

Perturbative Results Without Diagrams

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1. Introduction

Usually in perturbative calculation in Quantum (Field) Theory the number of diagrams grows factorially with the order

Example: number of diagrams for g-2 of the electron in QED (see Itzykson & Zuber p. 466, 467)

$$\Gamma(\alpha) = \frac{4z(1-S)}{S^3}, S = -2z \left[1 + \frac{K'_0(z)}{K_0(z)}\right], z = -\frac{1}{4\alpha}$$

expand in powers of $\alpha = 1/137.036$

 $\implies \Gamma(\alpha) = 1 + \alpha + 7 \alpha^{2} + 72 \alpha^{3} + 891 \alpha^{4} + 12672 \alpha^{5} + 202770 \alpha^{6} + \dots$

Consequence: huge cancellations between individual diagrams

heroic efforts needed for higher-order calculations Schwinger (1948), Petermann, Sommerfield (1957) Laporta & Remiddi (1996), Kinoshita et al. (1990-2005)

Need (more modestly: would be nice to have) new methods !



2. A new method (applied to the polaron g. s. energy)

Take as simple (but nontrivial) example the **polaron** problem – a non-relativistic field theory

polaron = electron slowly moving through polarizable crystal

model Hamiltonian H. Fröhlich (1954)

$$\widehat{H} \sim \frac{1}{2}\widehat{\mathbf{p}}^2 + \sum_k \widehat{a}_k^{\dagger} \widehat{a}_k + \sqrt{\alpha} \sum_k \frac{1}{|\mathbf{k}|} \left[\widehat{a}_k^{\dagger} e^{-i\mathbf{k}\cdot\widehat{\mathbf{x}}} + h.c. \right]$$

 α : dimensionless electron-phonon coupling constant

Ground-state energy of polaron:

$$E_0 := \sum_{n=1}^{\infty} \mathbf{e_n} \, \alpha^n \, , \, \mathbf{e_1} = -1$$

$$\mathbf{e_2} = -0.01591962 \, (1959) \, , \, \mathbf{e_3} = -0.00080607 \, \text{Smondyrev} \, (1986)$$



In field-theoretic language: have to evaluate self-energy diagrams with more and more loops

Long live the PATH INTEGRAL : phonons can be integrated out exactly! Feynman (1955)

$$Z(\beta) = \oint \mathcal{D}^3 x \, e^{-S_{\text{eff}}} \stackrel{\beta \to \infty}{\longrightarrow} e^{-\beta E_0}$$

where for large β

$$\Rightarrow S_{\text{eff}}[x] \sim \int_0^\beta dt \, \frac{1}{2} \dot{\mathbf{x}}^2 + \alpha \int_0^\beta dt_1 dt_2 \, e^{-|t_1 - t_2|} \, \int d^3k \, \frac{1}{\mathbf{k}^2} \exp\left[i\mathbf{k} \cdot (\mathbf{x}(t_1) - \mathbf{x}(t_2))\right] =: S_0 + S_1$$



Employ cumulant expansion of partition function

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

where $\lambda_n(\beta)$ are the cumulants w.r.t. S_1

Recursion relation with the moments $m_n(\beta) \equiv \langle S_1^n \rangle \propto \alpha^n$

$$\lambda_{n+1} = m_{n+1} - \sum_{k=0}^{n-1} {n \choose k} \lambda_{k+1} m_{n-k}$$

$$\lambda_{1} = m_{1}$$

$$\lambda_{2} = m_{2} - m_{1}^{2}$$

$$\lambda_{3} = m_{3} - 3m_{2}m_{1} + 2m_{1}^{3}$$

$$\lambda_{4} = m_{4} - 4m_{3}m_{1} - 3m_{2}^{2} + 12m_{2}m_{1}^{2} - 6m_{1}^{4}$$

$$\lambda_{5} = m_{5} - 5m_{4}m_{1} - 10m_{3}m_{2} + 20m_{3}m_{1}^{2} + 30m_{2}^{2}m_{1} - 60m_{2}m_{1}^{3} + 24m_{1}^{5}$$

$$\vdots$$

Note: $\lambda_n(\beta) \propto \alpha^n \implies \mathbf{e_n} = \lim_{\beta \to \infty} \frac{1}{\beta} \frac{(-)^{n+1}}{\alpha^n n!} \lambda_n(\beta)$



The path integral for the moments

$$m_n = C \oint \mathcal{D}^3 x \, S_1^n \, e^{-S_0[x]} , m_0 = 1$$

can be evaluated exactly. Write Coulomb propagator as

$$\frac{1}{\mathbf{k}^2} = \frac{1}{2} \int_0^\infty du \, \exp\left[-\frac{1}{2}\mathbf{k}^2 u\right]$$

 \implies all momentum integrations can be performed and one obtains

$$m_{n} = (-)^{n} \frac{\alpha^{n}}{(4\pi)^{n/2}} \prod_{m=1}^{n} \left(\int_{0}^{\beta} dt_{m} \int_{0}^{t_{m}} dt'_{m} \int_{0}^{\infty} du_{m} \right) \exp \left[-\sum_{m=1}^{n} (t_{m} - t'_{m}) \right] \\ \cdot \left[\det \mathbf{A} \left(t_{1} \dots t_{n}, t'_{1} \dots t'_{n}; u_{1} \dots u_{n} \right) \right]^{-3/2}$$

with $(n \times n)$ - matrix **A**



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Define

$$\mathbf{A}_{ij} =: \mathbf{a}_{ij} + u_i \,\delta_{ij}$$

Diagonal parts: $\mathbf{a}_{ii} = t_i - t'_i \equiv \sigma_i$

Non-diagonal matrix elements :



$$S := \frac{1}{2} \left(t_i + t'_i - (t_j + t'_j) \right)$$

$$r := \frac{1}{2} \left(\sigma_i - \sigma_j \right)$$

$$s := \frac{1}{2} \left(\sigma_i + \sigma_j \right)$$



3. Numerical procedures and results

For $m_n(\beta) \Rightarrow \lambda_n(\beta)$ one has to do a 3n-dimensional integral over t_i, t'_i, u_i Two u_i -integrations can be done analytically

$$\int_{0}^{\infty} du_n \det_n^{-3/2} A(1, 2, \dots, n) = \frac{2}{A_n \sqrt{\det_n A(u_n = 0)}}$$
$$\int_{0}^{\infty} du_{n-1} \int_{0}^{\infty} du_n \det_n^{-3/2} A(1, 2, \dots, n) = \frac{4}{\sqrt{A_{n-1,n} A_{n-1} A_n}} \frac{\arcsin \sqrt{x_{HF}}}{\sqrt{x_{HF}}}$$

where $A_n, A_{n-1}, A_{n-1,n}$ are **principal minors** of the determinant det_n $A \equiv A$

$$0 \leq x_{HF} := 1 - \frac{A_{n-1,n}A}{A_{n-1}A_n} \leq 1$$

because A_{ij} is a **positive semi-definite** matrix \implies Hadamard-Fischer inequality $A_{n-1}A_n \ge A_{n-1,n}A$

After performing u_n, u_{n-1} -integrations analytically

 \implies (3n-2)-dimensional integral left



Useful trick: calculate directly $\frac{\partial \lambda_n}{\partial \beta} \Longrightarrow$ (3n – 3)-dimensional integral !

Further advantage: asymptotic behaviour (thus extrapolation to $\beta \to \infty$) is much improved:

$$\mathbf{e}_{\mathbf{n}}(\boldsymbol{\beta}) := \frac{(-)^{n+1}}{\boldsymbol{\alpha}^{n} n!} \frac{\partial \lambda_{n}}{\partial \boldsymbol{\beta}} = \frac{\partial}{\partial \boldsymbol{\beta}} \left[\boldsymbol{\beta} \cdot \mathbf{e}_{\mathbf{n}} + \mathbf{c} \mathbf{\boldsymbol{\beta}} \mathbf{\boldsymbol{\beta}} \mathbf{\boldsymbol{\beta}} - \dots \right] \xrightarrow{\boldsymbol{\beta} \to \infty} \mathbf{e}_{\mathbf{n}} - \frac{a_{n}}{\sqrt{\boldsymbol{\beta}}} e^{-\boldsymbol{\beta}} \left(\boldsymbol{\beta} \right) + \dots$$

Exponential convergence to e_n : analytically proved for n = 1, 2

numerically for n = 3:

assume $\mathbf{e_n}(\beta) \rightarrow \mathbf{e_n} - a_n \, \beta^{-\kappa_n} \, e^{-\beta}$

fit to Monte-Carlo data gives $\kappa_3 = 0.55(3)$

Assume it also for $n > 3 \dots$



Numerical evaluation:

mapping to hypercube $\left[0,1\right]$, then:

Monte-Carlo integration

with **VEGAS** program or routines from the **CUBA** library

Note: Monte-Carlo integration can handle non-analytic,

even discontinous integrands



check n = 3 (6-dimensional integral):



analytical: $e_3 = -0.80607005 \cdot 10^{-3}$

but for n = 4 convergence is slow with number of function calls:



solution: perform the (n-2) remaining u_i -integrations by deterministic integration routine. Very efficient: **tanh-sinh-method** !







now for n = 4:





and also n = 5 (evaluation of (9+3)-dim. integral) is within reach:

Here tanh-sinh-integration seems to be slightly better than Gauss-Legendre









4. Summary

- Two additional perturbative coefficients e_4 , e_5 for the polaron g.s. energy have been determined by a new (mostly) numerical method. This amounts to performing a **4-loop** and **5-loop** calculation in Quantum Field Theory
- Method is based on a combination of **Monte-Carlo integration** techniques and deterministic **quadrature rules** for finite β (temperature) and on judicious extrapolation to $\beta \rightarrow \infty$ (zero temperature). Reproduces Smondyrev's coefficient e_3 with high accuracy
- Cancellation in nth order **not** among many individual diagrams but among much fewer terms in the integrand of the (3n 3)-dimensional integral
- Increased **computational power** would allow to improve accuracy for e_4 , e_5 and even e_6 seems accessible
- Application to **g-2 of the electron** under investigation (worldline representation of QED). Challenge: renormalization !?



5. Outlook: application to worldline QED

Generating functional

$$Z[\bar{\eta},\eta,j] = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi\mathcal{D}A \exp\left\{iS[\bar{\psi},\psi,A] + (\bar{\psi},\eta) + (\bar{\eta},\psi) + (j,A)\right\}$$
$$S[\bar{\psi},\psi,A] = \left(\bar{\psi},\left[\gamma \cdot (\underbrace{i\partial - eA}_{\equiv \Pi}) - M_0\right]\psi\right) + S_0[A]$$

2-point function:



result in momentum space : (Alexandrou, RR & Schreiber, PR A 59 (1999))

$$G_2(p) \sim \int_0^\infty dT \int d\chi \, e^{-i(M_0^2 T + M_0 \chi)} \int d^4 x \, e^{-ip \cdot x} \int \mathcal{D}A \, e^{iS_0[A]} \int \mathcal{D}^4 x \int \mathcal{D}^4 \zeta \, e^{iS[x,\zeta,\chi,A]} \Big|_{\Gamma \to \gamma}$$

orbital trajectory : x(0) = 0, x(T) = x

spin trajectory : $\zeta(0) + \zeta(T) = \Gamma$

$$S[x,\zeta,\chi,A] \sim \int_0^T dt \left(-\frac{1}{2} \dot{x}^2 + i\zeta \cdot \dot{\zeta} + \dot{x} \cdot \zeta \chi - e \, \dot{x} \cdot A - ie \, \zeta \cdot F \cdot \zeta \right)$$

$$\uparrow \qquad \uparrow \qquad \uparrow \qquad \uparrow$$

spin-orbit convection spin current

Photon field A can be integrated out exactly \implies effective action



In supersymmetric formulation: $t \rightarrow t, \theta$

2-point function

$$G_2(p) \sim \int_0^\infty d\mathbf{T} \int d\boldsymbol{\chi} \, \exp\left[i A(p, \boldsymbol{\Gamma}, \mathbf{T}) + i B(p, \boldsymbol{\Gamma}, \mathbf{T}) \, \boldsymbol{\chi}\right]$$

develops pole at $\gamma \cdot p = M_{\text{phys}}$ if for large T

$$\begin{array}{rcl} A(p, \Gamma, \mathbf{T}) & \longrightarrow & \left(p^2 - M_{\mathsf{phys}}^2 \right) \mathbf{T} \\ B(p, \Gamma, \mathbf{T}) & \longrightarrow & Z_2 \left(p \cdot \Gamma + M_{\mathsf{phys}} \right) \end{array}$$

Determine M_{phys} and wavefunction renorm. Z_2 – similar to polaron case !

From 3-point function $\langle \psi \bar{\psi} A \rangle$: electron-photon coupling, i.e. anomalous magnetic moment of electron