The Linear Delta Expansion and the Anharmonic Oscillator

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Plan of Talk

1. Shortcomings of Perturbation Theory

2. Linear Delta Expansion

3. LDE in [0] \((\int e^{-gx^4} dx)\)

4. LDE in [1] (AHO)

5. AHO Wave Function
1. Shortcomings of Perturbation Theory

(a)

- Conv\textsuperscript{\textit{n}L} perturb\textsuperscript{\textit{n}} series = Taylor series in \( g \)

- \( \therefore \) cannot produce non-analytic behaviour, such as \( \sqrt{g} \)

- Can't reproduce instanton-like behaviour like \( e^{-c/g^2} \). Taylor expansion \( \equiv 0! \)
(b)

- Even if series exists, only applicable for weak coupling

- In QFT running coupling constant is large at low energies

(c)

- Even for \( g \ll 1 \), perturbation series is asymptotic rather than convergent
Note:

In context of functional $\int$ formula of QFT, problem arises $\therefore$ expansion of integrand in

$$\int [d\varphi] \exp(-g S_{\text{int}}[\varphi])$$

not uniformly convergent. Hence interchange of $\Sigma$ and $\int$ not justified$^\dagger$

$^\dagger$S. A. Pernice and G. Oleaga, 
2. Linear Delta Expansion

Essential idea

AHO ($\phi^4$ theory in [1]):

$$H = \frac{1}{2}(p^2 + m^2 x^2) + g x^4 = H_0 + H_1 \quad (2.1)$$

Normal perturbation theory = expansion in $H_1$, i.e. $g$, giving an asymptotic series. E.g., expansion for ground-state energy is $E_0 = \sum c_n g^n$, where$^\dagger$

$$c_n \sim (-1)^{n+1} \frac{\sqrt{6}}{\pi^{3/2}} 3^n \Gamma(n + 1/2)$$

$^\dagger$C. M. Bender and T. T. Wu, *Phys. Rev.* D7 (1973) 1620
In above, split between $H_0$ and $H_I$ is fixed once and for all. Essence of LDE is that split changes (in an appropriate way) with the expansion order.

In particular, can add an additional mass term to $H_0$ and subtract it from $H_I$, to obtain

$$H_\delta = \frac{1}{2}(p^2 + \mu^2 x^2) + \delta(gx^4 - \lambda x^2) = H'_0 + H'_I \quad (2.2)$$

where $\mu^2 = m^2 + 2\lambda$, and $\delta$ is a dummy book-keeping parameter, to be set equal to 1 at end.

For $\delta \neq 1$, $H_\delta$ depends on parameter $\lambda$, which does not appear in original Hamiltonian $H$. Exact calculation with $H_{\delta=1}$ would not depend on $\lambda$, but any truncated expansion will contain a residual $\lambda$ dependence.
So how to fix $\lambda$? Most frequently used criterion is the Principle of Minimal Sensitivity (PMS)†:

$$\frac{\partial R_N}{\partial \lambda} = 0,$$

where $R_N = N$th-order expansion of some quantity $R$. This mimics, at least locally, independence of exact result on $\lambda$

†P. M. Stevenson, 
N.B. This makes $\lambda$ order-dependent:

$$\lambda = \lambda_N$$

This is crucial property that can give a convergent sequence. For *fixed* $\lambda$, expansion will share bad properties of perturbation theory.
Problems with PMS:

(i) No justification, other than “reasonableness”

(ii) May $\exists$ several stationary points. How to distinguish between them?

Partial answers:

(i) in some simple cases, can prove that PMS guarantees convergence

(ii) choose broadest maximum/minimum
3. LDE in [0] ($\int e^{-gx^4} \, dx$)

[0] analogue of $\varphi^4$ fn $\int$ is

$$Z \equiv \int_{-\infty}^{\infty} e^{-\frac{1}{2}m^2x^2-gx^4} \, dx \quad (2.1)$$

N.B. For $m = 0$, $Z = \frac{\Gamma(1/4)}{(2g^{1/4})}$. Non-analytic, \therefore no Taylor series!

Tackle this case, and define

$$Z(\delta) = \int_{-\infty}^{\infty} e^{-\lambda x^2+\delta(\lambda x^2-gx^4)} \, dx$$

$$= \int_{-\infty}^{\infty} dx e^{-\lambda x^2} \sum_{n=0}^{\infty} \frac{\delta^n}{n!} (\lambda x^2 - gx^4)^n \quad (2.2)$$

$$= \sum_{n} c_n(\lambda)\delta^n$$
(i) How does method give correct non-analytic behaviour in $g$?
Well, $\therefore$ PMS.
E.g. 1st-order result is

$$Z_1(\delta) = \sqrt{\frac{\pi}{\lambda}} \left[ 1 + \delta \left( \frac{1}{2} - \frac{3g}{4\lambda^2} \right) \right]$$

For fixed $\lambda$ this is a polynomial in $g$

But PMS cond$^n$ sets $\lambda = \lambda_1 = (5g/2)^{1/2}$, and then

$$Z_1 = \frac{6}{5} \left( \frac{2\pi^2}{5g} \right)^{1/4}$$
(ii) Again, for fixed $\lambda$, large-$n$ behaviour of $c_n$ is

$$c_n \sim (-1)^n \frac{g^n e^{-n}}{\lambda^{2n+1/2}} 4^n n^{n-1/2}$$

Alternates in sign and grows like $n^{n-1/2}$

But with PMS, divergence tamed by growth of $\lambda_n$

(iii) Very instructive to plot $Z_N(\lambda)$ against $\lambda$ for odd $N$ [$\not\exists$ soln of PMS cond^n for even $N$]
Note:

(i) \( \exists \) single maximum, which is less than the true value. Can prove this

(ii) \( \text{Pos}^n \) of maximum, \( \lambda_N \), increases with \( N \) (as \( \sqrt{N} \)). Max gets broader as \( N \) increases

(iii) For fixed \( \lambda \), as \( N \) increases \( Z_N(\lambda) \) eventually diverges, tending to \( -\infty \).

Turns out that maximum increases monotonically to true answer. Can show that error \( R_N := Z - Z_N(\lambda_N) \sim e^{-\#N} \)
Coefficients

What does PMS do to coefficients?

- for fixed $\lambda$, $c_n \sim (-gn)^n$ at large $n$ (saddle-point method/recursion relations)

- but for $\lambda = \lambda_N$, $c_n$ all have same sign, and decrease rapidly up to $n = N$ (bad behaviour occurs for $n > N$)
\( N = 11 \)

\[
\begin{array}{cccc}
\hline
\mathcal{C}_N & \lambda = 1 & \lambda = \lambda_{11} \\
\hline
\mathcal{C}_1 & -0.4 & 0.4025 \\
\mathcal{C}_2 & 3.1 & 0.2395 \\
\mathcal{C}_3 & -27.1 & 0.1395 \\
\mathcal{C}_4 & 336.6 & 0.0756 \\
\mathcal{C}_5 & -5498.6 & 0.0376 \\
\mathcal{C}_6 & 111471.8 & 0.0171 \\
\mathcal{C}_7 & -2700994.1 & 0.0072 \\
\mathcal{C}_8 & 76166358.6 & 0.0028 \\
\mathcal{C}_9 & \ldots & 0.0010 \\
\mathcal{C}_{10} & \ldots & 0.0003 \\
\mathcal{C}_{11} & \ldots & 0.0001 \\
\hline
\end{array}
\]
Convergence

Proof of convergence, using saddle-point methods

(i) Bound on $Z_N$

Easy to show that $Z_N < Z$ for $N$ odd, but not for $N$ even

Thus

$$Z_N = \int dx \, e^{-\lambda x^2} \left\{ e^{(\lambda x^2 - gx^4)} \right\}_N,$$

where $\{\ldots\}_N$ means series truncated at $N$th term

†I. R. C. Buckley, A. Duncan and HFJ, 
Rewrite as

\[ Z_N = \int dx \ e^{-gx^4} e^{-(\lambda x^2-gx^4)} \left\{ e^{(\lambda x^2-gx^4)} \right\}_N \]

\[ = \int dx \ e^{-gx^4} \Theta_N(z), \quad (2.3) \]

where

\[ \Theta_N(z) := e^{-z} \left\{ e^z \right\}_N \]
Graph shows that for \( N \) odd \( \Theta_N(z) \leq 1 \):
Can prove this by considering $d\Theta_N/dz$, to which only last term contributes:

$$\frac{d\Theta_N}{dz} = -\frac{z^N}{N!}e^{-z}$$  \hspace{1cm} (2.4)

∴ $Z_N(\lambda) < Z$ for all $\lambda$, and PMS max is best you can do
(ii) Estimate of $\lambda_N$

Eq. (2.4) involves only last term in series. \therefore\ can estimate $\lambda_N$ for large $N$, by saddle-point methods

Thus

$$\frac{dZ_N(\lambda)}{d\lambda} = -\frac{1}{N!} \int dx \ e^{-\frac{\lambda}{2}x^2}x^2(\lambda x^2 - gx^4)^N$$

For large $N$, integrand looks like:
For \( \lambda_N \) need two contributions to cancel. This gives

\[
\lambda_N = \left( \frac{2Ng}{\sinh \beta} \right)^{1/2} \propto \sqrt{N},
\]

where \( \beta = 1.199678\ldots \) is solution to \( \beta = \coth \beta \).

(iii) Estimate of error \( R_N \)

Error is

\[
R_N := Z - Z_N(\lambda) = \int dx \ e^{-gx^4} (1 - \Theta_N(z))
\]

\( \int \) Eq. (2.4) from 0 to \( z \), to get

\[
1 - \Theta_N(z) = \frac{(\text{sign } z)^{N+1}}{N!} \int_{0}^{\mid z \mid} d\omega \omega^N e^{-\omega(\text{sign } z)}
\]
Integral splits into two regions:

\[ A \equiv 0 \leq x \leq \sqrt{\lambda/g} \], where \( z > 0 \), and

\[ B \equiv \sqrt{\lambda/g} \leq x \], where \( z < 0 \)

Writing \( R_N = A_N + B_N \), and bounding each \( \int \) separately, can show that

\[
R_N < \frac{2}{N!} \int_0^{\infty} dx \ e^{-\lambda x^2} (\lambda x^2 - gx^4)^{N+1}
\]

\[ = (N + 1)c_{N+1} \]
\( c_{N+1} \) easily estimated by saddle-point integration for large \( N \), giving bound

\[
R_N < c N^{1/4} e^{-N/\sinh \beta} \approx c N^{1/4} e^{-0.663N}
\]

\[\therefore\] we have a convergent sequence of approximants, whose error decreases exponentially with \( N \)

**N.B.** We do not obtain a series in the conventional sense, because when \( N \) increases by 1, not only do we add an additional term, but we modify the already existing terms (\( \therefore \lambda \rightarrow \lambda_N \))
4. LDE in [1] - AHO

Direct analogue of Eq. (2.1) is partition function for AHO:

\[
Z \equiv \sum_{r=0}^{\infty} e^{-\beta E_r}
\]

\[
= \frac{1}{Z_0} \int_{x(\beta) = x(0)} \left[ dx \right] e^{-\int_0^{\beta} \mathcal{L}(x(\tau)) d\tau}
\]  

(4.1)

1st form good for numerical calculations

2nd form good for proof of convergence on similar (but much more complicated) lines to proof in [0]
(i) Numerics

Numerical evaln of Eq. (4.1) proceeds by first calculating energy levels \( E_r \) and then performing sum (truncated at some suitably large value of \( r \))

Equation to be solved, as an expansion in \( \delta \), is

\[
\left[ \frac{1}{2} \left( -\frac{\partial^2}{\partial x^2} + \mu^2 x^2 \right) + \delta(gx^4 - \lambda x^2) \right] \psi = E\psi \tag{4.2}
\]

where \( \mu^2 = m^2 + 2\lambda \)

**N.B.** Usual R-S perturbation method very cumbersome, but if \( V \) is polynomial, high orders in perturbation theory can be generated very efficiently using *recursion relations*, as first noted by Bender and Wu
First scale variables:
\[
\begin{align*}
  x &= y/\sqrt{\mu} \\
  g &= \mu^3 \tilde{g} \\
  \lambda &= g \bar{\lambda}/\mu \\
  E &= \mu \tilde{E}
\end{align*}
\]

so that Schrödinger equation becomes

\[
\left[-\frac{1}{2} \frac{d^2}{dy^2} + \frac{1}{2} y^2 + \delta \tilde{g}(y^4 - \bar{\lambda}y^2)\right] \psi = \tilde{E}_n \psi
\]

Writing \( \psi = e^{-y^2/2} \varphi \), get

\[-\varphi'' + 2y \varphi' + \varphi + 2\delta \tilde{g}y^2(y^2 - \bar{\lambda}) \varphi = 2\tilde{E} \varphi
\]

Substituting \( \tilde{E} = \sum e_n \delta^n \) and \( \varphi = \sum \varphi_n \delta^n \) gives (for \( n \geq 1 \))
\[-\varphi''_n + 2y\varphi'_n + 2\tilde{g}y^2(y^2 - \tilde{\lambda})\varphi_{n-1} = 2 \sum_{\ell=0}^{n-1} e_{n-\ell}\varphi_{\ell}.\]

Finally, consistent to take \(\varphi_n = \sum_{p=0}^{4n} a_{n,p}y^p\). This gives recursion relation

\[
a_{n,p} = \frac{1}{2p} \left[ (p+1)(p+2)a_{n,p} + 2 - 2\tilde{g}a_{n-1,p-4} + 2\tilde{g}\tilde{\lambda}a_{n-1,p-2} - 2 \sum_{\ell=0}^{n-1} a_{n-\ell,2} a_{\ell,p} \right]
\]

together with rel^n

\[e_n = -a_{n,2}\]
Can readily be solved using any recursive language (e.g. Mathematica, C++). Results very similar in general properties to [0] case. We\textsuperscript{†} were able to go to order $N = 75$ !

\textsuperscript{†}A. Duncan and HFJ, 
*Phys. Rev.* **D47** (1993) 2560
Numerically (corroborated by saddle-point estimates) we find

\[ \lambda_N \sim \sqrt{N}, \quad \text{while } R_N \sim e^{-cN^{2/3}} \]
(ii) Convergence

Again main tool is Eq. (2.5) for $1 - \Theta_N(z)$, applied to $\text{fn}^\ell \int$

$$Z = \frac{1}{Z_0} \int_{x(\beta) = x(0)} [dx] e^{-S_0 - \delta(S - S_0)}$$

with

$$S_0 = \int_0^\beta \frac{1}{2}(\ddot{x}^2 + \mu^2 x^2) d\tau$$

$$S = \int_0^\beta \left[ \frac{1}{2}(\ddot{x}^2 + m^2 x^2) + gx^4 \right] d\tau$$

Two regions $\mathcal{A} (S < S_0)$, and $\mathcal{B} (S > S_0)$ again have to be treated separately.
Saddle-point configuration in $\mathcal{A}$ is a constant configuration, giving
\[ A_N \sim \# N^{5/6} e^{-cN^{2/3}/\beta} \] (4.3)

while that in $\mathcal{B}$ is a localized instanton, giving
\[ B_N \sim \# N^{4/3} e^{-NS(\lambda)} \]

PMS value is obtained by finding $\lambda$ such that two behaviours match, giving an overall error
\[ R_N \sim \# e^{-cN^{2/3}} \]
But, factor of $1/\beta$ in exponent of (4.3) ⇒ can't take $\beta \to \infty$, essentially ∴ in QFT $Z$ is generator of all vacuum diagrams, including disconnected ones

Problem does not occur for $W \equiv \ln Z$, generator of connected vacuum diagrams

However, expansion for $W$ does not obey $W_N < W$, so $\nexists$ unique PMS point. Nonetheless, proof of convergence with appropriate scaling can be constructed in both zero† and one‡ dimensions

†C. M. Bender, A. Duncan and HFJ, *Phys. Rev.* D49 (1994) 4219
‡C. Arvanitis, HFJ and C. S. Parker *Phys. Rev.* D52 (1995) 3704
Completely different approach, using dispersion relations for $E(g)$, has been used by Guida et al.\textsuperscript{†} to prove convergence of LDE for the energy levels (with a suitable scaling instead of PMS)

\textsuperscript{†}R. Guida, K. Konishi and H. Suzuki
5. AHO Wave-Function

Get convergence for $E_n$, but WF is still of form $\psi = e^{-\mu x^2/2} \varphi$, where $\varphi$ is a polynomial

This is completely wrong: from Schrödinger eq

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + \frac{1}{2} m^2 x^2 + gx^4 \right] \psi = E_n \psi$$

should have $\psi \propto e^{-\gamma |x|^3}$ asymptotically, where $\gamma = (2g)^{1/2}/3$

How to remedy this? - Strong PMS! †

$$\frac{\partial}{\partial \mu} \psi(x; \mu) = 0 \quad \text{for each } x$$

† T. Hatsuda, T. Kumihiro and T. Tanaka

This means that $\mu$ becomes a function of $x$

Geometrically, strong PMS cond $\nabla$ $\frac{\partial}{\partial \mu} \psi(x; \mu) = 0$
defines envelope of series of curves given by $\psi(x; \mu)$

Simplest example is hyperbola $y = 1/x$, obtained as envelope of its tangents $y = (2\mu - x)/\mu$
To first order, WF obtained from R-S pert\textsuperscript{h} th\textsuperscript{y} is

\[
\psi = \left\{ 1 - \delta \left[ \frac{m^2 - \mu^2}{8\mu^2} (2z^2 - 1) + \frac{g}{8\mu^3} (2z^4 + 6z^2 - 9/2) \right] \right\} e^{-z^2/2}
\]

where \( z = x\sqrt{\mu} \)

Solving \( \partial \psi / \partial \mu = 0 \) gives 2 branches for \( \mu(x) \) (\( m = 1, g = 1/2 \))
Green one is sensible one, giving envelope
Superimposed on individual WFs:

Asymptotic behaviour of envelope $\Psi(x)$ is

$$\Psi(x) \sim \exp(-\frac{1}{2}|x|^3) \ (\text{vs.} \ \exp(-\frac{\sqrt{2}}{3}|x|^3))$$
Another idea\textsuperscript{†}:

Write $\psi = \exp\left(-\frac{1}{2}\mu x^2 - \gamma |x|^3\right)\varphi$, to enforce correct asymptotic behaviour.

Then eq\textsuperscript{n} for $\varphi$ is

$$\varphi'' - 2\mu x \varphi' + (2E - \mu)\varphi = 6\gamma x^2 \varphi' + \left(-6\gamma \mu x^3 + (m^2 - \mu^2)x^2 + 6\gamma x\right) \varphi$$

- Multiply RHS by $\delta$ and do a $\delta$ exp\textsuperscript{n}
- Start with $\varphi^{(0)} = 1$
- In any order $\varphi$ is a polynomial in $x$
- Fix $\mu_N$ by standard PMS: $\partial E_N/\partial \mu = 0$

\textsuperscript{†}P. Amore, A. Aranda and A. De Pace

Get excellent results† (more accurate than standard LDE (N=47))

But no proof of convergence

†P. Amore et al.
5. **Summary**

LDE gives a convergent sequence of approximants for

- $Z, W \equiv \log Z$ in $[0]$

- $Z, W, E$ in QM

Generalizations of LDE give

- good approximations for WF

- faster convergence