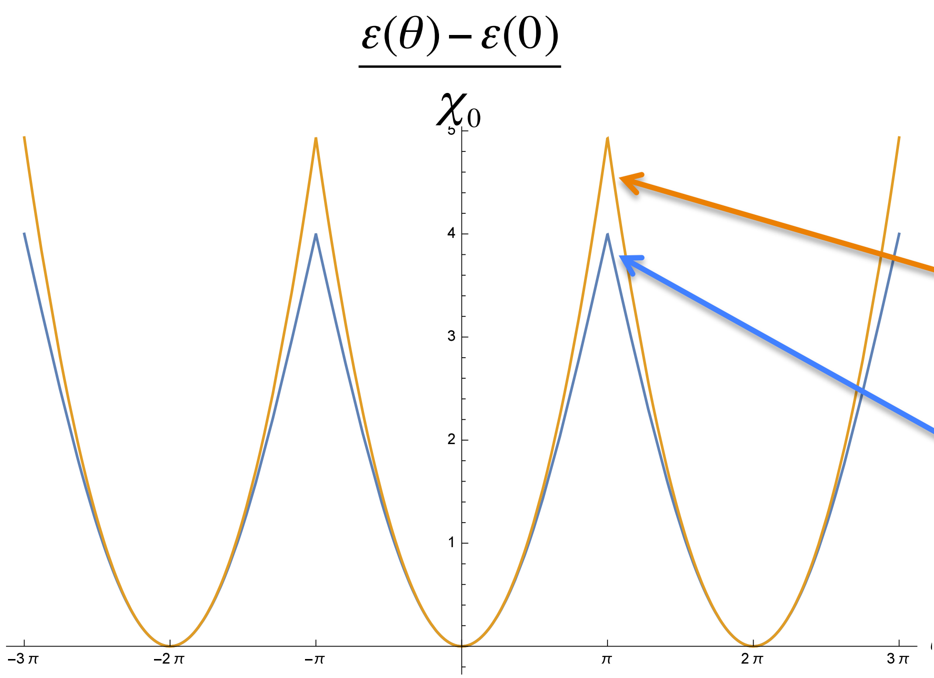

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Infinitely many colors

Two flavors of infinitesimally light quarks

The energy was given in units of χ_0

$$\chi_0 \equiv \varepsilon''(0) = \lim_{V\to\infty}\left(\frac{\frac{1}{V}\sum_{Q\in Z} Q^2 Z_Q(V)}{\sum_{Q\in Z} Z_Q(V)}\right)$$

The topological susceptibility at zero

Sets the scale for variations of $\varepsilon(\theta)$

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- **Intuitively Yes**: Both quantities are intensive quantities independent of volume. They describe the same system. They must contain the same info.
- ***Intuitively No***: *The sum over Q to obtain $\mathcal{Z}(\theta, V)$ requires* an exponentially accurate knowledge (in V) of the $\mathcal{Z}_Q(V)$ while we have dropped power law terms to get infinite volume limit.

Which Intuition is correct?

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To pose this mathematically let us define a new quantity:

$$\underline{\varepsilon}(\theta) = -\lim_{V\to\infty}\frac{1}{V}\log\left(\sum_{Q} e^{-\tilde{\varepsilon}\left(\frac{Q}{V}\right)V}\, e^{i\theta Q}\right)$$

Uses $\tilde{\varepsilon}\left(\frac{q}{V}\right)$ **rather than** $\tilde{\varepsilon}\left(\frac{q}{V},V\right)$ **as is used to compute** $\varepsilon(\theta)$

The issue amounts to answer does $\underline{\varepsilon}(\theta)=\varepsilon(\theta)$?

The dilute instanton gas

- To get insight we first focused on a problem that is **NOT** QCD (in any known limit) but for which
  - The θ dependence is known and most aspects of the system are easily calculable
  - The system is known not to break CP spontaneously at $\theta=\pi$.
- We considered any theory that in some controlled limit is accurately described by a dilute instanton gas with instantons of fixed action.
- The virtue of systems of this type is that the calculable nature of the problem allows us to test ideas.

The dilute instanton gas

$\mathcal{Z}_Q(V)$ Is easy to compute

$$\boxed{\mathcal{Z}_Q(V) = \mathcal{Z}_0 \sum_{n=0}^{\infty} \frac{\left(\frac{1}{2}\, c\, e^{-S_0} V\right)^{|Q|+2n}}{n!\,(n+|Q|)!} = I_Q(ce^{-S_0}V)}$$

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Thus

$$\boxed{\varepsilon(\theta) = \varepsilon_0 + \chi_0(1-\cos(\theta))}$$

$$\text{with } \chi_0 \equiv ce^{-S_0}$$

$$\text{and } \varepsilon_0 \equiv \frac{-\log\left(\mathcal{Z}_0\right)}{V} - ce^{-S_0}$$

Get the standard dilute instanton gas result with a cosinusoidal dependance on θ; no kink.

Energy density for dilute instanton gas as a function of topological charge density can be extracted From $\mathcal{Z}_Q(V)$

$$\tilde{\varepsilon}(q,V) = -\log\left(I_{qV}(\chi_0 V)\right)$$

Known "uniform expansion" of modified Bessel function valid for $I_\nu(\nu x)$ in the limit of large V can be used to extract the infinite volume limit

$$\boxed{\tilde{\varepsilon}(q) = \varepsilon_0 + \chi_0 + q\sinh^{-1}\left(\frac{q}{\chi_0}\right) - \sqrt{\chi_0^2 + q^2}}$$

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Does $\underline{\varepsilon}(\theta) = \varepsilon(\theta)$?

- Ideally one could do this sum analytically for arbitrary V, obtain a functional form and then take the large V limit of the expression.
  - Unfortunately given the functional form for the energy density, it is not known how to obtain a closed form expression for this sum.
  - Instead, we can do the sum numerically for large but finite V (the relevant combination is $\chi_0 V$) and a number of values for θ.

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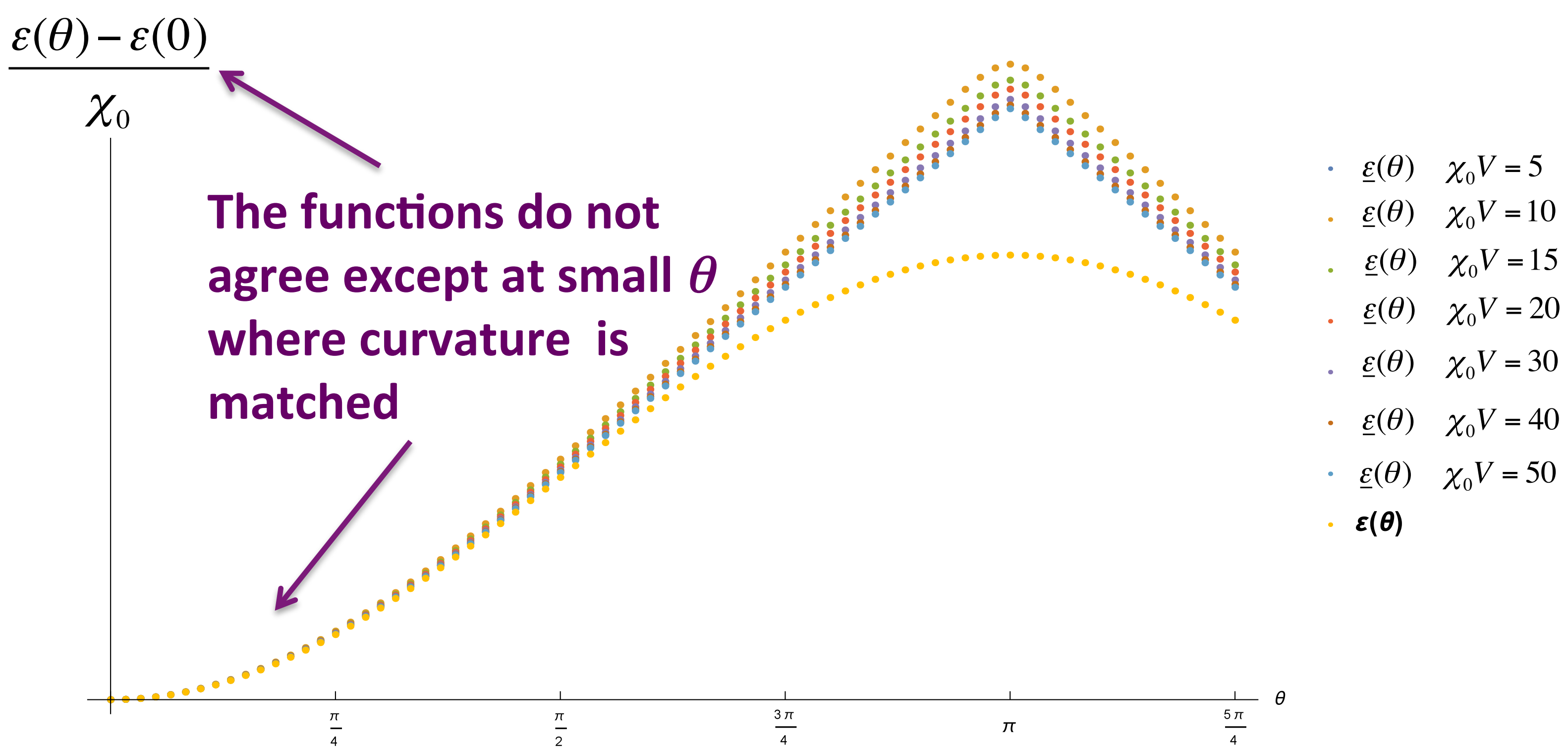

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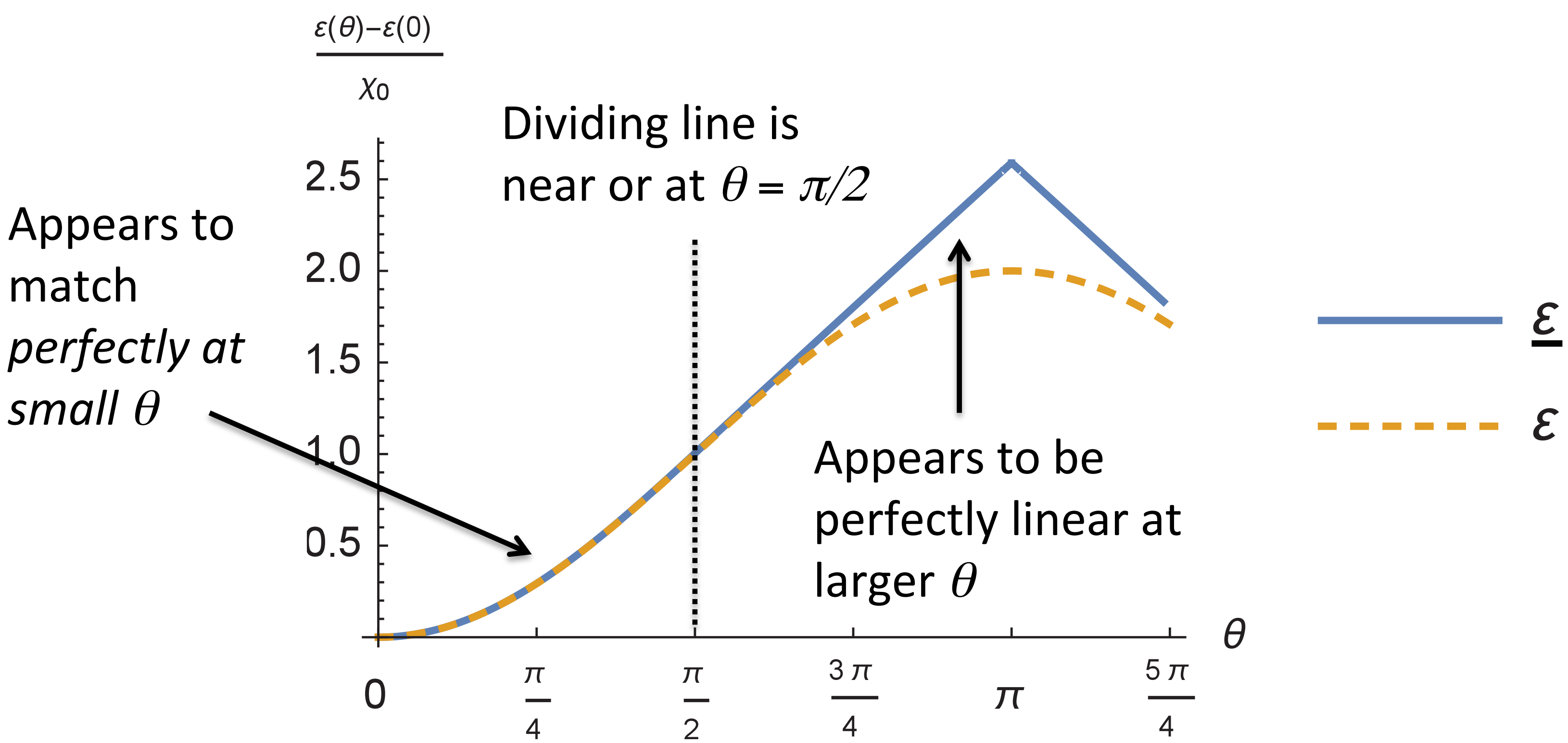

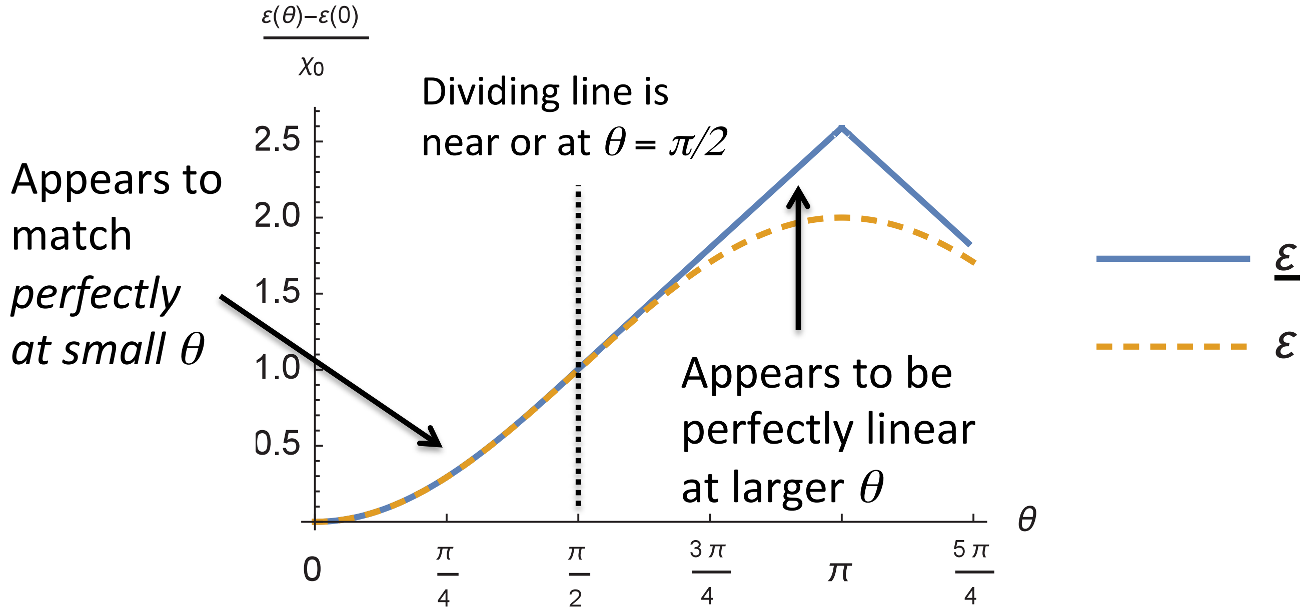

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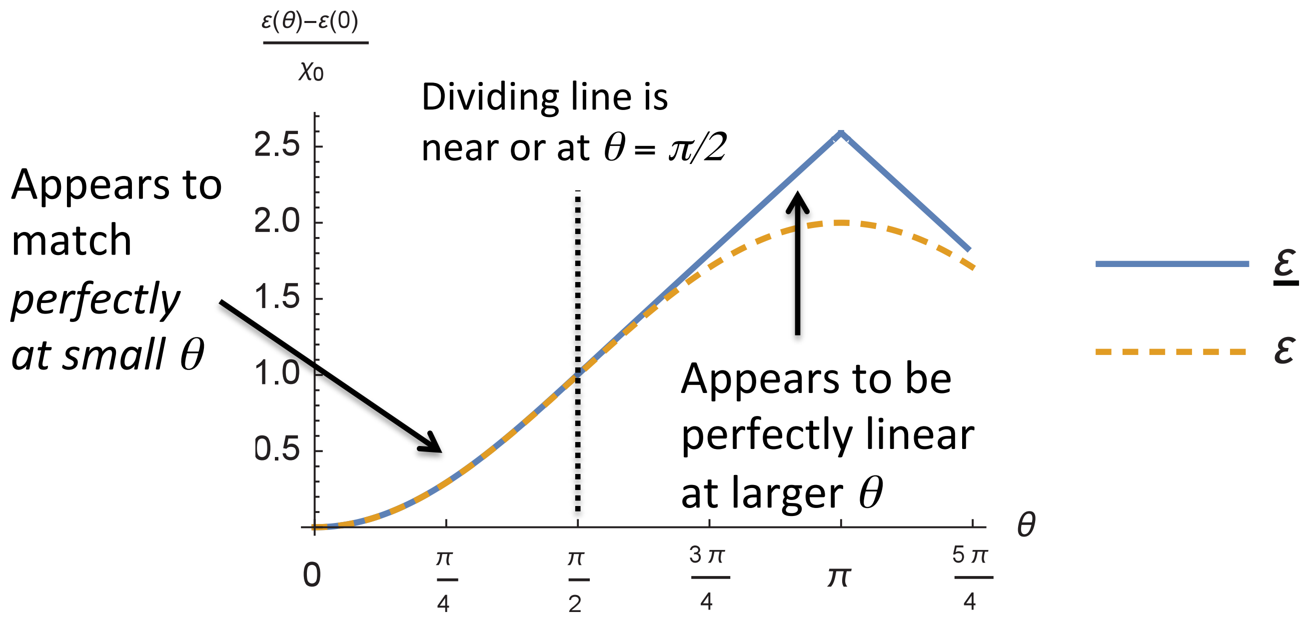

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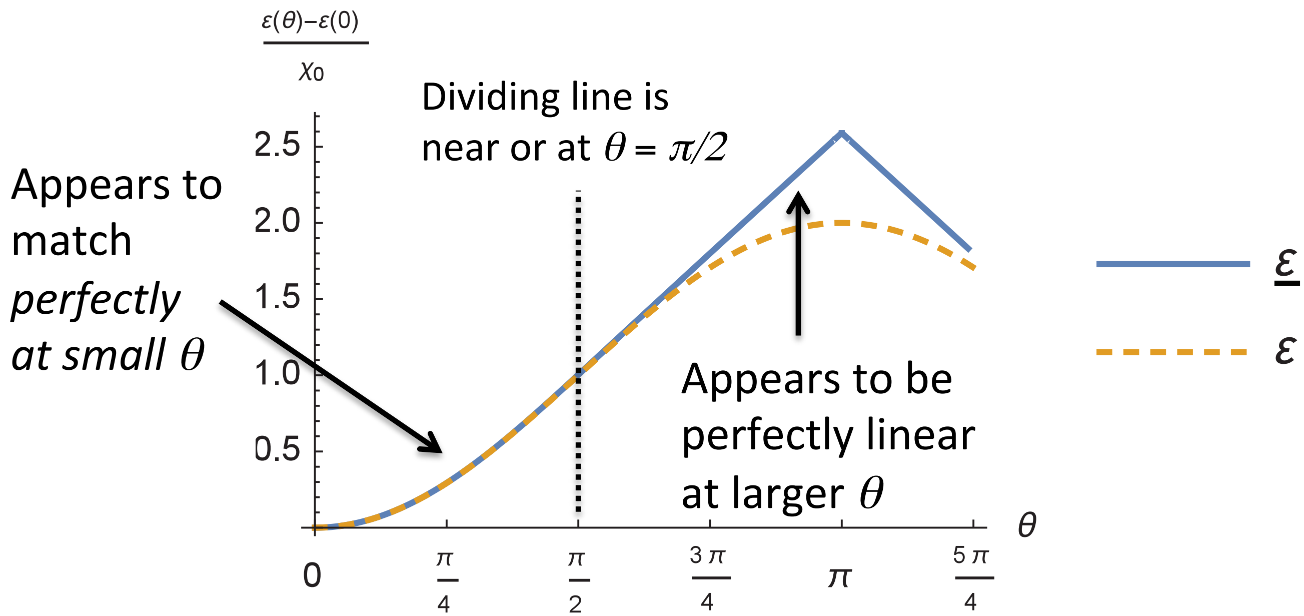
  - Why is it possible to reconstruct $\varepsilon(\theta)$ via direct summation of topological sectors in some regions of θ but not others?
    - Why doesn't exponential sensitivity of sign problem ruin things at small θ?
    - Why isn't exact knowledge of energy density as a function of topological charge density sufficient at larger θ?



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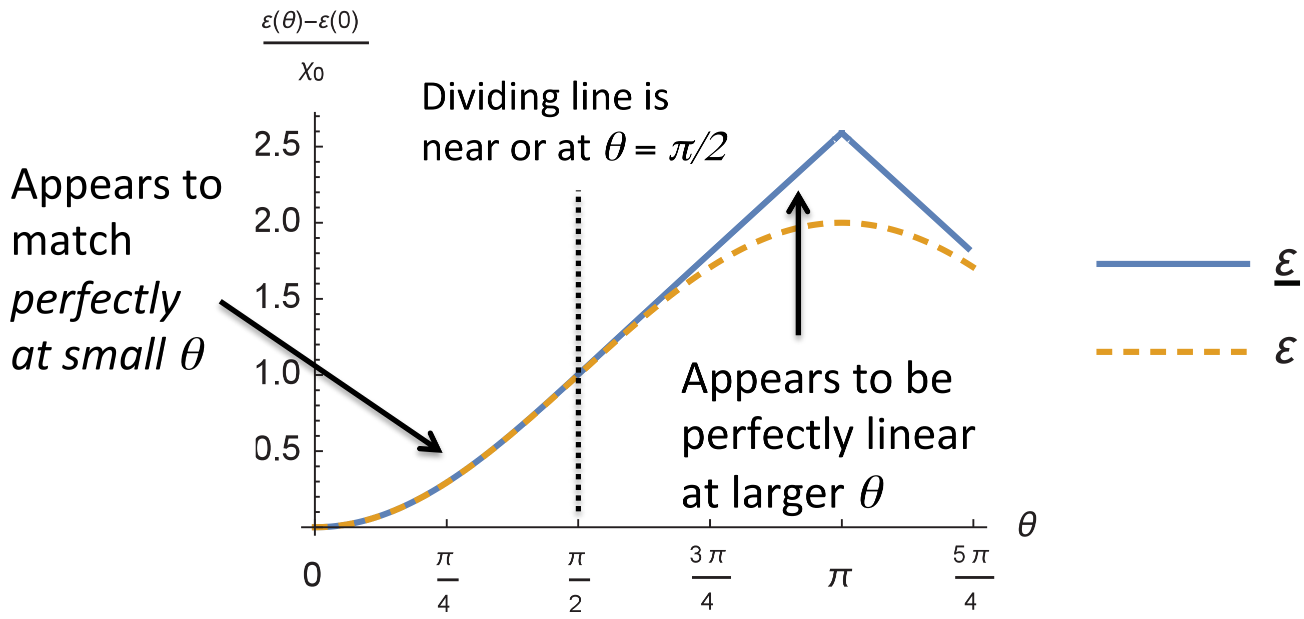

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  - Why is the function linear beyond this point?

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    - It can be shown in general (i.e. not just for dilute instanton gas) that below the first point of inflection in $\varepsilon(\theta)$, $\underline{\varepsilon}(\theta) = \varepsilon(\theta)$
      - For theories without points of inflection for entire range $-\pi < \theta < \pi$, $\underline{\varepsilon}(\theta) = \varepsilon(\theta)$ over the range.
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      - Such theories must have a kink at $\theta = \pm\pi$
    - It can also be shown in general (i.e. not just for dilute instanton gas) that above the first point of inflection in $\varepsilon(\theta)$, $\underline{\varepsilon}(\theta)$ is linear

- Why does $\underline{\varepsilon}(\theta) = \varepsilon(\theta)$ below the point of inflection?
  - The dilute instanton gas gives a major hint:

  The energy densities are related by a generalized Legendre transformation when θ is below the point of inflection.

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Like an ordinary Legendre transformation but with a critical factor of *i* different. This necessitates analytically continuing the energy density functions into the complex plane.

This Legendre transform can be shown to hold in the general case (not just the dilute instanton gas) below all points of inflection. The existence of this transformation ultimately implies $\underline{\varepsilon}(\theta) = \varepsilon(\theta)$

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Derivation of the generalized Legendre transformation and proof that it yields $\underline{\varepsilon}(\theta) = \varepsilon(\theta)$ below an inflection point and linearity above is somewhat complicated.

It will just be sketched here.

A magical Identity (which holds for $-\pi<\theta<\pi$)

$$\underline{\varepsilon}(\theta) = -\lim_{V\to\infty} \frac{1}{V} \log \left(\sum_Q e^{-\tilde{\varepsilon}(\frac{Q}{V})V} e^{i\theta Q} \right)$$

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One can replace the sum by an integral. This seems trivial—but it is anything but trivial—recall that the Q=0 term in the sum is exponentially bigger than the total. **It really is magical—but can be proved!**

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At large V this is the kind of integral for which the saddles point/stationary phase approximation becomes accurate—if a saddle point exists. If one does exist it will be on the imaginary axis.

Assuming a saddle point along the imaginary axis exists

$$\underline{\varepsilon}(\theta) = \tilde{\varepsilon}(q_\theta^{\mathrm{sp}}) - i\theta q_\theta^{\mathrm{sp}} \quad \textbf{with} \quad \left.\frac{\partial\left(\tilde{\varepsilon}(q) - i\theta q\right)}{\partial q}\right|_{q=q^{\mathrm{sp}}} = 0$$

This is the form of a generalized Legendre transformation!!
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But one can repeat the analysis for ε assuming a saddle point exists.

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\varepsilon(\theta) &= -\lim_{V\to\infty}\frac{1}{V}\log\left(\sum_Q e^{-\tilde{\varepsilon}(\frac{Q}{V},V)V}\, e^{i\theta Q}\right) \\
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&= \tilde{\varepsilon}(q_\theta^{\rm sp}) - i\theta q_\theta^{\rm sp}
\end{aligned}$$

with

$$\lim_{V\to\infty}\left.\frac{\partial\left(\tilde{\varepsilon}(q,V) - i\theta q\right)}{\partial q}\right|_{q=q^{\rm sp}} = \left.\frac{\partial\left(\tilde{\varepsilon}(q) - i\theta q\right)}{\partial q}\right|_{q=q^{\rm sp}} = 0$$

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ε is given by a generalized Legendre transformation –the same one as $\underline{\varepsilon}$ assuming it has a saddle point !!

- **Thus ε and $\underline{\varepsilon}$ are equal when a saddle point exists to dominate the relevant integral for $\underline{\varepsilon}$.**
  - In these circumstances the generalized Legendre form emerges naturally.
  - This explains why $\varepsilon = \underline{\varepsilon}$ at small θ

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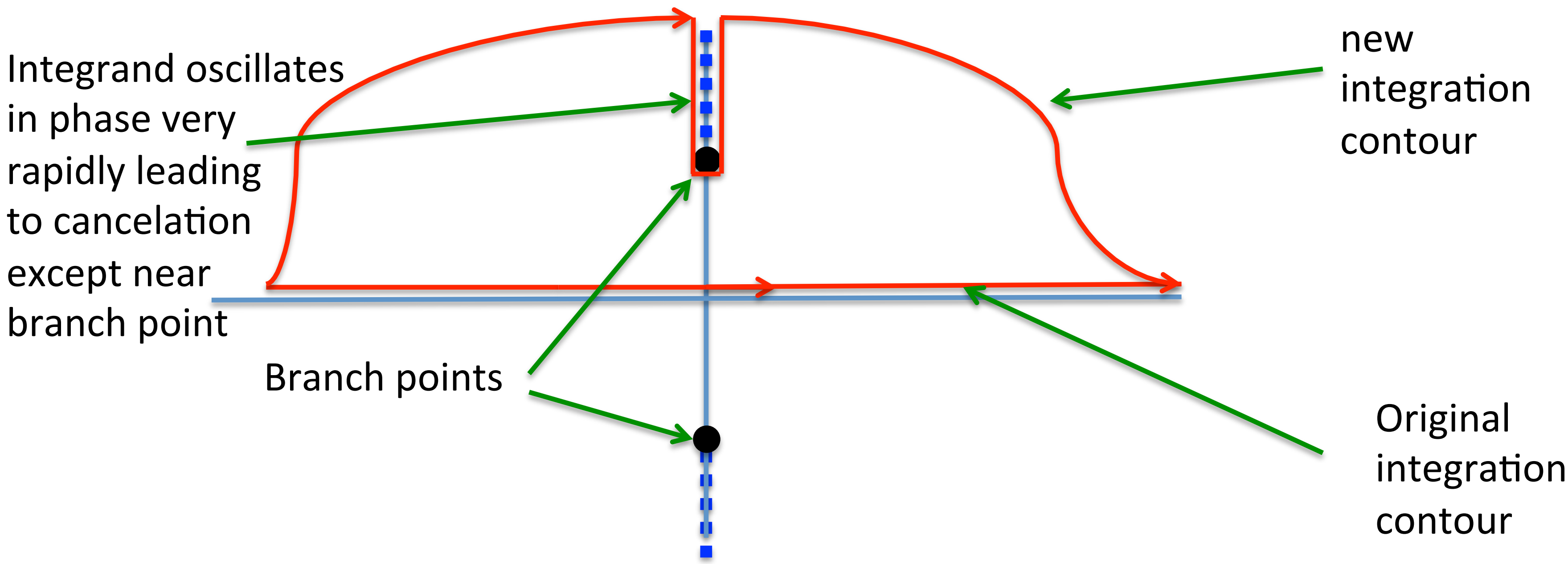
Thus, the structure will break down at points along the imaginary axis, where $\underline{\varepsilon}$ becomes nonanalytic and beyond which it is not well-defined. This occurs at branch points.

A theorem: Whenever a saddle point exists $\left.\frac{\partial^2 \varepsilon(\theta)}{\partial \theta^2}\,\frac{\partial^2 \tilde{\varepsilon}(q)}{\partial q^2}\right|_{q_\theta^{\rm sp}} = 1$

Thus as a point of inflection in $\varepsilon(\theta)$ is approached a nonanalytic point in q is also approached. It is easy to see that it is a branch point. One can also prove the converse—whenever a branch point is approached in q is a point of inflection in θ is approached.

Note that just as saddle points can dominate integrals, so can branch points.



- **In the absence of a saddle point a branch point will dominate integral for $\underline{\varepsilon}$.**
  - Note that the position of branch point is independent of the value of θ.
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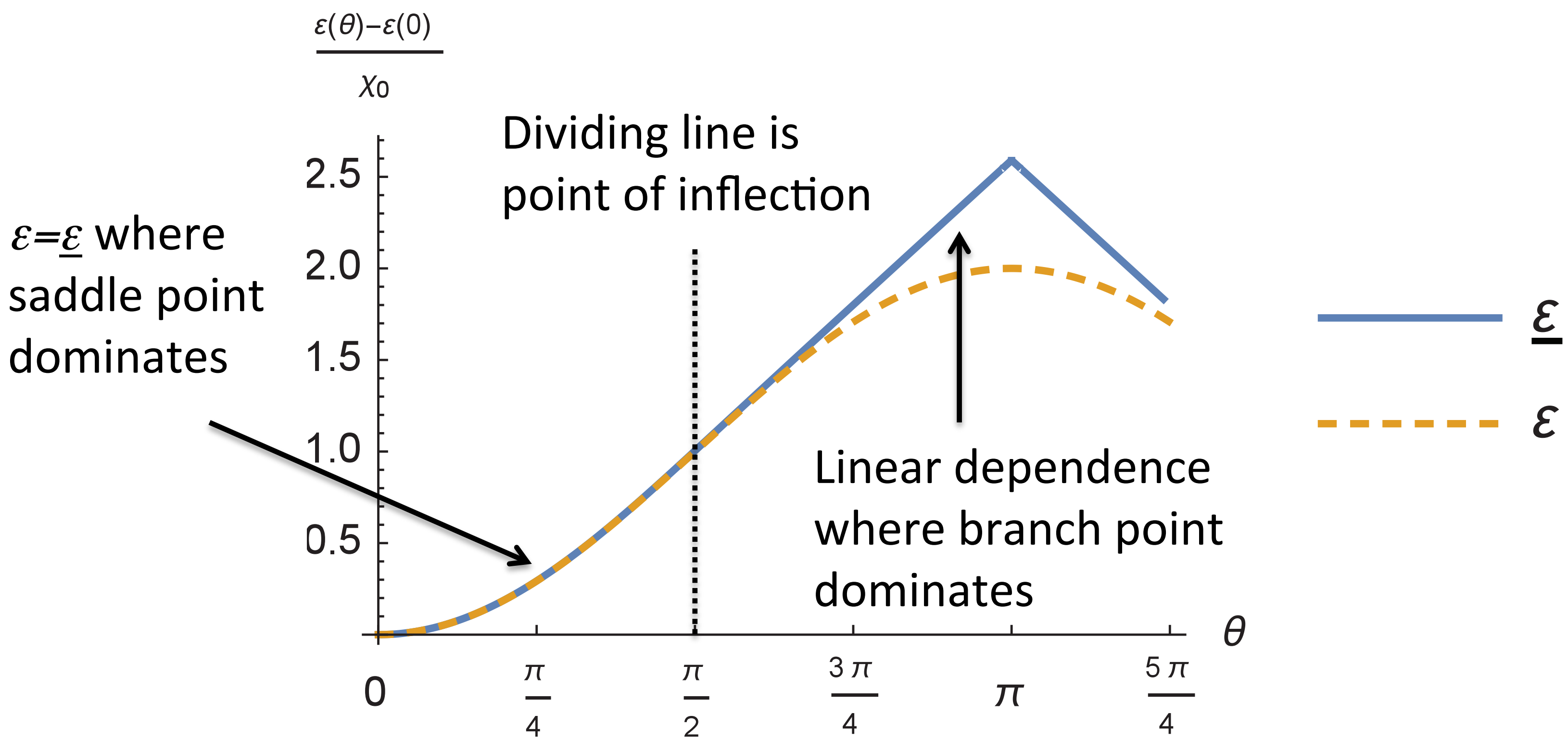
Qualitative behavior seen in dilute instanton gas, follows from this general analysis.



All of this analysis depended on the magical identity which allowed the replacement of the sum by an integral.

Thus it is useful to see why this identity works.

As a first step one can equate a periodic sum sum of δ functions to a sum of complex exponentials

$$\sum_{n=-\infty}^{\infty} \delta(x-n) = \sum_{k=-\infty}^{\infty} \exp\left(i2\pi kx\right)$$

From this it follows that

A sum

$$\sum_{n=-\infty}^{\infty} \exp\left(-\lambda f\left(\frac{n}{\lambda}\right)\right) \exp(i\theta\, n) =$$

$$\sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} dx \exp\left(-\lambda f\left(\frac{x}{\lambda}\right)\right) \exp(i\theta x) \exp(i2\pi kx) =$$

A sum of integrals

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Note each integral is of the type where at large λ the integral is dominated by a special point—eg. a saddle point or branch point and, up to power law corrections, they are given at large λ by $\exp[-\lambda\{f(y_{sp}+iy_{sp}(\theta+2\pi k)\}]$.

The sum of integrals is exponentially dominated by the term with the smallest exponential; this is typically the k=0 term when $-\pi<\theta<\pi$. In infinite λ limit only one term contributes.

$$\lim_{\lambda \to 0} \frac{1}{\lambda} \log \left(\sum_{n=-\infty}^{\infty} \exp\left(-\lambda f\left(\frac{n}{\lambda}\right)\right) \exp(i\theta\, n) \right)$$

$$= \lim_{\lambda \to 0} \frac{1}{\lambda} \log \left(\lambda \int_{-\infty}^{\infty} dy \exp\left(-\lambda\left(f(y) + i(\theta)\, y\right)\right) \right)$$

The sum is replaced by a single integral; the magical identity is established!

This validates the analysis and justifies the previous conclusions about the role of the subtle interplay of the sign problem and the infinite volume limit.

Conclusions

- **The answer to the question "Does the infinite volume expression for the energy density as a function of *q* yield the correct $\varepsilon(\theta)$ via direct summation over topological sectors or is the sign problem so severe as to prevent this?" is "It depends".**

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  - **Theories without points of inflection in $\varepsilon(\theta)$ for $0<\theta<\pi$, the answer is "yes"for whole region; such theories have kinks at $\theta=\pm\pi$.**

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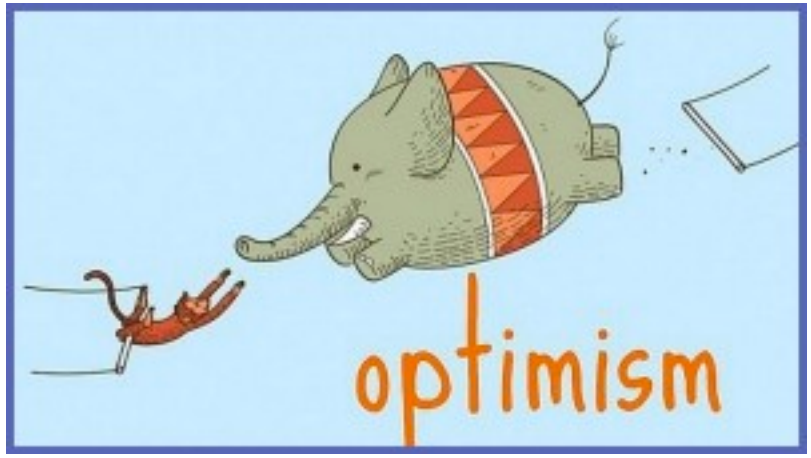
An optimistic take on things



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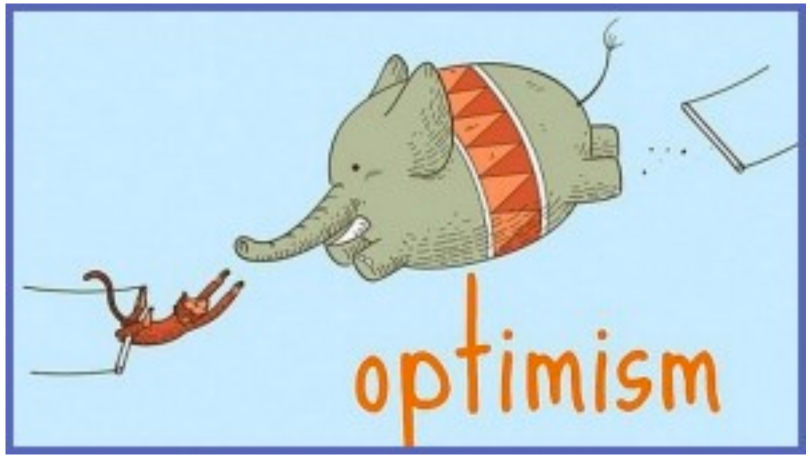

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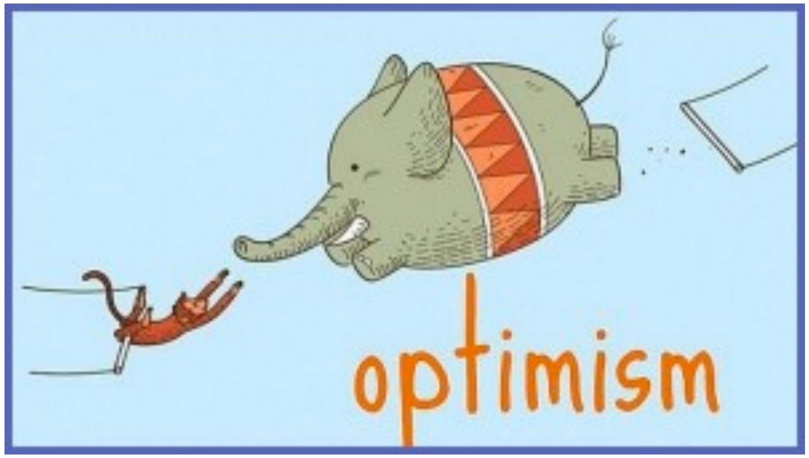

Despite the apparent need for exponentially accuracy, we can drop power law terms in some circumstances and still get a reasonable result—at least in some cases.

This suggests that maybe with enough cleverness perhaps the problem can be solved without the need for exponential accuracy.

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