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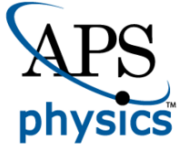
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Breakdown of the coherent state path integral: two simple examples

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We show how the time-continuous coherent state path integral breaks down for both the single-site Bose-Hubbard model and the spin path integral. Specifically, when the Hamiltonian is quadratic in a generator of the algebra used to construct coherent states, the path integral fails to produce correct results following from an operator approach. As suggested by previous authors, we note that the problems do not arise in the time-discretized version of the path integral.

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Path integrals are widely known for being an alternate formulation of quantum mechanics, and appear in many textbooks as a useful calculational tool for various quantum and statistical mechanical problems (e.g., perturbative expansions, non-perturbative techniques including the instanton method, and effective theories [1–3]). From their inception, there has been the problem of writing down a path integral for any system that can be described by a Hilbert space equipped with a Hamiltonian. One way to approach this problem is with what is known now as the generalized coherent state path integral [4, 5] which generalizes the coherent state path integral for a harmonic oscillator. The key observation with path integration [2] is that, given a Hamiltonian H , the propagator, e^{-itH} , at some time t can be broken up into N slices, $(e^{-itH/N})^N$, and in between each multiplicative term one inserts an (over-)complete set of states parametrized by a continuous parameter. If we take $N \rightarrow \infty$ we get the time-continuous formulation. This formulation of path integrals, applied to coherent states, has become widely and routinely used in many areas of physics (see the many papers collected in [6]), yet despite the many successes of path integrals, they have been on very shaky mathematical grounds (for a small “slice” of this history, see [7]).

Glauber coherent states [8] are usually understood as the most classical states associated with the harmonic oscillator. They obey the classical equations of motion for a harmonic oscillator and are minimal uncertainty states. Perelomov and Gilmore [9, 10] extended the definition of coherent states to Lie algebras other than the Heisenberg algebra (i.e., the harmonic oscillator algebra). Since then, these “generalized” coherent states have been used in a number of applications (see [11, 12]). In particular, the coherent states form an overcomplete basis (with a continuous label) which is a necessary ingredient for the construction of a path integral. For the harmonic oscillator, coherent states are represented by a complex number, but for coherent states constructed with $\mathfrak{su}(2)$ (spin), they are points on the Bloch sphere, S^2 .

For the case of the harmonic oscillator, it is commonly known that one can easily go between the normal-ordered Hamiltonian (all annihilation operators commuted to the right) and the coherent state path integral [1]; this is due to the fact that coherent states are eigenvectors of the annihilation operator. For the general coherent state path integral, the “classical” Hamiltonian in the path integral is just the expectation value of the quantum Hamiltonian with a coherent state. This prescription results in some notable exactly solvable cases, but all such cases involve *non-interacting* terms which are essentially linear in the algebra generators used to construct the coherent-states. When the Hamiltonian involves terms that are non-linear in generators (interactions), this prescription fails, as this letter demonstrates.

In previous literature, the spin coherent state path integral has sometimes produced (quantitatively) incorrect results [13–17] unless the time-discretized version is employed [16, 18]. These problems with the time-continuous path integral were mostly solved by Stone *et al.* [19] by identifying an anomaly in the fluctuation determinant which added an extra phase to the semi-classical propagator. Kochetov had also found this phase in a general context [20]. Furthermore, Pletyukhov [21] related the extra phase in the spin path integral back to Weyl ordering the Hamiltonian in the case of the harmonic oscillator (in the simplest case, Weyl ordering corresponds to symmetrically ordering annihilation and creation operators). Additionally, Weyl ordering has been considered in the Bose-Hubbard case in [22]. Unfortunately, this solution does not explain the present breakdown under consideration.

In this letter, we outline another problem with the time-continuous coherent state path integral. This problem manifests itself in two simple examples: (i) the spin-coherent state path integral and (ii) the harmonic oscillator coherent state path integral (in particular, the single-site Bose-Hubbard model). The single-site Bose-Hubbard Hamiltonian is a minimal model that demonstrates the problem with the normal-ordered path integral. However, the problem itself is more general than the toy model considered here and clearly persists in more complicated models, including lattice Bose-Hubbard models. We use an exact method of calculating the partition function mathematically developed by Alekseev *et al.* [23] (and more recently used by Cabra *et al.* [24] for the spin path integral with $H = S_z$), and demonstrate that the exact result differs from the correct partition function in the cases of both normal-ordering of operators (as prescribed by most textbooks) and when using Weyl ordering (i.e., it cannot be accounted for with the phase anomaly found by Solari and Kochetov [18, 20] and elaborated on by Stone *et al.* [19]).

We begin with the coherent state path integral for spin with the standard $SU(2)$ algebra defined on the operators $\{S_x, S_y, S_z\}$ with $[S_i, S_j] = i\epsilon_{ijk}S_k$, and we define our Hilbert space by taking the matrix representation of the $SU(2)$ group in $(2s+1)$ -by- $(2s+1)$ matrices (s being the spin of the system). Irrespective of the algebra, we can in general define a Hermitian matrix H that acts on states in our Hilbert space, and this will be our Hamiltonian. Usually, H is polynomial of algebra generators.

If $|s\rangle$ is the maximal state of S_z in our spin- s system, then we can define spin-coherent states as $|\mathbf{n}\rangle = e^{-i\phi S_z} e^{-i\theta S_y} |s\rangle$ where (θ, ϕ) are coordinates on the sphere S^2 along the unit vector \mathbf{n} (i.e., a point on the standard Bloch sphere). These coherent states are overcomplete such that $\frac{2s+1}{4\pi} \int_{S^2} d\mathbf{n} |\mathbf{n}\rangle \langle \mathbf{n}| = 1$ where $d\mathbf{n} = d\phi d(\cos\theta)$ is the standard measure on S^2 . Using this continuous, overcomplete basis, one can derive the standard path integral for the partition

function for spin from $\mathcal{Z} = \text{tr} e^{-\beta H}$ in the standard way [1] discussed in the introduction:

$$\mathcal{Z}' = \int \mathcal{D}\mathbf{n}(\tau) \exp \left\{ - \int_0^\beta d\tau [- \langle \mathbf{n}(\tau) | \partial_\tau \mathbf{n}(\tau) \rangle + \langle \mathbf{n}(\tau) | H | \mathbf{n}(\tau) \rangle] \right\}. \quad (1)$$

We call the partition function as given by the time-continuous path integral \mathcal{Z}' in order to distinguish it from $\mathcal{Z} = \text{tr} e^{-\beta H}$ since we will find that in general they may not agree. The path integral is over all closed paths (since it is the partition function). The first term in the action for Eq. (1), $\langle \mathbf{n} | \partial_\tau \mathbf{n} \rangle$, is the Berry phase term and in (θ, ϕ) coordinates $-\langle \mathbf{n} | \partial_\tau \mathbf{n} \rangle = -is(1 - \cos \theta) \partial_\tau \phi$.

We assume $\langle \mathbf{n} | H | \mathbf{n} \rangle = H(\cos \theta)$ for some function $H(x)$ (this is true if and only if H is diagonal). This puts the ϕ dependence of the action solely in the Berry phase term of the action. We then integrate the Berry phase term by parts; the boundary term is just $\Delta \phi (1 - \cos \theta(0))$ with $\Delta \phi = \phi(\beta) - \phi(0) = 2\pi k$ for any integer k and $\cos \theta(\beta) = \cos \theta(0)$ since our paths are closed. We must sum over the different topological sectors defined by the integer k (i.e., how many times ϕ wraps around the sphere). Thus, our only ϕ dependence is multiplying $\frac{d \cos \theta}{d\tau}$ from integrating by parts, and we use standard identity for functional integrals $\int \mathcal{D}\phi e^{-i \int_0^\beta d\tau \phi(\tau) f(\tau)} = \delta(f)$, to get that $\cos \theta$ must be constant (i.e., $\frac{d \cos \theta}{d\tau} = 0$). This δ -function allows us to do the path integral over $\mathcal{D}(\cos \theta)$, except for the initial value which we call $x := \cos \theta(0)$. Taking all of this into account, the path integral can then be written as

$$\mathcal{Z}' = \sum_{k=-\infty}^{\infty} \int_{-1}^1 dx e^{2\pi i k s (1-x) - \beta H(x)}. \quad (2)$$

The sum over k can be evaluated as a sum of delta functions of the form $\delta(s(1-x) - n)$ for all integers n . Since x is in the interval -1 to $+1$, only finitely many n contribute ($n = 0$ to $n = 2s$ to be exact). We can rewrite the sum over n as a sum over $m := s - n$ and we get the answer (dropping overall constants)

$$\mathcal{Z}' = \sum_{m=-s}^s e^{-\beta H(m/s)}. \quad (3)$$

Eq. (3) looks very promising, but $H(m/s)$ is not the same as $\langle m | H | m \rangle$. First let us see where it *does* work. Take the simple Hamiltonian $H = S_z$, then $\langle \mathbf{n} | H | \mathbf{n} \rangle = s \cos \theta$, and thus $H(x) = sx$. This immediately yields

$$\mathcal{Z}'_{H=S_z} = \sum_{m=-s}^s e^{-\beta m}, \quad (4)$$

and it is easily calculated (in operator language) that $\mathcal{Z}'_{H=S_z} = \mathcal{Z}_{H=S_z}$. The two methods agree for the particular Hamiltonian $H = S_z$ (the case considered by Cabra *et al.* [24]). On the other hand, if we take $H = S_z^2$ and $s = 1$, we can evaluate $\langle \mathbf{n} | S_z^2 | \mathbf{n} \rangle = \frac{1}{2} (\cos^2 \theta + 1)$; from which we have

$$H(x) = \frac{1}{2} (x^2 + 1). \quad (5)$$

Thus, $\mathcal{Z}'_{H=S_z^2} = 2e^{-\beta} + e^{-\beta/2}$, but this conflicts with $\mathcal{Z}_{H=S_z^2} = 2e^{-\beta} + 1$ by more than just a multiplicative constant. Thus, we have $\mathcal{Z}'_{H=S_z^2} \neq \mathcal{Z}_{H=S_z^2}$ for $s = 1$, and in fact $\mathcal{Z}'_{H=S_z^2} \neq \mathcal{Z}_{H=S_z^2}$ for all $s > 1/2$.

Importantly, the two methods agree for any Hamiltonian when $s = 1/2$. This comes from the fact that any (diagonalized) Hamiltonian for a two state system ($s = 1/2$) can be written as $H = a + bS_z$ (in fact $H = S_z^2 = 1/4$), and the above method gives $\mathcal{Z}' = \mathcal{Z}$ when $H = a + bS_z$.

Also, if we take the Hamiltonian $H = S_z^2/s^2$, then when $s \gg 1$ Eq. (3) reproduces the correct result. This is a general result for Hamiltonians that are finite polynomials of S_z/s , and suggests that “semiclassically” (i.e. s tends to infinity), we will still arrive at sensible results.

Agreement can be forced by considering $H(x) = x^2$ instead of Eq. (5), but this corresponds to replacing S_z with $\langle S_z \rangle$ in the Hamiltonian *instead* of just considering $\langle H \rangle$. In the $H = S_z^2$ case, it is the difference between considering $\langle S_z^2 \rangle$ and $\langle S_z \rangle^2$; the latter gives correct results.

To motivate looking for this same issue in a system with the Weyl-Heisenberg algebra (i.e., the harmonic oscillator algebra), it is known [25] that one can contract $\mathfrak{u}(2)$ (since we constructed our coherent states for spins with $\mathfrak{su}(2)$) into

the Weyl-Heisenberg algebra by considering $\mathfrak{u}(2) = \text{span}\{S_0, S_x, S_y, S_z\} = \mathfrak{u}(1) \oplus \mathfrak{su}(2)$, where we define $[S_0, S_i] = 0$. Then define the operators $J_0 := S_0$, $J_{1,2}(\epsilon) := \epsilon S_{y,x}$, and $J_3(\epsilon) := S_0 + \epsilon^{-2} S_z$ to get the commutation relations $[J_3, J_{1,2}] = \mp i J_{2,1}$, $[J_1, J_2] = -i\epsilon^2 J_3 + iJ_0$, and $[J_0, J_i] = 0$. If we let $\epsilon \rightarrow 0$, we recover exactly the Weyl-Heisenberg algebra: $\mathfrak{h}_4 = \text{span}\{1, x, p, a^\dagger a\}$ with $[x, p] = i$, $[a^\dagger a, x] = -ip$, $[a^\dagger a, p] = ix$. Observe that S_z is related to $a^\dagger a$ in this contraction, so we might suspect that terms quadratic in $a^\dagger a$ give problems like those found with S_z^2 in the spin-coherent state path integral.

A Hamiltonian that uses the Weyl-Heisenberg algebra to construct its coherent states is the Bose-Hubbard model. For a single site, we can write

$$H = -\mu n + \frac{U}{2} n(n-1), \quad (6)$$

where $n = a^\dagger a$ and the a (a^\dagger) is the annihilation (creation) operator for the algebra $[a, a^\dagger] = 1$. The form $n(n-1) = a^\dagger a^\dagger a a$ comes from the normal ordering required from a path integral of the form

$$\mathcal{Z}' = \int \mathcal{D}^2 z \exp \left\{ - \int_0^\beta d\tau \left[\frac{1}{2} (z^* \dot{z} - \dot{z}^* z) - \mu |z|^2 + \frac{U}{2} |z|^4 \right] \right\}. \quad (7)$$

We can solve this path integral with the same method used to obtain Eq. (3) in the spin-coherent state path integral. Let $z = \sqrt{n} e^{i\theta}$, so that the measure becomes $\mathcal{D}^2 z = \mathcal{D}n \mathcal{D}\theta$ and the action becomes $S = \int d\tau (in\dot{\theta} - \mu n + \frac{U}{2} n^2)$. Integrating by parts on the $n\dot{\theta}$ term then integrating over $\mathcal{D}\theta$ will fix n to be constant, and the boundary term will fix n to be an integer. Since n is radial, it can only be positive so we directly obtain

$$\mathcal{Z}' = \sum_{n=0}^{\infty} e^{\mu n \beta - \frac{U}{2} n^2 \beta}. \quad (8)$$

But this differs from the partition function that we can easily calculate in operator language:

$$\mathcal{Z} = \sum_{n=0}^{\infty} e^{\mu n \beta - \frac{U}{2} n(n-1) \beta}. \quad (9)$$

We see that a similar problem to that of the spin coherent state path integral here. To see it explicitly, for $U \gg 1$, we have $\mathcal{Z}' \sim 1 + e^{\mu - U/2} + \dots$, but $\mathcal{Z} \sim 1 + e^\mu + e^{2\mu - U} + \dots$. With different asymptotics, \mathcal{Z} and \mathcal{Z}' are different expressions. Note that if we let $\mu \rightarrow \mu + \frac{U}{2}$ in \mathcal{Z}' , that we will get same result. This substitution for μ corresponds to replacing n in Eq. (6) by $\langle n \rangle = |z|^2$ when writing down our action (so instead of $\langle n^2 \rangle$, one gets $\langle n \rangle^2$).

We now compare this to the semiclassical result. Still considering Eq. (6), let us change our algebra slightly to incorporate a small parameter (akin to the standard $\hbar \rightarrow \infty$ for normal semiclassics): h ; h^{-1} is the representation index (called γ in [20]). We note here that different h 's change the coherent states $|z\rangle$ in the following way: if $z = \frac{1}{\sqrt{2}}(u + iv)$, then $u = q/c$, $v = p/d$, and $h = \hbar/(cd)$ (and $[a, a^\dagger] = h$). We have used q and p as the standard position and momentum for the harmonic oscillator. Up until now we have been considering $h = 1$.

We can write the propagator between two coherent states $|z_i\rangle$ and $|z_f\rangle$ using a Hubbard-Stratonovich transformation and the propagator for the harmonic oscillator:

$$\begin{aligned} K(z_f^*, z_i; t) &= \langle z_f | e^{-iHT/h} | z_i \rangle \\ &= \sqrt{\frac{iT}{2\pi U h}} \int d\omega e^{\frac{1}{h} \Phi_\omega + \frac{1}{2} i\omega T + \frac{1}{8} U h T}, \end{aligned} \quad (10)$$

where we have defined

$$\Phi_\omega = z_f^* z_i e^{i(\omega + \mu)T} + \frac{iT}{2U} \omega^2 - \frac{1}{2} (|z_i|^2 + |z_f|^2).$$

Eq. (10) is an exact statement.

In order to contrast Eq. (10) with semiclassics, we write out the propagator in path integral notation [20]

$$K(z_f^*, z_i; T) = \int_{z(0)=z_i}^{z^*(T)=z_f^*} \mathcal{D}^2 z \exp \{ \Phi[z, z^*]/h \},$$

where $\Phi = \Gamma + S$,

$$\begin{aligned}\Gamma &= \frac{1}{2} [z_f^* z(T) + z^*(0) z_I - |z_f|^2 - |z_I|^2], \\ S &= \frac{1}{2} \int_0^T dt (z \dot{z}^* - z^* \dot{z}) - i \int_0^T dt \langle z | H | z \rangle.\end{aligned}$$

Performing the standard semiclassical analysis and algebra (see [20] and [19]) the semiclassical propagator takes the form

$$K_{\text{sc}}(z_f^*, z_i; T) = \sum_{\omega} \left(\frac{iT}{\hbar U} \right)^{1/2} \left(\frac{1}{\hbar} \frac{\partial^2 \Phi_{\omega}}{\partial \omega^2} \right)^{-1/2} \times \exp \left[\frac{1}{\hbar} \Phi_{\omega} + \frac{i}{2} (\omega + \mu) T - i\Delta \right], \quad (11)$$

where the sum is over solutions to the consistency equation given by $\frac{\partial \Phi_{\omega}}{\partial \omega} = 0$ or $\omega = -U z_f^* z_i e^{i(\omega + \mu)T}$, and we have defined $\Delta = \frac{1}{2}(\mu + 2\omega)T$. The term Δ comes from the fixing of the fluctuation determinant anomaly described in detail by Stone *et al.* [19] for the SU(2) case. However, if we try to get Eq. (11) by using the method of steepest descent on Eq. (10) with $\hbar \rightarrow 0$, we will not get the same result. This is because of what has been shown by others [20, 21]: that the semiclassics will give results consistent with the Weyl ordering of the Hamiltonian (naïvely ordering all a and a^\dagger 's symmetrically). The usual normal ordered Hamiltonian takes the form (inserting \hbar 's) $H = -\mu n + \frac{U}{2} n(n - \hbar)$ while the Weyl ordered Hamiltonian takes the form (up to a constant) $H_W = -\mu n + \frac{U}{2} n(n + \hbar)$. If we derive Eq. (10) for H_W , we will find the the steepest descent exactly agrees with Eq. (11) just as expected [20, 21].

While the semiclassical result is not a new one, it shows that the path integral is not dealing with the same Hamiltonian. Unfortunately, our exact calculation of \mathcal{Z}' (see Eq. (8)) suggests that the path integral is dealing with $H' = -\mu n + \frac{U}{2} n^2$ while semiclassics suggests it is dealing with $H_W = -\mu n + \frac{U}{2} n(n + 1)$ (going back to $\hbar = 1$). These two methods differ but both are not dealing with the Hamiltonian under consideration, Eq. (6). In the case of the Weyl ordered Hamiltonian, we can write our original Hamiltonian in Eq. (6) as $H = H_W - U n$ which is Weyl ordered (up to a constant). This ordering can be used to modify the path integral by an extra term: $-U|z|^2$. This correction to the path integral suggested by Weyl ordering does not fix the exact calculation of \mathcal{Z}' as can be easily shown, but it does motivate an *ad hoc* correction to the path integral to “fix” our exact calculation. We use the following action:

$$S = \int dt \left(-\mu |z|^2 + \frac{U}{2} |z|^2 (|z|^2 - 1) \right). \quad (12)$$

This action is constructed by just changing the operator n to a function $|z|^2$; while this gives correct results with the method which gives Eq. (8), there is no *a priori* reason to suspect this of being the action. Similarly, if in the spin-coherent state path integral, we replace the operator S_z with its expectation value $\langle \mathbf{n} | S_z | \mathbf{n} \rangle$ everywhere, we will get the correct result. This means, in particular, for $H = S_z^2$ that instead of $\langle S_z^2 \rangle$ in the spin-path integral we have $\langle S_z \rangle^2$. In general, if one substitutes the generators of the coherent states in the Hamiltonian with their expectation value, one obtains the correct result for \mathcal{Z} with the methods used to derive Eq. (3) and Eq. (8).

Corrections aside, a simple way to see what has gone wrong is to return to Eq. (5). This $H(x)$ function can not achieve the value 0, but $H = S_z^2$ clearly has such an eigenvalue. This is due to the fact that for higher dimensional representations of SU(2) not every eigenvector of S_z can be rotated into another with a standard SU(2) rotation. On the other hand, the coherent states we used are a complete set for even higher dimensional representations, so in principle, we should not lose any information about the $m = 0$ state. Continuity in \mathbf{n} seems to be the culprit: $H(x)$ came from a time discretized form (between time slices j and $j + 1$) $\langle \mathbf{n}_{j+1} | S_z^2 | \mathbf{n}_j \rangle$, and we have $\langle \mathbf{n} | S_z^2 | -\mathbf{n} \rangle = 0$, so $\langle \mathbf{n}_{j+1} | S_z^2 | \mathbf{n}_j \rangle$ can attain zero, but not for any paths that are “close” to each other (i.e. $\mathbf{n}_j \approx \mathbf{n}_{j+1}$) as the continuous time path integral assumes. As such, the discrete time path integral (before a continuity assumption is imposed) can unambiguously give the correct results to a calculation.

To conclude, in the time-continuous formulation of the path integral, neither the action suggested by Weyl-ordering nor the action constructed by normal ordering gives correct results when evaluating \mathcal{Z} via path integrals.

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