Path Integrals over Poisson Trajectories: Analytical and Numerical Estimates of Ground State Energies

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Abstract

The aim of this contribution is to demonstrate both a path integral method based on birth and death processes and a related numerical technique by applying them to a simple (but nontrivial) model of an electron in interaction with a boson field mode.

1 Introduction

Recently a path integral technique based on generalized Poisson processes has been introduced in [1,2]. The physical motivation is, that this technique seems to be useful to study models describing boson-boson interactions and electron-boson interactions. The method provides an analogue of the Feynman-Kac formula giving a solution of the (imaginary time) Schrödinger equation in the occupation number representation. The solution is obtained as a sum over paths of jump processes in the space of integers representing the occupation numbers of field modes.

Here, we demonstrate this method, together with a numerical technique based on it, by applying it to a simple model system. We derive analytical bounds on ground state energies in terms of path integrals over generalized

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Poisson processes and present numerical estimates of ground state energies by Monte-Carlo calculations.

The model we study may be regarded as a restricted version of the Fröhlich-Hamiltonian [7] where the electron interacts with only one mode of the lattice vibrations. This simplified model is also known as the symmetrical Gross' model [5,4]. For a review of the polaron problem, see [6].

2 The Model System

We consider the following Hamiltonian describing a non-relativistic electron in interaction with one mode of a quantized field:

$$\begin{aligned} H &= \tfrac{1}{2}p^2 + a_1{}^+a_1 + \lambda(a_1 e^{-ikx} + a_1{}^+e^{+ikx}) \\ &\quad + a_2{}^+a_2 + \lambda(a_2 e^{+ikx} + a_2{}^+e^{-ikx}) \end{aligned} \tag{1}$$

where x is the position of a non-relativistic electron, p is the conjugate momentum, $a_1{}^+, a_1$ and $a_2{}^+, a_2$ are the annihilation and creation operators for field modes (called phonons for simplicity from now on) of momentum k and $-k$, respectively; the frequency of the field modes has been set to 1, and the coupling constant λ may be taken to be real positive without loss of generality. Since the total momentum $q = p + k(a_1{}^+a_1 - a_2{}^+a_2)$ commutes with the Hamiltonian, we can unitarily transform H into

$$\begin{aligned} H' &= \tfrac{1}{2}(q - k(a_1{}^+a_1 - a_2{}^+a_2))^2 + a_1{}^+a_1 + a_2{}^+a_2 \\ &\quad + \lambda(a_1 + a_1{}^+ + a_2 + a_2{}^+) \end{aligned} \tag{2}$$

where q is now a c-number. Since we will be interested in the ground state energy of H we can restrict our considerations to the zero total momentum sector, and we will therefore only consider $q = 0$ in the following. With the methods of [1,2] we can then express the probability amplitude (in imaginary time) for the system to remain in the state with 0 phonons by the following probabilistic formula:

$$P(t) = \mathbf{E}[\delta_{0,N_1(t)}\delta_{0,N_2(t)} \exp\{-\frac{k^2}{2}\int_0^t (N_1(\tau) - N_2(\tau))^2\, d\tau + 2\lambda^2 t\}]. \tag{3}$$

The expectation is taken with respect to the birth and death processes N_i, $i = 1, 2$, associated with the phonon numbers in modes k and $-k$, respectively. For both processes N_i the probability rate of births is constant

and equal to λ^2 while the probability rate of deaths is equal to the phonon number $N_1(t)$ in mode k and $N_2(t)$ in mode $-k$, respectively. The processes all start in 0 at time 0. Furthermore, due to the product of Kronecker deltas appearing under the expectation, only trajectories ending in 0 contribute. Since the ground state energy of H' (in the $q = 0$ sector) is given by

$$E_0 = \lim_{t\to\infty} -\frac{1}{t} \ln P(t) \tag{4}$$

we will look for lower bounds of $P(t)$ in order to obtain upper bounds for E_0.

We remark that, since the integral $\int_0^t (N_1(\tau) - N_2(\tau))^2 \, d\tau$ in the exponential in (3) is positive, we immediately obtain

$$P(t) \leq e^{2\lambda^2 t} \mathbf{E}[\delta_{0,N_1(t)} \delta_{0,N_2(t)}] \tag{5}$$

and, since $\mathbf{E}[\delta_{0,N_1(t)} \delta_{0,N_2(t)}]$ tends to a constant, we have the trivial lower bound

$$E_0 \geq -2\lambda^2 \, . \tag{6}$$

3 Analytical Estimates

In this section we present a variational approach to our problem introducing appropriately chosen trial actions. After having performed a Radon-Nikodym derivative as shown in [2], $P(t)$ may be rewritten as an expectation with respect to two new processes N_i' :

$$\begin{aligned} P(t) = \mathbf{E}[\delta_{0,N_1'(t)} \delta_{0,N_2'(t)} \exp\{ & -\frac{k^2}{2} \int_0^t (N_1'(\tau) - N_2'(\tau))^2 \, d\tau \\ & - \int_0^t (N_1'(\tau) + N_2'(\tau)) \, d\tau \\ & + \int_0^t \left(\frac{\lambda^2}{A(N_1'(\tau)+1)} + \frac{\lambda^2}{A(N_2'(\tau)+1)} \right) d\tau \\ & + \int_0^t (A(N_1'(\tau))N_1'(\tau) + A(N_2'(\tau))N_2'(\tau)) \, d\tau \}] \end{aligned} \tag{7}$$

where the processes N_i' are identical and characterised by birth rates $\lambda^2/A(N_i'(t)+1)$ and death rates $A(N_i'(t))N_i'(t)$. The integrals containing $A(n)$ will serve as trial actions that we will adjust in order to estimate the ground state energy.

From (7), Jensen's inequality, the independence of the two processes and the fact, that an extra factor $\mathbf{E}[\delta_{0,N'(t)}]$ will disappear in the limit $t \to \infty$, we have, for any choice of the trial function $A(n)$,

$$E_0 \leq \lim_{t\to\infty} -\frac{2}{t}[-\frac{k^2}{2}\int_0^t (\langle N'^2(\tau)\rangle - \langle N'(\tau)\rangle^2)\,d\tau - \int_0^t \langle N'(\tau)\rangle\,d\tau + \int_0^t (\langle \frac{\lambda^2}{A(N'(\tau)+1)}\rangle + \langle A(N'(\tau))N'(\tau)\rangle)\,d\tau] \quad (8)$$

where N' is a process which is characterized by the same probability rates as N_1 and N_2, and where we made use of the definition

$$\frac{1}{t}\int_0^t \langle f(N'(\tau))\rangle\,d\tau \equiv \frac{1}{t}\int_0^t \frac{\mathbf{E}[f(N'(\tau))\delta_{0,N'(t)}]}{\mathbf{E}[\delta_{0,N'(t)}]}\,d\tau\,. \quad (9)$$

If the process N', which is identical to the processes N_i', possesses an equilibrium distribution, we can replace expression (9), in the limit $t \to \infty$, by the expectation value $\overline{f(N')} = \sum_{n=0}^{\infty} P_e(n)f(n)$ with respect to this equilibrium distribution where

$$P_e(n) \equiv \frac{(\lambda^2)^n}{n!\,\prod_{i=1}^n [A(i)]^2} \Big/ \sum_{n=0}^{\infty} \frac{(\lambda^2)^n}{n!\,\prod_{i=1}^n [A(i)]^2}\,. \quad (10)$$

Let us try, first, to estimate the elements of the sum in (8) with the help of a process-independent trial function, $A(n) \equiv A$. The process N' will then have a constant rate of birth λ^2/A and a death rate proportional to $AN'(t)$. It turns out that the best choice is $A = 1 + k^2/2$ which leads to

$$E_0 \leq -\frac{2\lambda^2}{1+\frac{k^2}{2}} \equiv F\,. \quad (11)$$

Note that, in this case, the equilibrium distribution is a Poisson distribution with parameter $\lambda^2/(1+\frac{k^2}{2})^2$.

Now, we want to use a different trial action which will give improved results when the process spends most of the time in the neighbourhood

of the 0-phonon configuration. This will be the case for small couplings which should be understood here in terms of $y \equiv \lambda^2/(1+\frac{k^2}{2})^2$. We set $A(n) = 1 + \frac{k^2}{2}n$ and obtain therefore from (8)

$$E_0 \leq -2\left(\frac{k^2}{2}\overline{N'}^2 + \lambda^2\overline{(1+\tfrac{k^2}{2}(N'+1))^{-1}}\right) \tag{12}$$

where the expectations are taken over the equilibrium distribution of a process N' which has birth rate $\lambda^2/(1+\frac{k^2}{2}(N'(t)))$ and death rate $(1+\frac{k^2}{2}(N'(t)+1))N'(t)$. The evaluation of the right hand side of this

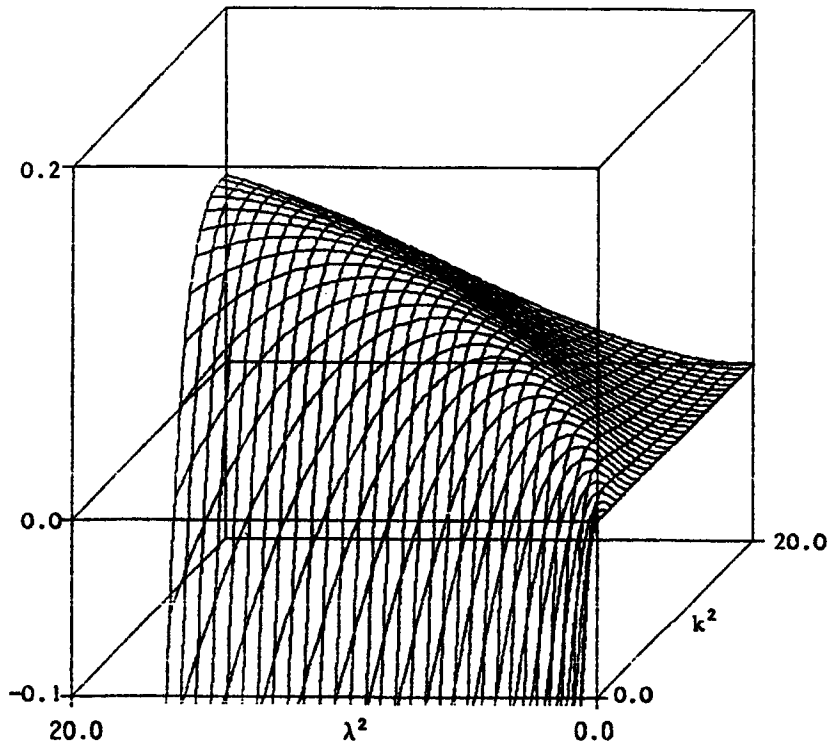

Figure 1: $F(\lambda^2, k^2) - G(\lambda^2, k^2)$
Comparison of the bounds F, eq. (11), and G, eq. (13); note that G improves F where $F - G \geq 0$.

expression is nontrivial; however, for small y, we do not loose much information by taking into account only those contributions to (12) which come from the equilibrium probabilities of the 0- and 1-phonon configurations.

Proceeding in this way, we arrive at the following, still exact, bound:

$$E_0 \leq -2\Big(\frac{k^2}{2}\frac{\lambda^4}{(1+\frac{k^2}{2})^4}\exp\{\frac{-2\lambda^2}{(1+\frac{k^2}{2})^2}\} + [\frac{\lambda^2}{(1+\frac{k^2}{2})} + \frac{\lambda^4}{(1+\frac{k^2}{2})^2(1+k^2)}]\exp\{\frac{-\lambda^2}{(1+\frac{k^2}{2})^2}\}\Big) \equiv G\,. \quad (13)$$

Expanding G in powers of y,

$$G = F - \frac{k^4}{2(1+k^2)}\frac{\lambda^4}{(1+k^2/2)^4} + \mathcal{O}((\frac{\lambda^2}{(1+k^2/2)^2})^3) \quad (14)$$

one realizes that G gives an improved bound for small y (see also figure 1). In order to obtain an estimate of the ground state energy E_0, we collect (11) and (13) into

$$E_0 \leq \min(F, G)\,. \quad (15)$$

Of course, different trial functions could be considered in order to obtain improved estimates for given coupling regions. We plan to investigate this possibility in a more systematic fashion. Here, we want to show other possibilities of our approach and go on to discuss our numerical results.

4 Numerical Results

The bounds on E_0 which where derived in Section 3 are based on the application of Jensen's inequality together with a variational procedure. We now want to improve these bounds by calculating directly the expression for $P(t)$ in eq. (7). Since it is impossible to evaluate the nonlinear functionals of the processes involved analytically, we will calculate the expectation values numerically by a direct Monte-Carlo method, i.e. as averages over realizations of paths of the processes. While this procedure can be applied to any choice of the trial function, obtaining in principle the same result, we will demonstrate the working of our numerical technique only in the case corresponding to the Jensen bound F.

Let us look again at equation (7). Using the process independent trial function $A(n) = 1 + k^2/2$ and evaluating the process independent integrals

we obtain (we drop the prime in the notation for the processes)

$$P(t) = \exp(\frac{2\lambda^2 t}{1+\frac{k^2}{2}})\mathbf{E}[\delta_{0,N_1(t)}\delta_{0,N_2(t)} \exp\{-\frac{k^2}{2}\int_0^t [(N_1(\tau)-N_2(\tau))^2-(N_1(\tau)+N_2(\tau))]\,d\tau\}] \quad (16)$$

and, hence, for the ground state energy

$$E_0 = F + \Delta E_0 \quad (17)$$

where

$$\Delta E_0 = -\lim_{t\to\infty}\frac{1}{t}\ln(\mathbf{E}[\delta_{0,N_1(t)}\delta_{0,N_2(t)} \exp\{-\frac{k^2}{2}\int_0^t [(N_1(\tau)-N_2(\tau))^2-(N_1(\tau)+N_2(\tau))]\,d\tau\}]) \quad (18)$$

gives the correction to the Jensen bound

$$F = -\frac{2\lambda^2}{1+\frac{k^2}{2}}\,. \quad (19)$$

In calculating ΔE_0 numerically we have to deal with finite times. To facilitate the following discussion, let us introduce some auxiliary notation:

$$\Delta\mathcal{E}(t) \equiv -\frac{1}{t}\ln(\mathbf{E}[\delta_{0,N_1(t)}\delta_{0,N_2(t)} \exp\{-\frac{k^2}{2}\int_0^t [(N_1(\tau)-N_2(\tau))^2-(N_1(\tau)+N_2(\tau))]\,d\tau\}]) \quad (20)$$

$$\mathcal{E}(t) \equiv F + \Delta\mathcal{E}(t)\,. \quad (21)$$

We now have to appeal to the quantum mechanical interpretation of $P(t)$ as the transition probability from the 0-phonon to the 0-phonon configuration to see that

$$\mathcal{E}(t) = E_0 - \frac{1}{t}\ln(\sum_{i=0}^{\infty}|\psi_i(0,0)|^2 e^{-(E_i-E_0)t}) \geq E_0 \;\; \forall t \in \mathbf{R}^+ \quad (22)$$

where $\psi_i(n,m)$ denote the energy eigenfunctions in the occupation number representation and E_i the corresponding energy values. Hence, we not only have

$$\Delta E_0 \;=\; \lim_{t\to\infty} \Delta\mathcal{E}(t) \tag{23}$$

but we obtain, for every finite t, a true bound on the ground state energy:

$$\Delta E_0 \;\leq\; \Delta\mathcal{E}(t)\;\; \forall t \in \mathbb{R}^+ \; . \tag{24}$$

This estimate may be improved upon using knowledge about the ground state wave function of the forced harmonic oscillator. However, we will then no longer obtain a true bound but an expression which will be closer to the actual ground state energy being only an approximate bound. Writing $\gamma = |\psi_0(0,0)|^2$, $\epsilon_i = E_i - E_0$, we have

$$\begin{aligned} E_0 \;&=\; \mathcal{E}(t) + \frac{1}{t}\ln(\gamma) + \frac{1}{t}\ln(1 + \frac{1}{\gamma}\sum_{i=1}^{\infty} |\psi_i(0,0)|^2 e^{-\epsilon_i t}) \\ &\leq\; \mathcal{E}(t) + \frac{1}{t}\ln(\gamma) + \frac{1}{t}\frac{1}{\gamma} e^{-\epsilon_1 t} \; . \end{aligned} \tag{25}$$

Neglecting the last term which is decaying fast and approximating γ by $|\Omega(0,0)|^2 = \exp(-2\lambda^2/(1+\frac{k^2}{2})^2)$, where $\Omega(n,m)$ is the ground state of the two uncoupled harmonic oscillators corresponding to the processes appearing in (16), we obtain a better estimate of ΔE_0. However, due to the uncontrolled approximations this is now, as anticipated, only an approximate bound:

$$\Delta E_0 \;\lesssim\; \Delta\mathcal{E}(t) - \frac{1}{t}\frac{2\lambda^2}{(1+\frac{k^2}{2})^2} \;\equiv\; \Delta\mathcal{E}^b(t) \; . \tag{26}$$

The t-dependent correction term will be important for small couplings where, indeed, $\psi_0(n,m)$ is very close to $\Omega(n,m)$.

The method we employ to evaluate $\Delta\mathcal{E}(t)$ numerically is a direct Monte-Carlo technique. Sample paths of the two processes are generated using the exponential distribution of waiting times between jumps and the integrals along paths are calculated. Averages over many realizations, observing the condition that both processes have to end at zero for the integrand to be nonvanishing, provide an estimate of $\Delta\mathcal{E}(t)$. Several independent repetitions of this procedure are performed in order to estimate the mean and the variation of this estimator.

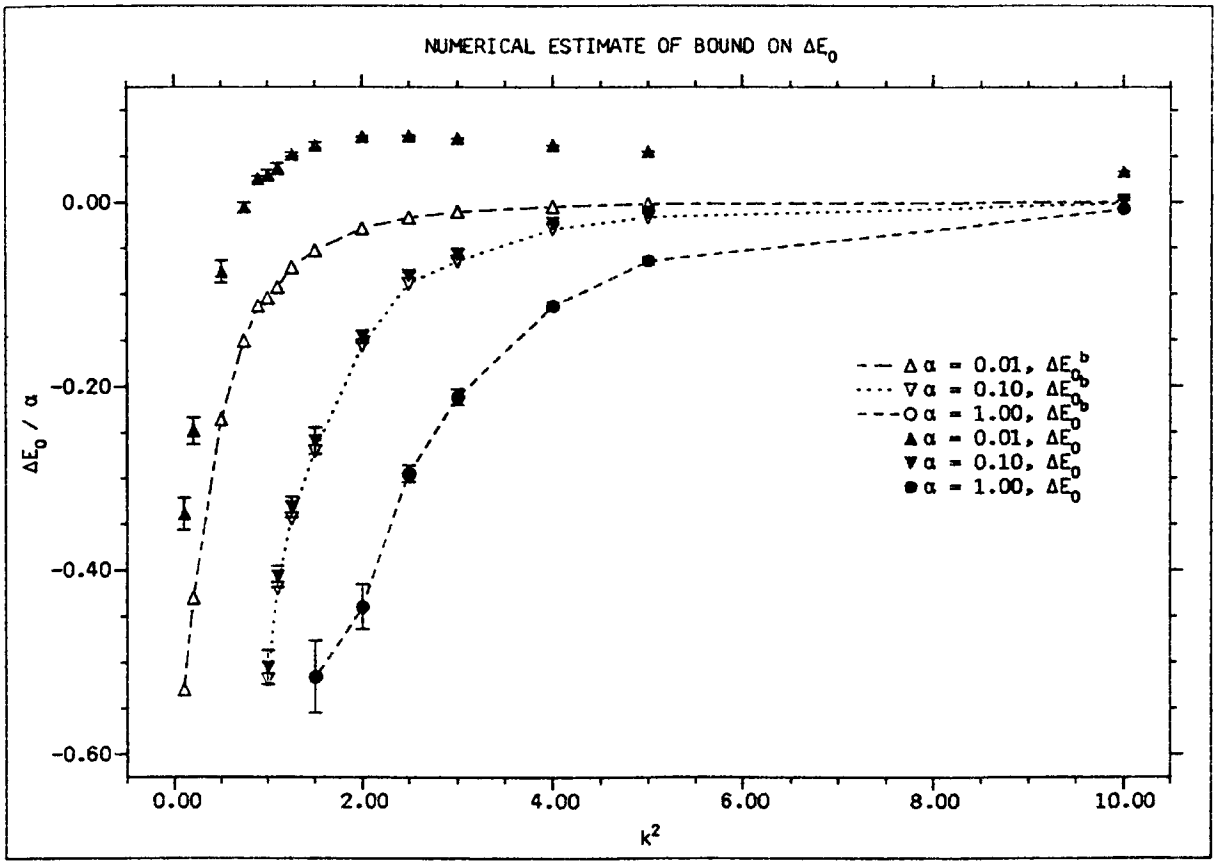

Figure 2: Monte-Carlo calculation of bound on ΔE_0

Results of Monte-Carlo calculation of bound on correction to Jensen bound (solid symbols, conf. eq. (24), denoted ΔE_0) and of approximate bound (open symbols, conf. eq. (26), denoted ΔE_0^b) for three values of the parameter α. The latter are obtained from the former by addition of the t-dependent correction term in (26). The energy axis is scaled by α. For $\alpha = 0.01$, the true bound gives, for most values of k^2, no improvement over the Jensen bound. For $\alpha = 1.0$, the correction term has no distinguishable effect at the scale of this plot. For clarity, error bars are drawn only with solid symbols, interpolating line segments only with open symbols. Error bars correspond to the mean error of the mean over 10 independent estimations of $\Delta\mathcal{E}(t)$.

We have calculated $\Delta\mathcal{E}(t)$ for a wide range of values of λ^2, k^2 and for different t. The latter is important because it is not clear from the theoretical considerations how one should balance length of the sample paths, i.e. time t, against number of realizations. We present here, in figure 2, a representative selection of results parametrized by $\alpha = \lambda^2 k^2/(2\sqrt{2}\pi)$. For each value of $k^2, \lambda^2(\alpha, k^2)$ the result shown corresponds to an average over 10 independent estimations of $\Delta\mathcal{E}(t)$, each comprising 1000 realizations of the trajectories of the processes N_1, N_2; the time t is chosen to be the same on a scale where t is proportional to the expected number of jumps of the processes. Hence, the results for the different parameter values all have 'the same statistics' in the sense that the same numerical effort went into one realization of the sample path. The statistical significance of the results is gauged by the mean error $s/\sqrt{n}$ of the average over the $n = 10$ independent estimations, where s denotes the standard deviation. Since the number of estimations is fixed for all parameter values one can also draw conclusions on the strength of the fluctuations of the processes as they influence the estimates of $\Delta\mathcal{E}(t)$.

Let us make a few remarks to assess the results of our numerical calculations. First, note that the type of convergence of a Monte-Carlo procedure is convergence in probability. Second, we are in a large deviation situation with a strongly fluctuating random variable of exponential type while the quantity of physical interest is obtained as its logarithm; hence, it is the variation in the estimates of $\Delta\mathcal{E}(t)$ itself which is of physical significance. Third, $\Delta\mathcal{E}(t)$ provides a bound on ΔE_0 which is improving with increasing t. On the other hand, the computational effort to construct a sample path of the processes is also increasing with t. Therefore, one has to balance, in the amount of computer time spent, the number of realizations of the processes, i.e. improved statistics, against the length of sample paths, i.e. principally better bounds. Finally, observe that we are calculating numerically only the correction to the Jensen bound F and that our Monte-Carlo procedure depends on an appropriate choice of the trial action. Both facts are aspects of what is called importance sampling in Monte-Carlo terminology: we have integrated out analytically a most important contribution, namely F, and our integration measure is concentrated on significant contributions of the remainder. In fact, the form of the integrand in equation (16) was motivated by the instability of Monte-Carlo calculations based on another choice of the trial action. A more thorough discussion of the numerical procedure and the results may be found in [3].

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