The Breakdown of the Coherent State Path Integral

Justin H. Wilson

Advisor: Victor Galitski

University of Maryland, College Park, MD

Presentation Based on:

PRL **106**, 110401 (2011)

Preprint: arXiv:1012.1328

Quantum Vacuum Meeting

17 May 2012

Introduction

- Path integrals have a jaded mathematical history.
- Semiclassics have produced incorrect results (fixed with the discovery of a phase anomaly).
- We will find that we get *quantitatively* wrong results with an exact calculation.
  - We try to fix this *a posteriori.*
  - Nothing incorrect appears when the Hamiltonian is a linear sum of generators of the Lie algebra

Glauber coherent states are an over-complete set of states.

$$\mathfrak{h}_4 = \{1, a, a^\dagger, a^\dagger a\} \qquad\qquad [a, a^\dagger] = 1$$

$$|z\rangle = e^{-|z|^2/2} e^{z a^\dagger} |0\rangle$$

$$a|z\rangle = z|z\rangle \qquad\qquad \int \frac{\mathrm{d}^2 z}{\pi} |z\rangle\langle z| = 1$$

Partition function/Path integral

$$\mathcal{Z} = \mathrm{tr}\, e^{-\beta H} = \int \mathcal{D}^2 z \exp\left\{ -\int_0^\beta [z^* \dot{z} + \langle z|H|z\rangle] \right\}$$

R. J. Glauber, Phys. Rev. **131**, 2766 (1963)

The single-site Bose-Hubbard model can be written in terms of a Hamiltonian or a path integral.

- Hamiltonian: $$H = -\mu\hat{n} + \frac{U}{2}\hat{n}(\hat{n}-1)$$

  $a^\dagger a$ $\quad$ $a^\dagger a^\dagger a a$

- Partition Function:

$$\mathcal{Z} = \operatorname{tr} e^{-\beta H} \stackrel{?}{=} \int \mathcal{D}^2 z \, e^{-\int_0^\beta \mathrm{d}\tau \left[z^* \dot{z} - \mu |z|^2 + \frac{U}{2} |z|^4\right]} =: \mathcal{Z}'$$

The evaluation of the path integral...

$$\mathcal{Z}' := \int \mathcal{D}^2 z \, e^{-\int_0^\beta \mathrm{d}\tau \left[z^* \dot{z} - \mu |z|^2 + \frac{U}{2} |z|^4\right]}$$

$$z = \sqrt{n}\, e^{i\theta} \qquad\qquad \mathcal{D}^2 z = \mathcal{D}n \, \mathcal{D}\theta$$

$$\mathcal{Z}' = \int \mathcal{D}n \mathcal{D}\theta \, e^{-\int_0^\beta \mathrm{d}\tau \left[in\dot{\theta} - \mu n + \frac{U}{2} n^2\right]}$$

Integrate by parts

$$\mathcal{Z}' = \int \mathcal{D}n \mathcal{D}\theta \, e^{-i(n(\beta)\theta(\beta) - n(0)\theta(0)) - \int_0^\beta \mathrm{d}\tau \left[-i\dot{n}\theta - \mu n + \frac{U}{2} n^2\right]}$$

Method:
A. Alekseev *et al.*, J. Geom. Phys. **5**, 391 (1988)
D.C. Cabra *et al.*, J. Phys. A **30**, 2699 (1997)

$$\mathcal{Z}' = \int \mathcal{D}n\mathcal{D}\theta\, e^{-i(n(\beta)\theta(\beta)-n(0)\theta(0))-\int_0^\beta \mathrm{d}\tau\left[-i\dot{n}\theta-\mu n+\frac{U}{2}n^2\right]}$$

$$n(\beta) - n(0) = 0$$

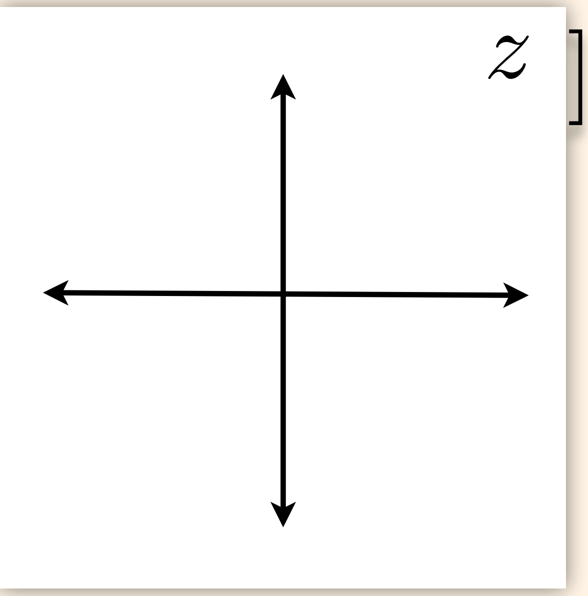
$$\theta(\beta) - \theta(0) = 2\pi k$$

$$\mathcal{Z}' = \sum_k \int \mathcal{D}n\mathcal{D}\theta\, e^{-i2\pi k n(0)+i\int_0^\beta \theta\dot{n}-\int_0^\beta \mathrm{d}\tau\left[-\mu n+\frac{U}{2}n^2\right]}$$

$$\int \mathcal{D}\theta(\tau) e^{-i\int_0^\beta \mathrm{d}\tau\, f(\tau)\theta(\tau)} = \delta(f)$$

$$\mathcal{Z}' = \sum_k \int \mathcal{D}n\, \delta(\dot{n})\, e^{-i2\pi k n(0)-\int_0^\beta \mathrm{d}\tau\left[-\mu n+\frac{U}{2}n^2\right]}$$

$$\mathcal{Z}' = \int \mathcal{D}n\mathcal{D}\theta\, e^{-i(n(\beta)\theta(\beta)-n(0)\theta(0))-\int_0^\beta \mathrm{d}\tau \cdots]}$$



$$n(\beta) - n(0) = 0$$

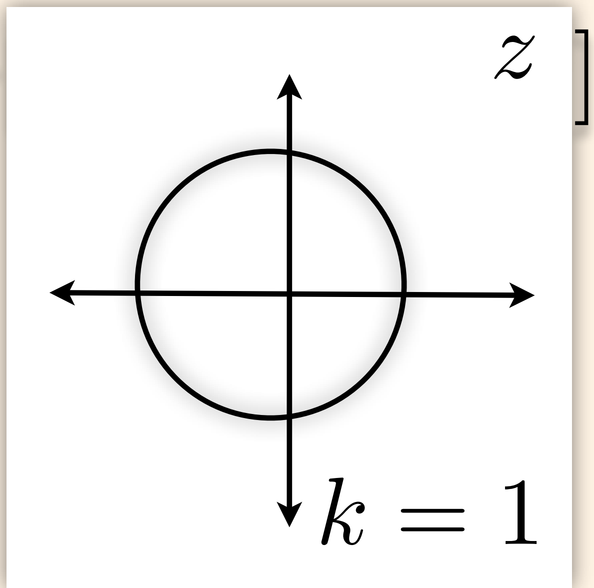
$$\theta(\beta) - \theta(0) = 2\pi k$$

$$\mathcal{Z}' = \sum_k \int \mathcal{D}n\mathcal{D}\theta\, e^{-i2\pi k n(0)+i\int_0^\beta \theta\dot{n}-\int_0^\beta \mathrm{d}\tau\left[-\mu n+\frac{U}{2}n^2\right]}$$

$$\int \mathcal{D}\theta(\tau) e^{-i\int_0^\beta \mathrm{d}\tau\, f(\tau)\theta(\tau)} = \delta(f)$$

$$\mathcal{Z}' = \sum_k \int \mathcal{D}n\,\delta(\dot{n})\, e^{-i2\pi k n(0)-\int_0^\beta \mathrm{d}\tau\left[-\mu n+\frac{U}{2}n^2\right]}$$

$$\mathcal{Z}' = \int \mathcal{D}n\mathcal{D}\theta\, e^{-i(n(\beta)\theta(\beta)-n(0)\theta(0))-\int_0^\beta \mathrm{d}\tau\,]}$$



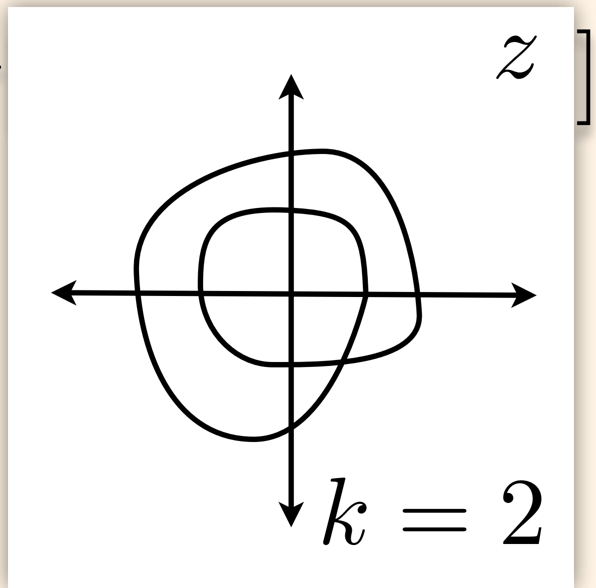
$$n(\beta) - n(0) = 0$$
$$\theta(\beta) - \theta(0) = 2\pi k$$

$$\mathcal{Z}' = \sum_k \int \mathcal{D}n\mathcal{D}\theta\, e^{-i2\pi k n(0)+i\int_0^\beta \theta\dot{n}-\int_0^\beta \mathrm{d}\tau\left[-\mu n+\frac{U}{2}n^2\right]}$$

$$\int \mathcal{D}\theta(\tau) e^{-i\int_0^\beta \mathrm{d}\tau\, f(\tau)\theta(\tau)} = \delta(f)$$

$$\mathcal{Z}' = \sum_k \int \mathcal{D}n\, \delta(\dot{n})\, e^{-i2\pi k n(0)-\int_0^\beta \mathrm{d}\tau\left[-\mu n+\frac{U}{2}n^2\right]}$$

$$\mathcal{Z}' = \int \mathcal{D}n\mathcal{D}\theta \, e^{-i(n(\beta)\theta(\beta) - n(0)\theta(0)) - \int_0^\beta \mathrm{d}\tau \;]}$$



$$n(\beta) - n(0) = 0$$
$$\theta(\beta) - \theta(0) = 2\pi k$$

$$\mathcal{Z}' = \sum_k \int \mathcal{D}n\mathcal{D}\theta \, e^{-i2\pi k n(0) + i\int_0^\beta \theta \dot{n} - \int_0^\beta \mathrm{d}\tau \left[-\mu n + \frac{U}{2} n^2\right]}$$

$$\int \mathcal{D}\theta(\tau) e^{-i\int_0^\beta \mathrm{d}\tau \, f(\tau)\theta(\tau)} = \delta(f)$$

$$\mathcal{Z}' = \sum_k \int \mathcal{D}n \, \delta(\dot{n}) \, e^{-i2\pi k n(0) - \int_0^\beta \mathrm{d}\tau \left[-\mu n + \frac{U}{2} n^2\right]}$$

$$\mathcal{Z}' = \int \mathcal{D}n\mathcal{D}\theta\, e^{-i(n(\beta)\theta(\beta) - n(0)\theta(0)) - \int_0^\beta \mathrm{d}\tau \left[-i\dot{n}\theta - \mu n + \frac{U}{2} n^2\right]}$$

$$n(\beta) - n(0) = 0$$

$$\theta(\beta) - \theta(0) = 2\pi k$$

$$\mathcal{Z}' = \sum_k \int \mathcal{D}n\mathcal{D}\theta\, e^{-i2\pi k n(0) + i\int_0^\beta \theta\dot{n} - \int_0^\beta \mathrm{d}\tau \left[-\mu n + \frac{U}{2} n^2\right]}$$

$$\int \mathcal{D}\theta(\tau) e^{-i\int_0^\beta \mathrm{d}\tau\, f(\tau)\theta(\tau)} = \delta(f)$$

$$\mathcal{Z}' = \sum_k \int \mathcal{D}n\, \delta(\dot{n})\, e^{-i2\pi k n(0) - \int_0^\beta \mathrm{d}\tau \left[-\mu n + \frac{U}{2} n^2\right]}$$

$$\mathcal{Z}' = \sum_k \int \mathcal{D}n \, \delta(\dot{n}) \, e^{-i2\pi k n(0) - \int_0^\beta \mathrm{d}\tau \left[-\mu n + \frac{U}{2} n^2\right]}$$

$n(t)$ is a constant in time

$$\mathcal{Z}' = \sum_k \int_0^\infty \mathrm{d}x \; e^{-i2\pi k x - \beta\left[-\mu x + \frac{U}{2} x^2\right]}$$

$n(t) = x \geq 0$

$$\sum_k e^{2\pi i k x} = \sum_n \delta(x-n)$$

$$\mathcal{Z}' = \sum_n \int_0^\infty \mathrm{d}x \; \delta(x-n) e^{-\beta\left[-\mu x + \frac{U}{2} x^2\right]}$$

$$\boxed{\mathcal{Z}' = \sum_n e^{\beta \mu n - \beta \frac{U}{2} n^2}}$$

They are *not* the same expression.

$$U \gg 1$$

$$\mathcal{Z}' = \sum_{n=0}^{\infty} e^{\beta\mu n - \beta\frac{U}{2}n^2} \sim 1 + e^{\beta\mu}e^{-\beta U/2} + \cdots$$

$$\mathcal{Z} = \sum_{n=0}^{\infty} e^{\beta\mu n - \beta\frac{U}{2}n(n-1)} \sim 1 + e^{\beta\mu} + e^{2\beta\mu}e^{-\beta U} + \cdots$$

$$\Longrightarrow \qquad \mathcal{Z} \neq \mathcal{Z}'$$

This is a new issue.

$$Z' := \int \mathcal{D}^2 z \, e^{-\int_0^\beta \left[z^* \dot{z} - \mu |z|^2 + \frac{U}{2} |z|^4 \right]} := \mathrm{tr}\, e^{-\beta H'}$$

- Semiclassics suggest[3,4]:

$$H' = H_W = -\mu \hat{n} + \frac{U}{2} \hat{n}(\hat{n} + 1) \quad \text{(Up to a constant)}$$

- Exact calculation suggests:

$$H' = -\mu \hat{n} + \frac{U}{2} \hat{n}^2$$

- Original Hamiltonian:

$$H = -\mu \hat{n} + \frac{U}{2} \hat{n}(\hat{n} - 1)$$

[3] Kochetov, J. Phys. A. **31**, 4473 (1998)
For spin-path integral:
[4] M. Stone *et al.*, J. Math. Phys. (N.Y.) **41**, 8025 (2000)

How to “fix” the path integral

$$\mathcal{Z} = \int \mathcal{D}^2 z \, e^{-\int_0^\beta \mathrm{d}\tau \left[z^* \dot{z} - \mu |z|^2 + \frac{U}{2} |z|^2 (|z|^2 - 1) \right]}$$

Prescription:
Replace operator n in Hamiltonian by $|z|^2$

Path integral used previously: $$Z' := \int \mathcal{D}^2 \, e^{-\int_0^\beta \mathrm{d}\tau \left[z^* \dot{z} - \mu |z|^2 + \frac{U}{2} |z|^4 \right]}$$

How to “fix” the path integral

$$\mathcal{Z} = \int \mathcal{D}^2 z \, e^{-\int_0^\beta \mathrm{d}\tau \left[z^* \dot{z} - \mu |z|^2 + \frac{U}{2} |z|^2 (|z|^2 - 1) \right]}$$

Equality when doing our exact calculation.

Prescription:
Replace operator n in Hamiltonian by $|z|^2$

Path integral used previously:

$$Z' := \int \mathcal{D}^2 \, e^{-\int_0^\beta \mathrm{d}\tau \left[z^* \dot{z} - \mu |z|^2 + \frac{U}{2} |z|^4 \right]}$$

How to “fix” the path integral

$$\mathcal{Z} = \int \mathcal{D}^2 z \, e^{-\int_0^\beta \mathrm{d}\tau \left[z^* \dot{z} - \mu |z|^2 + \frac{U}{2} |z|^2 (|z|^2 - 1) \right]}$$

Equality when doing our exact calculation.

Prescription:
Replace operator n in Hamiltonian by $|z|^2$

Drawbacks:

1. No *a priori* reason to suspect this.
2. Semiclassics give the wrong result.

Path integral used previously:

$$Z' := \int \mathcal{D}^2 \, e^{-\int_0^\beta \mathrm{d}\tau \left[z^* \dot{z} - \mu |z|^2 + \frac{U}{2} |z|^4 \right]}$$

The calculation works when the Hamiltonian is a linear sum of generators.

Same problem comes up in the spin coherent state path integral

e.g. $$H = S_z^2$$ for spin-1

Everything works out for Hamiltonians that are *linear* in generators of the algebra

e.g.
$$H_{\text{spin}} = AS_x + BS_y + CS_z + D$$
$$H_{\text{HO}} = E + Fa + F^*a^\dagger + Ga^\dagger a$$

Therefore, it always works for spin-1/2.

Conclusion

- Path integral breaks down by the exact calculation shown. This extends to other models (spin path integrals, general Bose Hubbard, etc.).
  - It works when the Hamiltonian is a linear sum of Lie algebra generators.
  - Agreement can be achieved by naively replacing the operator n by $|z|^2$ in the path integral.
  - In the time discretized path integral (before any continuity assumption), everything works out OK.