PERTURBATIVE RESULTS WITHOUT DIAGRAMS

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Higher-order perturbative calculations in Quantum (Field) Theory suffer from the factorial increase of the number of individual diagrams. Here I describe an approach which evaluates the total contribution numerically for finite temperature from the cumulant expansion of the corresponding observable followed by an extrapolation to zero temperature. This method (originally proposed by Bogolyubov and Plechko) is applied to the calculation of higher-order terms for the ground-state energy of the polaron. Using state-of-the-art multidimensional integration routines 2 new coefficients are obtained corresponding to a 4- and 5-loop calculation.

Keywords: high-order perturbative calculations, cumulant expansion, Monte-Carlo integration

1. Introduction

Highly accurate measurements require precise theoretical calculations which perturbation theory can yield if the coupling constant is small. However, in Quantum Field Theory (QFT) the number of diagrams grows factorially with the order of perturbation theory and they become more and more complicated. The prime example is the anomalous magnetic moment of the electron where new experiments\(^1\) need high-order quantum-electrodynamical calculations but the number of diagrams for them “explodes” as shown by the generating function\(^2\)

\[
\Gamma(\alpha) = 1 + \alpha + 7 \alpha^2 + 72 \alpha^3 + 891 \alpha^4 + 12672 \alpha^5 + 202770 \alpha^6 + \ldots\]  

There are ongoing efforts\(^3\) to calculate all 12672 diagrams in \(\mathcal{O}(\alpha^5)\) — a huge, heroic effort considering the complexity of individual diagrams and the large cancellations among them.

Obviously new and more efficient methods would be most welcome for a cross-check or further progress.
2. A new method (applied to the polaron g.s. energy)

Here I present a “new” method which – as I learned during the conference – was already proposed 20 years by Bogolyubov (Jr.) and Plechko (BP)⁴. However, to my knowledge it has been never applied numerically which turned out to be quite a challenging task.

The BP method is formulated for the polaron problem, a non-relativistic (but non-trivial) field theory describing an electron slowly moving through a polarizable crystal. Due to medium effects its energy is changed and it acquires an effective mass:

\[ E_p = E_0 + \frac{p^2}{2m^*} + \ldots \]

The aim is to calculate the power series expansion for the g.s. energy

\[ E_0(\alpha) = \sum_{n=1}^\infty e_n \alpha^n \]  \hspace{1cm} (2)

as function of the dimensionless electron-phonon coupling constant \( \alpha \). The lowest-order coefficients are well-known⁵ (\( e_1 = -1, \ e_2 = -0.01591962 \)) but since Smodyrev’s calculation⁶ in 1986

\[ e_3 = -0.00080607 \] \hspace{1cm} (3)

there has been no progress towards higher-order terms.

This will be remedied by the first numerical application of the BP method. For this purpose the path integral formulation of the polaron problem will be used where the phonons have been integrated out exactly⁷. For large Euclidean times \( \beta \) this gives the following effective action

\[ S_{\text{eff}}[x] = \int_0^\beta \frac{dt}{2} \dot{x}^2 - \frac{\alpha}{\sqrt{2}} \int_0^\beta dt \int_0^t dt' e^{-(t-t')} \int \frac{d^3k}{2\pi^2} \exp \left[ ik \cdot (x(t) - x(t')) \right] \] \hspace{1cm} (4)

which will be split into a free part \( S_0 \) and an interaction term \( S_1 \). The g.s. energy may be obtained from the partition function

\[ Z(\beta) = \int D^3x \ e^{-S_{\text{eff}}[x]} \ \xrightarrow{\beta \to \infty} \ e^{-\beta E_0} \] \hspace{1cm} (5)

at asymptotic values of \( \beta \), i.e. zero temperature. The central idea is to use the *cumulant expansion* of the partition function

\[ Z(\beta) = Z_0 \exp \left[ \sum_{n=1}^\infty \frac{(-\beta)^n}{n!} \lambda_n(\beta) \right] \] \hspace{1cm} (6)

where the \( \lambda_n(\beta) \)'s are the cumulants w.r.t. \( S_1 \). These are obtained from the *moments*

\[ m_n := \mathcal{N} \int D^3x \ (S_1[x])^n \ e^{-S_0[x]} \ , \ m_0 = 1 \] \hspace{1cm} (7)
by the recursion relation (see, e.g. Eq. (51) in Ref. 8)

\[ \lambda_{n+1} = m_{n+1} - \sum_{k=0}^{n-1} \binom{n}{k} \lambda_{k+1} m_{n-k} \] (8)

Explicitly the first cumulants read

\[ \lambda_1 = m_1 , \lambda_2 = m_2 - m_1^2 , \lambda_3 = m_3 - 3 m_2 m_1 + 2 m_1^3 \]
\[ \lambda_4 = m_4 - 4 m_3 m_1 - 3 m_2^2 + 12 m_2 m_1^2 - 6 m_1^4 \]
\[ \lambda_5 = m_5 - 5 m_4 m_1 - 10 m_3 m_2 + 20 m_3 m_1^2 + 30 m_2^2 m_1 - 60 m_2 m_1^3 + 24 m_1^5 \] (9)

By construction \( m_n \propto \alpha^n \) and Eq. (8) shows that the cumulants share this property. Thus we immediately obtain

\[ e_n = \lim_{\beta \to \infty} \frac{1}{\beta} \frac{(-\beta)^{n+1}}{\alpha^n n!} \lambda_n(\beta). \] (10)

The functional integral for the moments can be done since it is Gaussian. The integrals over the phonon momenta \( k_m, m = 1 \ldots n \) can also be performed if the \( m \)th propagator is written as

\[ \frac{1}{k_m^2} = \frac{1}{2} \int_0^\infty du_m \exp \left[ -\frac{1}{2} k_m^2 u_m \right]. \] (11)

Then one obtains

\[ m_n = \frac{(-\alpha^n)}{(4\pi)^{n/2}} \prod_{m=1}^n \left( \int_0^\beta dt_m \int_0^{t_m} dt_m' \int_0^\infty du_m \right) \exp \left[ - \sum_{m=1}^n (t_m - t_m') \right] \]
\[ \cdot \left( \det A(t_1 \ldots t_n, t_1' \ldots t_n'; u_1 \ldots u_n) \right)^{-3/2}. \] (12)

Here the \( (n \times n) \)- matrix \( A \)

\[ A_{ij} = \frac{1}{2} \left[ -|t_i - t_j| + |t_i - t_j'| + |t_i' - t_j| - |t_i' - t_j'| \right] + u_i \delta_{ij}. \] (13)

is non-analytic in the times \( t_i, t_i' \), but analytic in the auxiliary variables \( u_i \).

3. Numerical procedures and results

The task is now to perform the \( (3n) \)-dimensional integral over \( t_i, t_i', u_i \) for large enough \( \beta \) in the expression for the cumulants/moments. It is clear that any reduction in the dimensionality of the integral will greatly help in obtaining reliable numerical results in affordable CPU-time. A closer inspection of the structure of the integrand reveals that 2 integrations over
the auxiliary variables (say \( u_n, u_{n-1} \)) can always be done analytically. Furthermore, we do not use Eq. (10) to extract the energy coefficient \( e_n \) but

\[
e_n = \frac{(-1)^{n+1}}{\alpha^n n!} \lim_{\beta \to \infty} \frac{\partial \lambda_n(\beta)}{\partial \beta} =: \lim_{\beta \to \infty} e_n(\beta). \tag{14}
\]

This “kills two birds with one stone”: first the derivative w.r.t. \( \beta \) takes away one further integration over a time (see Eq. (12) where \( \beta \) appears as upper limit) requiring that only a \((3n - 3)\)-dimensional integral has to be done numerically. Second, it vastly improves the convergence to \( e_n \equiv e_n(\beta = \infty) \) because now

\[
e_n(\beta) \xrightarrow{\beta \to \infty} \frac{\partial}{\partial \beta} \left[ \beta \cdot e_n + \text{const} - \frac{a_n}{\sqrt{\beta}} e^{-\beta} + \ldots \right] = e_n + \frac{a_n}{\sqrt{\beta}} e^{-\beta} + \ldots. \tag{15}
\]

In other words: we obtain an exponential convergence to the value \( e_n \) whereas previously the approach would be very slow, like \( \text{const}/\beta \). This exponential convergence of the derivative version has been demonstrated analytically for \( n = 1, 2 \) and numerically for \( n = 3 \) (see below). In the following we will assume that it holds for all \( n \). After mapping to the hypercube \([0, 1]\) the remaining \((3n - 3)\)-dimensional integral can be evaluated by Monte-Carlo techniques utilizing the classic VEGAS program\(^9\) or the more modern programs from the CUBA library\(^10\).

We first have tested this approach by comparing with the analytical result given in Eq. (3). Fig. 1 shows \( e_3(\beta) \) and the best fit to the data.

![Fig. 1. (color online). Monte-Carlo results for the derivative of the 3rd cumulant as function of the Euclidean time \( \beta \). The total number of function calls is denoted by \( n_{\text{tot}} \) and the full (open) circles are the points used (not used) in the fit.](image-url)
assuming the $\beta$-dependence (15). Since the asymptotic behaviour is not valid for low values of $\beta$ we have eliminated small-$\beta$ points successively until the resulting $\chi^2$/dof of the fit reaches a minimum. Excellent agreement with Smodyrev’s result (3) is found. If one allows for a different power of $\beta$ in the prefactor of Eq. (15) then the fit gives an exponent $-0.55(3)$ instead of $-0.5$ assumed before.

However, when extending these calculations to the case $n = 4$ a very slow convergence of the numerical result with the number of function calls $n_{\text{tot}}$ is observed at fixed $\beta$. Fortunately, a solution was found by performing the remaining $(n - 2)$ $u_i$-integrations not by stochastic (Monte-Carlo) methods but by deterministic quadrature rules. This is possible since the $u_i$-dependence of the integrand is analytic (see Eq. (13)). We have used the very efficient “tanh-sinh-integration” method[11] but Gaussian quadrature is nearly as good. A dramatic improvement in stability results together with a reduction of $n_{\text{tot}}$ needed for the much smaller values of $|e_n|$, $n > 3$. This allows a reliable evaluation of $e_4$ (see Fig. 2 a) and also makes the determination of $e_5$ feasible as shown in Fig. 2 b.

Fig. 2. (a) Same as Fig. 1 but for the 4th cumulant. (b) Data for the derivative of the 5th cumulant. Open triangles denote results (not used in the fit) which have a $\chi^2 > 1.5$ indicating that successive Monte-Carlo iterations are not consistent with each other.

The best fit values for $e_4$ and $e_5$ displayed in Figs. 2 a, b are still preliminary as a more detailed error analysis has to be made. Also for the $n = 5$ case the Monte-Carlo statistics should be improved. Note that each high-statistic point in Fig. 2 b took about 30 days runtime on a Xeon 3.0 GHz machine.
4. Summary and Outlook

- Two additional perturbative coefficients $e_4, e_5$ for the polaron g.s.
  energy have been determined by the method of Bogolyubov and
  Plechkov (rediscovered independently). This amounts to performing
  a 4-loop and 5-loop calculation in Quantum Field Theory.
- The method is based on a combination of Monte-Carlo integration
  techniques and deterministic quadrature rules for finite $\beta$ (tem-
  perature) and on a judicious extrapolation to $\beta \to \infty$ (zero tem-
  perature). As a check the value of $e_3$ calculated analytically by
  Smolyrev has been reproduced with high accuracy.
- The cancellation in $n^{th}$ order is not among many individual dia-
  grams but among the much fewer terms in the integrand of the
  $(3n-3)$-dimensional integral (see Eq. (9)).
- The method can be simply extended to the calculation of higher-
  order terms in the small-coupling expansion of the effective mass
  $m^*(\alpha)$ for a moving polaron.
- Generalizing this approach to relativistic QFT in the world line
  representation and calculation of higher-order terms for the
  anomalous magnetic moment of the electron is under investiga-
  tion. New challenges arise from the divergences which now occur
  and the need for renormalization.

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