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LETTER TO THE EDITOR

Exactly soluble coherent state path integral with non-polynomial action

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Abstract. We present an example of an exactly soluble bosonic coherent state path integral with non-polynomial action.

Exact evaluation of path integrals is a separate branch of path integral science. The list of exactly soluble Feynman's path integrals in various coordinate spaces can be found in [1]. It was pointed out [2] that 'most systems for which Schrodinger's equation is exactly soluble¨ have been solved exactly by path integration'.

   In this letter we present an example of exact calculation of a coherent state path integral with non-polynomial action. This path integral is a partition function of a bosonic Hamiltonian originating from the problem of a single electron interacting with molecular phonons in a Holstein dimer. This problem contains the evaluation of the partition function over electron and phonon variables. The first step consists in the diagonalization of the initial Hamiltonian in electron subspace by means of the Fulton–Gouterman transformation [3,4]. This transformation of a Holstein dimer Hamiltonian with one electron leads to two pure bosonic problems. The corresponding path integral representation of partition function was investigated in [5]. The non-trivial part of the phonon problem is a path integral with nonpolynomial action:

$$Z_{\pm} = Z \, \mathrm{D}\bar{u} \, \mathrm{D}u \, \exp(S_{\pm}) \tag{1}$$

with action

$$S_{\pm} = -\int_0^{\beta} \left[\bar{u}\dot{u} + \omega\bar{u}u - \frac{g}{\sqrt{2}}(\bar{u}+u) \pm t \exp(-2\bar{u}u) \right] \mathrm{d}\tau \tag{2}$$

where ω is a phonon frequency, t is an electron hopping integral, g is an electron– phonon coupling and the paths $u, \bar{u}$ are subject to the periodic boundary conditions $\bar{u}(0) = u(\beta), u(0) = u(\beta)$. These actions correspond to the following Hamiltonians:

$$H^{(\pm)} = \omega u^+ u - \frac{g}{\sqrt{2}}(u^+ + u) \pm t\cos[-\pi u^+ u]$$

(3)

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The term $\exp(-2uu)^-$ in the action (2) corresponds to the operator $\cos[-\pi u^+ u]$ in (3) because we must represent the operator in normal form before replacing the creation and annihilation operators u^+ and u by trajectories u^- and u when we derive the action based upon a Hamiltonian.

These Hamiltonians describe the symmetric and antisymmetric states of an electron in the dimer with respect to phonon permutation symmetry [5]. The path integrals $Z_\pm$ have nontrivial character even at the limit $g = 0$ due to the highly nonlinear term $\exp(-2uu)^-$. In the present work we calculate exactly the path integrals (1), (2) for $g = 0$ based on time-sliced approximation.

We start with the following expansion of the action:

$$Z_+ = Z\,Du^-\,Du\,\exp\left[-\int_0^\beta (\bar{u}\dot{u} + \omega^- uu + te^{-2\bar{u}u})\,d\tau\right]$$
$$= \int D\bar{u}\,Du\,\sum_{n=0}^\infty \frac{(-t)^n}{n!}\left(\int_0^\beta e^{-2\bar{u}u}\,d\tau\right)^n\exp\left[-\int_0^\beta (\bar{u}\dot{u} + \omega\bar{u}u)\,d\tau\right]. \quad (4)$$

Equation (4) can be obtained on the basis of the N time-sliced approximation (see [6]), namely

$$Z^{(N)} = \sum_{n=0}^\infty Z_{(n)}^{(N)} = \sum_{n=0}^\infty \frac{(-t)^n}{n!}\int\prod_{m=0}^{N-1} d\mu_n\left[\sum_{l=0}^{N-1} e^{-2\bar{u}_{l+1}u_l}\cdot\frac{\beta}{N}\right]^n$$
$$\times\exp\left\{\sum_{m=0}^{N-1}(-|u_m|^2 + \bar{u}_{m+1}u_m(1-\beta\omega/N))\right\}. \quad (5)$$

Here the measure $d\mu_i = \frac{du_i\,d\bar{u}_i}{2\pi i}$ ____. In equation (4) the nth power of the exponential sum is as follows:

$$\left[\sum_{l=0}^{N-1} e^{-2\bar{u}_{l+1}u_l}\times\frac{\beta}{N}\right]^n = \sum_{n_0+n_1+\cdots+n_{N-1}=n} C(n_0, n_1, n_2, \ldots, n_{N-1})$$
$$\times(e^{-2\bar{u}_1 u_0})^{n_0}(e^{-2\bar{u}_2 u_1})^{n_1}\cdots(e^{-2\bar{u}_N u_{N-1}})^{n_{N-1}} \quad (6)$$

where

$$C(n_0, n_1, n_2, \ldots, n_{N-1}) = \binom{n}{n_0}\binom{n-n_0}{n_1}\binom{n-n_0-n_1}{n_2}\cdots\binom{n-n_0-\cdots-n_{N-2}}{n_{n-1}}$$
$$= \frac{n!}{n_0!n_1!\ldots(n-n_0-n_1-\cdots-n_{N-1})!}.$$

The number of terms in expansion equation (5) with the same set $\{n_i\}$ of summands in index of summation, $\{n_0, n_1, \ldots, n_{N-1}\}$ equals

$$W = N(N-1)\ldots(N-P)\times\frac{1}{q_1!\ q_2!\ldots q_m}. \qquad !$$

where P denotes the number of n_i ($n_i \neq 0$). In this expression the set $\{n_0, n_1, n_2, \ldots, n_{N-1}\}$ can be split into m subsets of equal n_i with the number q_j of coinciding elements in the jth subset.

To clarify this step, let us put fixed indices $n_1 = 0$ $n_3 = 8$, $N = 12$ into the series of equation (6) and choose the single summand as $(e^{-2u^- u})^3(e^{-2u^- u})^2(e^{-2u^- u})^3$. The corresponding coefficient

C is the product $\binom{8}{3} \times \binom{5}{2} \times \binom{3}{3}$. It should be noted that the following summands have the same structure, $(e_{-2u}\bar{}_{2u1})3(e_{-2u}\bar{}_{3u2})3(e_{-2u}\bar{}_{7u6})2$ or $(e_{-2u}\bar{}_{1u0})2(e_{-2u}\bar{}_{4u3})3(e_{-2u}\bar{}_{12u11})3$. The summands with an identical structure give an equal contribution to $Z^{(N)}$ in equation (5). In the example cited above the number of the summands with an identical structure equals

$W = 12 \times 11 \times 10 \times \frac{1}{2!}$. In the denominator of the latter equality the factorial 2! counts the number of the coinciding indices $n_i(= 3)$.

Let us bear in mind that we calculate the path integral as a limit $Z_+ = \lim_{N\to\infty} Z^{(N)}$. So, only the terms $\sim O(1)$ are essential, whereas the terms $\sim O(1/N)$ should be omitted. We must keep the factor $[\sum_{l=0}^{N-1} e^{-2\bar{u}_{l+1}u_l} \cdot \frac{\beta}{N}]^n$. Really, the denominator of the multiplier $\left(\frac{\beta}{N}\right)^n$ (equation (5)) can be cancelled only in the case where every summand equals unity, $n_i = 1$, in the index of summation of series equation (6). Only these terms should be kept in the series equation (6). As a result, in equation (5) each non-vanishing summand $Z_{(\stackrel{N}{n})}$ is the product of the n multipliers of the type $\exp(-|u_m|^2 + \bar{u}_{m+1}u_m(1 - \beta\omega/N) - 2\bar{u}_{m+1}u_m) = \exp(-|u_m|^2 + \bar{u}_{m+1}u_m(-1 - \beta\omega/N))$ and $N - n$ multipliers of the kind

$$\exp(-|u_m|^2 + \bar{u}_{m+1}u_m(1 - \beta\omega/N)).$$

In the corresponding Nth-multiple integral of equation (5) the non-vanishing terms contain the factor

$$\frac{(-t)^n}{n!} \left(\frac{\beta}{N}\right)^n n!N(N-1)\ldots(N-n+1) \times \frac{1}{n!}. \tag{7}$$

Integrations in equation (5) with respect to $\prod_{i=0}^{N-1} d\mu_i$ lead to the following expressions:

$$Z_n^{(N)} = \frac{(-\beta t)^n}{n!} \frac{1}{1 - (-1 - \frac{\beta\Omega}{N})^n(1 - \frac{\beta\Omega}{N})^{N-n}}. \tag{8}$$

In equation (8) the factor $\frac{(-\beta t)^n}{n!}$ appeares as a result of the limiting procedure. Under the same limit (N tends to infinity) the factor of equation (7) is equal to $\frac{(-\beta t)^n}{n!}$.

Putting equation (8) into the total partition function, equation (5), with a passage to the limit $N \to \infty$ in the whole expression one can get the final result

$$Z_+ = \lim_{N\to\infty} Z^{(N)} = \frac{\cosh\beta t}{1 \quad e^{-\beta\Omega}} - \frac{\sinh\beta t}{1 + e^{-\beta\Omega}} \quad _- \quad .$$

For the partition function Z_- the same sequence of calculations leads to

$$Z_-|_{g=0} = \frac{\cosh\beta t}{1 - \exp(-\beta\Omega)} + \frac{\sinh\beta t}{1 + \exp(-\beta\Omega)}.$$

At last, the total partition function is expressed as follows:

$$Z = Z_-|_{g=0} + Z_+|_{g=0} = \frac{2\cosh\beta t}{1 - \exp(-\beta\Omega)}.$$

So, we calculated the partition functions (1), (2) for the limiting case g = 0. Since the eigenvalues of the Hamiltonian, equation (3), for g = 0 are known,

$$E_n^\pm = \Omega n \pm (-1)^n \times t \qquad n = 0, 1, 2, \ldots$$

the partiton function can be easily calculated without the explicit use of path integration. The cited integration is of interest due to the fact that it presents a rare example of exactly calculable path integral with nonlinear action.

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