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880.05 Lecture 3

Handouts:

a. Plots of errors for model partition function approximations
b. Problem Set #1
c. (online) MATLAB matrix documentation

Logistics:

- The first problem set is just intended to reinforce some basics of matrices and some topics from the first few lectures.
- Comment on Zinn-Justin excerpt and other handouts: you are not supposed to understand all this before class! It is a supplement; it would just be helpful to look at before class (and then revisit parts later)

Recap:

- Last time we looked at solving a (not too) many-body problem by expanding the many-body wave function in a convenient basis.
  - Solving the eigenvalue problem is equivalent to finding the variationally best set of coefficients.
  - We can use a nonorthogonal basis (like gaussians of different widths) by solving the generalized eigenvalue problem.
  - The SVM approach uses such a basis.
- We will want to return to the idea of expanding in an orthonormal basis, $|\varphi_i\rangle, \{i=1,2,\ldots\infty\}$ with $\langle\varphi_j|\varphi_i\rangle = 1$.
  - For example, harmonic oscillator wave functions.

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Plan for today:

· The more general plan is to cast our many-body calculations in the form of equilibrium thermodynamics using statistical mechanics. (We'll come back and consider the response of a system to a time-dependent perturbation.) This means evaluating partition functions in the presence of external "sources" that are the analog of applied magnetic fields. We'll evaluate these partition functions in terms of (very large-dimensional) multiple integrals

$\Rightarrow$ These will be our path integrals.

- We'll see the connection to the "sum-over-all-paths" idea originated by Feynman.
- We will have in mind actual numerical calculations of the path integrals, so we think about them by making continuous space and time discrete and infinities become finite. (At least much of the time!)
- By casting the problem in terms of integrals, we can take advantage of experience in approximating integrals; to see the connection we will explore repeatedly a very simple integral that illustrates many of the techniques we will use.
- The pedagogic strategy is to toss out many ideas in analog form and then return repeatedly to them — which is called a "spiral" approach — adding detail and generalizing or applying to new problems.

· To get started we review some basic thermodynamics and statistical mechanics, as in the excerpt handout from Fetter and Walecka, with an added important point from the Morse handout.

- Note that notations for thermodynamic functions and variables can differ in textbooks and the literature! You just need to get used to switching back and forth.

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Recall that there are three "ensembles":

i) microcanonical : fixed E and N

ii) canonical: system exchanges <u>energy</u> with a heat bath
$\Rightarrow$ fixed N and fixed average E

Probability of system having E is $\boxed{\propto e^{-E/k_BT} = e^{-\beta E}}$ $\beta \equiv \frac{1}{k_BT}$

iii) grand canonical: system exchanges energy <u>and</u> particles with heat/particle bath. Neither N nor E is fixed.
Probability of system having E and N is
$$\boxed{\propto e^{-(E-\mu N)/k_BT} = e^{-\beta(E-\mu N)}}$$

- The grand canonical ensemble will be the most <u>natural</u> to calculate with many-body path integrals.
  - If we have a very large number of particles, then the differences between the ensembles is negligible (e.g. $\propto \frac{1}{\sqrt{N}}$)
  - For some physical phenomena such as superfluidity, this is actual a physical feature of the system.
  - But we also have to think about systems like finite nuclei, helium drops, or metallic clusters where N is not so large. In these cases, using a grand canonical treatment can make errors that are too large to neglect.
  - This is a current issue in nuclear structure physics, where pairing (as in "Cooper pairs") is an important contribution to the ground state energy of some nuclei that have order 100 particles. Dealing with this consistently in a density functional theory approach, which we will introduce later in terms of path integral "effective actions", is a topic of active investigation (maybe you will come up with a good idea!).

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- To define the grand partition function, we need a complete set of states that are eigenstates of energy E and particle number N: $\boxed{\hat{H}|N\,j\rangle = E|N\,j\rangle}$ and $\boxed{\hat{N}|N\,j\rangle = N|N\,j\rangle}$
  - given N, we'll use j to enumerate all of the different states with N particles. (So really j should have an N label as well). We treat this as a discrete set.
  - The energy of the j^{th} state with N is labeled E_j.
  - Then the grand partition function Z_G is

$$\boxed{Z_G \equiv \sum_N \sum_j e^{-\beta(E_j - \mu N)}}$$

with μ the chemical potential.

- The key connection to thermodynamics is that

$$\boxed{\Omega(T,V,\mu) = -\frac{1}{\beta}\ln Z_G}$$

(V is volume ⇒ we always keep it finite at least until the end of a calculation)

where Ω is the thermodynamic potential.

- Let's recall the laundry list of thermodynamic variables and functions

intensive variables: T P μ $\mathcal{H}$ ← magnetic field ...

extensive variables: S V N $\mathcal{M}$ ← magnetization ← paramagnet ⇒ $\mathcal{M} = \mu_0 V \chi \mathcal{H}$ ← induced magnetic moment

taken to be extensive here

(Note: we're assuming one component systems, so a single chemical potential)

energy $E = E(S,V,N)$

Helmholtz free energy $F = F(T,V,N)$ · minimized for a mechanically isolated system at constant T

Gibbs free energy $G(T,P,N)$ · equilibrium at constant T and P when minimized

* thermodynamic potential $\Omega(T,V,\mu)$

- Note that we can consider μ in different ways, e.g. as a Lagrange multiplier. Or, as something analogous to $\mathcal{H}$: a source that changes a property of the system ($\mathcal{M}$ or N respectively). We will later consider them to be space (time) dependent!

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- The First Law of Thermodynamics specifies how the internal energy (called U in the Moore excerpt) changes when the independent variables change:

$$\boxed{dE = TdS - PdV + \mu dN}$$

- with a magnetic field, we would add $\mathcal{H}\, d\mathcal{M}$ and so on with other sources.

← work done to line up atomic moments

This implies

$$\boxed{T = \left(\frac{\partial E}{\partial S}\right)_{V,N,\mathcal{M}};\ P = -\left(\frac{\partial E}{\partial V}\right)_{S,N,\mathcal{M}};\ \mu = \left(\frac{\partial E}{\partial N}\right)_{S,V,\mathcal{M}};\ \mathcal{H} = \left(\frac{\partial E}{\partial \mathcal{M}}\right)_{S,V,N}}$$

- At $T=0$ in the ground state, $S=0 \Rightarrow \boxed{\mu \overset{T=0}{=} \left(\frac{\partial E}{\partial N}\right)_V}$

- We perform <u>Legendre transformations</u> to obtain the other thermodynamic functions from E
  $\Rightarrow$ change the independent variables.
  - This is usually motivated by what variables are under control in an experimental process.
  - We'll want to do a functional generalization later to derive DFT and to have functionals that are better to approximate (stay tuned!). The generalization is that the variables will depend on space-time.

$$\boxed{F = E - \left(\frac{\partial E}{\partial S}\right)_{V,N} S = E - TS} \Rightarrow \boxed{dF = dE - TdS - SdT = -SdT - PdV + \mu dN}$$

$$\boxed{G = F + PV = E - TS + PV \Rightarrow dG = -SdT + VdP + \mu dN}$$

$$\boxed{\Omega = F - \mu N = E - TS - \mu N \Rightarrow d\Omega = -SdT - PdV - Nd\mu}$$

so that

try these →

$$\boxed{S = \left(-\frac{\partial \Omega}{\partial T}\right)_{V\mu}} \quad \boxed{P = -\left(\frac{\partial \Omega}{\partial V}\right)_{T\mu}} \quad \boxed{N = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{TV}}$$

* In more detail, to switch from $E(S)$ to $F(T)$, we first construct $T(S) = \left(\frac{\partial E}{\partial S}\right)_{V,N} S$ and then <u>invert</u> this equation to find $S(T)$. Then we use this function to construct $F(T) = E(S(T)) - TS(T)$. (with V,N dependence suppressed).

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• Now consider $\boxed{P = -\left(\frac{\partial \Omega}{\partial V}\right)_{T,\mu}}$

• T and μ are both intensive but V and Ω are extensive. So if we double the size of the system, T and μ are unchanged but Ω and V both double. Thus,

$\Omega = (\text{const.})V$ with (const) independent of V

• Then $P = -\frac{\partial \Omega}{\partial V}$ implies $\boxed{\Omega = -PV}$ or $\boxed{P = -\Omega/V}$

• Since $\boxed{\Omega = E - TS - \mu N = -PV} \Rightarrow \boxed{E = TS - PV + \mu N}$

and $\boxed{F = -PV + \mu N}$ $\boxed{G = \mu N}$

• The idea that quantities like the energy should be "size extensive" is an important one for finite systems treated with the type of basis expansion of the wave function we considered last time. It turns out that some apparently reasonable approximations violate this property.

• Another way to see the result for E is to make a scale change by $\lambda = 1 + \eta$ with η infinitesimal (ie really small so $\eta^2 \lll \eta$).

All extensive quantities ⇒ λ * extensive

$\Rightarrow \boxed{\lambda E = E(\lambda S, \lambda V, \lambda N)}$

or Taylor expanding

$$\boxed{(1+\eta)E = E + \eta S\left(\frac{\partial E}{\partial S}\right)_{V,N} + \eta V\left(\frac{\partial E}{\partial V}\right)_{S,N} + \eta N\left(\frac{\partial E}{\partial N}\right)_{S,V}}$$

which yields $\boxed{E = ST + V(-P) + N\mu = TS - PV + \mu N}$ as above.

• Check: How would you go from $E(\mathcal{M})$ to $\Gamma(\mathcal{H})$? (with N, V, S still)

What is Γ in terms of the other variables?

ans: $\Gamma = E - \left(\frac{\partial E}{\partial \mathcal{M}}\right)_{S,V,N}\mathcal{M} = E - \mathcal{H}\mathcal{M}$, $d\Gamma = TdS - PdV + \mu dN - \mathcal{M}\,d\mathcal{H}$.

$= TS - PV + \mu N - \mathcal{H}\mathcal{M}$

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- So we see that we can find all the equilibrium many-body thermodynamics if we know $\Omega(T,V,\mu)$.

- Back to the partition function and a more general expansion:

$$\boxed{\begin{aligned} Z_G &= \sum_N \sum_j e^{-\beta(E_j-\mu N)} \\ &= \sum_N \sum_j \langle N_j | e^{-\beta(\hat{H}-\mu\hat{N})} | N_j \rangle \\ &= \mathrm{Tr}\left(e^{-\beta(\hat{H}-\mu\hat{N})}\right) = e^{-\beta\Omega(T,V,\mu)} \end{aligned}}$$

since diagonal in this basis

now think of this as a big matrix (finite, because we truncate the sums in practice)

- Question: Is $\langle a | e^{-\beta\hat{H}} | b \rangle \stackrel{?}{=} e^{-\beta\langle a|\hat{H}|b\rangle}$ for fixed general $|a\rangle, |b\rangle$?

ans: No, it only works if $|a\rangle, |b\rangle$ are eigenstates of $\hat{H}$ and also that $|a\rangle = |b\rangle$. We can see the failure by doing the Taylor expansion on both sides

- Recall some properties of traces.

If $\underline{A}$ is real, symmetric, and positive definite, then there is an orthogonal transformation $\underline{\underline{O}}$ that diagonalizes $\underline{A}$:

$$\boxed{\underline{\underline{O}}\,\underline{\underline{A}}\,\underline{\underline{O}}^T = \underline{\underline{A}}_D = \begin{pmatrix} a_1 & & 0 \\ & \ddots & \\ 0 & & a_n \end{pmatrix}} \quad \text{where } \boxed{\underline{\underline{O}}\,\underline{\underline{O}}^T = \underline{\underline{I}}} \quad \boxed{\det \underline{\underline{O}} = 1}$$

eigenvalues

$$\Rightarrow \mathrm{Tr}\,\underline{A} = \mathrm{Tr}(\underline{\underline{O}}^T\underline{\underline{O}}\,\underline{A}) = \mathrm{Tr}(\underline{\underline{O}}\,\underline{A}\,\underline{\underline{O}}^T) = \mathrm{Tr}(A_D) = \sum \text{eigenvalues}.$$

cyclic property of trace

(How you construct $\underline{\underline{O}}$: See PS#1 for a MATLAB reminder!)

- But this holds for any orthogonal (or unitary, more generally) transformation, which corresponds to a change of <u>basis</u>

* $\Rightarrow$ the final expression above holds for the trace over any complete basis $\Rightarrow$ much more general than where we started.

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Let's explore this last expression a bit more:

- What happens as $T \to 0$? Then $\beta \to \infty$ and we project out the ground state (only it survives the trace) and $-\frac{1}{\beta}\ln Z_G \to E - \mu N$ where E is the ground-state energy

- The ensemble average or expectation value of an operator is

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}(\hat{O}\, e^{-\beta(\hat{H}-\mu\hat{N})})}{\mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})}} = \frac{1}{Z_G}\mathrm{Tr}(\hat{O}\, e^{-\beta(\hat{H}-\mu\hat{N})})$$

we'll use this idea

- For example: $\hat{O} = \hat{N}$

$$\boxed{\langle \hat{N} \rangle = \frac{\mathrm{Tr}(\hat{N} e^{-\beta(\hat{H}-\mu\hat{N})})}{\mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})}} = \frac{\frac{1}{\beta}\frac{\partial}{\partial\mu}\mathrm{Tr}(e^{-\beta(\hat{H}-\mu\hat{N})})}{\mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})}} = \frac{1}{\beta}\frac{1}{Z_G}\frac{\partial Z_G}{\partial\mu} = \frac{1}{\beta}\frac{\partial}{\partial\mu}\ln Z_G}$$

Check: $\ln Z_G = -\beta\Omega \Rightarrow \langle \hat{N} \rangle = -\frac{1}{\beta}\frac{\partial}{\partial\mu}\beta\Omega = -\frac{\partial\Omega}{\partial\mu} = N$ ✓

- Make sure this is clear: we will be doing many similar manipulations!
  - Note that we could take $\hat{H} \to \hat{H} + \alpha\hat{O}$ and solve this problem as a function of α. Then $\langle \hat{O} \rangle_\alpha = -\frac{1}{\beta}\frac{\partial}{\partial\alpha}\ln Z_G$ and then we could take $\alpha \to 0$.

- So why not just evaluate $\mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})}$ numerically in a convenient basis? This only works in very limited cases:
  - i) The matrices are small, so that we can calculate the exponential numerically (e.g. in MATLAB). This is too small for many-body problems of interest.
  - ii) Take the trace in the basis that diagonalizes $\hat{H} - \mu\hat{N}$. Fine, but if we could do this, we would already have solved our problem!
  - iii) If β is very small. Otherwise it becomes impractical (or impossible) to evaluate the exponential.

Case iii) is the only reasonable one, but we don't want just small β (indeed, for the ground state we want to take $\beta \to \infty$!).

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· The strategy is then to use the observation that we could divide β into a large number M of pieces of size $\varepsilon \Rightarrow \beta = M\varepsilon$, which lets us write (let $\hat{H} - \mu\hat{N} \equiv \hat{H}'$)

$$\mathrm{Tr}\, e^{-\beta\hat{H}'} = \mathrm{Tr}\big(\underbrace{e^{-\epsilon\hat{H}'} e^{-\epsilon\hat{H}'} \cdots e^{-\epsilon H'}}_{M \text{ copies}}\big)$$

· If $\varepsilon \equiv \epsilon$ is small enough, we can truncate the expansion of each exponential $e^{-\epsilon\hat{H}'} \doteq 1 - \epsilon\hat{H}' + \ldots$ and we can separate $\hat{H}'$ into kinetic and potential parts if desired.

· We can insert complete sets of states between each copy, evaluate $\hat{H}'$ (details depend on what kind of path integral we are evaluating), and then re-exponentiate. [This works because ϵ is small so that $e^{-\epsilon(T+V)} \doteq e^{-\epsilon T} e^{-\epsilon V}$ or $e^{-\frac{\epsilon}{2}T} e^{-\epsilon V} e^{-\epsilon\frac{T}{2}}$ works since the $[T, V]$ extra pieces are small $O(\epsilon)$ or $O(\epsilon^2)$ corrections]

· The complete set would be position and momentum states if we are doing one particle quantum mechanics or the many-body generalizations, or could be states appropriate for field theory (later!).

· So we'll have full integrals as we step from $0 \cdot \epsilon$ to $M\varepsilon$ and the exponent will look like a discretized integral over τ from 0 to β. Imaginary time! [Note: τ is just the conventional label for this parameter]. This is our path integral — as you can tell from the choices of states inserted and whether $\hat{H}'$ is in first or second quantization, we'll get different looking path integrals.

A transition amplitude from t_i to t_f would result in a real-time path integral with the same manipulations.

· Note that the trace will mean there is a boundary condition relating $\tau = 0$ and $\tau = \beta$.

· We'll fill in details later. For now we want to reduce to a very simple limiting model, that still enables us to exhibit many of the approximations and manipulations we will do with our full path integrals.

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Model Partition Function

- Our model partition function is just an integral:

$$\boxed{Z = \int d\xi \, e^{-f(\xi)}}$$

- We can think of this as a classical partition function for a particle in a potential, with $\xi \to x$ and $f \to V$:

$$Z = \int dx \, e^{-V(x)}$$ as Negele and Orland do (Section 2.1)

or imagine that ξ is a field variable at one discrete lattice site that doesn't couple at all to other sites. (I.e. f is like the action.)

- Let's think about analogs to EFT.
  - At low energies we will have an expansion of f that here takes the form of a Taylor expansion:

  $$f(\xi) = f(0) + \xi f'(0) + \frac{\xi^2}{2} f''(0) + \ldots$$

  - Now suppose the physics tells us there is a symmetry under $\xi \to -\xi$, meaning Z should be unchanged.
    $\Rightarrow$ only the even terms in $f(\xi)$ contribute.
  - The constant $f(0)$ just gives an overall normalization that is additive to $\ln Z$ and thus doesn't change physics, so we can write a general expansion up to quartic order as

$$Z_\lambda = \int_{-\infty}^{\infty} \frac{d\xi}{\sqrt{2\pi/a}} \, e^{-\frac{a\xi^2}{2} - \frac{\lambda}{4}\xi^4}$$

[Note: Mathematica can do this integral in terms of Bessel functions.]

where we follow N+O in choosing the limits and notation.

- We've called this Z_λ because we plan to investigate approximations as a function of λ.
- We could rescale ξ to get rid of a, but we'll keep it because it serves as the analog of what will eventually be identified as an inverse propagator. Also, we want to consider both $a>0$ and $a<0$.

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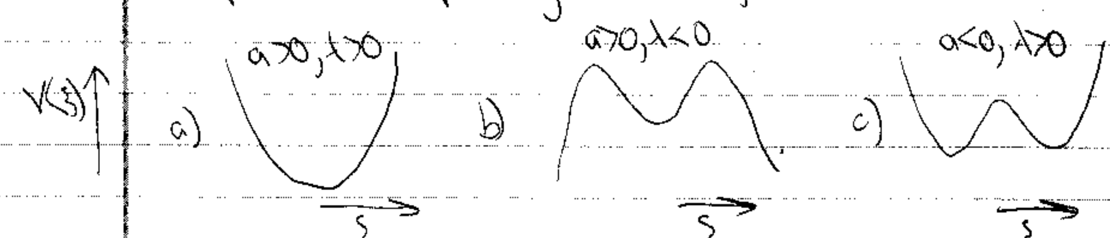
- The quadratic term is analogous to what will be the kinetic term + one-body potential like a trap (although it is just a harmonic potential here). A correction term would be a ξ^6 term, for example. We need a "power counting" that estimates its contribution to tell us we can neglect it at low enough energy. $\frac{\lambda}{4}\xi^4$ is our interaction with strength λ.
    - [Looking ahead: quadratic $\to \psi^\dagger[\cdots]\psi$ and quartic $\to \frac{\lambda}{2}\psi^\dagger\psi^\dagger\psi\psi$.

- The integral reminds us we can change integration variables without changing the value of Z_λ and therefore the physics is invariant. This implies we might find a transformation that makes our <u>approximate</u> calculations better or simpler.
    - In the real case, we exploit this both in RG and EFT.

- As we go through our discussion of the single integral, you should keep in mind then when we do the partition functions of interest, the integral will become a multiple integral over (say) $\xi_1, \xi_2, \ldots$ and the ξ_i and ξ_j are coupled in general. So $-\frac{1}{2}a\xi^2 \to -\frac{1}{2}\xi_i A_{ij}\xi_j$ with $\underline{A}$ a matrix.

- Thinking of $V(\xi) = \frac{a\xi^2}{2} + \frac{\lambda}{4}\xi^4$, we have several regimes possible depending on the signs of a and λ



- We will consider physical situations analogous to a) and c). b) in general is problematic since it is unbounded by below. (The situation when we have perturbative expansions in an EFT is interesting to consider — are they asymptotic? In some cases, like two-body scattering for small scattering length, they are not. But what about the finite density many-body problem?)

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- The first approximation strategy we consider is perturbation theory, which is based on treating the physics as being continuous as a small parameter is increased from 0.
  - In practice, we want that parameter to take us from a solvable problem to the one of interest, $H = H_0 + H_1$
  - An obvious candidate for the small parameter is λ, because at $\lambda=0$ we have a nice Gaussian integral.

- [Note: We chose (actually we adopted N+O's choice :) of $\frac{1}{4}\lambda$ as the coefficient of ξ^4. Obviously we could have chosen another coefficient, which would simply scale λ. However, we generally like to choose it so that λ or its analog can be used directly in assessing whether we expect the EFT to be in a region where it is valid and to estimate corrections. In this case, we'd like λ to be considered small when $\lambda \ll 1$. However, we'll see from the numerics that $\tilde{\lambda} = 6\lambda$, so that the quartic term is $\frac{1}{4!}\tilde{\lambda}\xi^4$ would have been a better choice. The 4! is a natural combinatoric factor that should be factored out so that $\tilde{\lambda} \ll 1$ is the relevant comparison (in other words, $\tilde{\lambda} \approx 1$ means a breakdown of the expansion).]

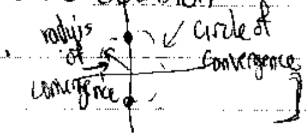
- If λ is small, then we can expand the exponent in Z_λ:

$$e^{-\frac{\lambda}{4}\xi^4} = 1 - \frac{\lambda}{4}\xi^4 + \frac{1}{2!}\left(\frac{\lambda}{4}\right)^2 \xi^8 + \ldots$$

and do the integral term by term. This is conventional perturbation theory in an interaction.

- The expansion above converges for any value of λ because there are no singularities of $e^{-\alpha}$ in the complex λ plane (and therefore the radius of convergence about $\lambda=0$ is infinite).

[Recall that $\frac{1}{1+\lambda^2}$, for example, has poles at $\lambda = \pm i$, so the expansion about $\lambda=0$ even for real λ only converges for $|\lambda| < 1$.



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In general, however, we expect that perturbative expansions for partition functions are asymptotic – meaning the radius of convergence is zero!

Let's try doing it for Z_λ, including some numerical calculations.

- The expansion is $\left| Z_\lambda = \sum_{n=0}^{\infty} Z_n \lambda^n \right|$ [Take $a=1$ for convenience]

where

$$\lambda^n Z_n = \frac{(-\lambda)^n}{n!}\frac{1}{4^n}\int_{-\infty}^{\infty}\frac{d\xi}{\sqrt{2\pi}}e^{-\xi^2/2}\xi^{4n}$$

$$= \frac{(-\lambda)^n (4n-1)!!}{n!\,4^n}$$

$$= \frac{(-\lambda)^n (4n)!}{n!\,16^n (2n)!} \sim \frac{1}{\sqrt{n\pi}}\left(\frac{4\lambda n}{e}\right)^n$$

$$\leftarrow \int_{-\infty}^{\infty} d\xi\, \xi^{4n} e^{-\xi^2} d\xi = 2\int_0^\infty d\xi\, \xi^{4n} e^{-\xi^2} \overset{\xi = t^{1/2}}{=} \int_0^\infty t^{(2n+1/2)-1} e^{-t} dt = \Gamma(2n+\tfrac{1}{2})$$

using $\boxed{n! \doteq \sqrt{2\pi n}\, n^{n+1/2} e^{-n}}$

The utility of a perturbative expansion is that we can calculate at least the low order terms. In our simple case, we can do all of them easily. ⇒

- We've used Mathematica to see how well a finite number of terms works by calculating and plotting (see the hand out

$$\boxed{R_n(\lambda) \equiv \left| Z(\lambda) - \sum_{m=0}^{n} Z_m \lambda^m \right|} \quad \text{vs. the \# of terms } n$$

(normalized to R_0).

- We see that for very small $\lambda \sim 0.01$, we can get very accurate results from perturbation theory, but even then only up to a certain # of terms, after which it degrades. } asymptotic series!
- The turnaround point gets smaller as λ increases, looking at the blown-up plot, for $\lambda = 0.1$, which seems small, we have to stop at the 2^{nd} or 3^{rd} term and the accuracy is only 25%.
- Looking on the back at the error as a function of $\hat{\lambda} = 6\lambda$ for $n=1$ and $n=2$ (first and 2^{nd} order or "LO and NLO") [with a different normalization of the error, sorry] we see that $n=2$ ceases to be a correction to $n=1$ at $\hat{\lambda} \simeq 1$, so this is a good scaling, Then $\lambda = 0.1 \Rightarrow \hat{\lambda} = 0.6$

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so we are not surprised that it is failing quickly.

· We can see the problem by bounding R_n

$$\boxed{R_n = \left|Z_\lambda - \sum_{m=0}^{n} Z_m \lambda^m\right| \le \int_{-\infty}^{\infty} \frac{d\xi}{\sqrt{2\pi}} e^{-\xi^2/2} \frac{1}{(n+1)!}\left(\frac{\lambda \xi^4}{4}\right)^{n+1} = \lambda^{n+1}|Z_{n+1}|}$$

so as long as successive terms decrease, the approximation gets better.

· But there is a minimum in the terms as a function of n for $n \sim 1/4\lambda$ (or $1/\lambda \approx 1$) so the minimum error goes like

$$\boxed{|\lambda^n Z_n|_{min} \sim \sqrt{\frac{4\lambda}{\pi}}\, e^{-1/4\lambda}}$$

(The truncation error is the order of the first omitted term.)

· This can be very small from $e^{-\frac{1}{4\lambda}}$ if λ is small (weak coupling).

· Later we'll connect the growth in Z_n to the number of diagrams generated, which is where the $(4n-1)!!$ factor that kills us comes from. We can think of this as the competition between the smallness of λ and the factorial growth from combinatorics of how many "partial amplitude" contribution there are at order n.

· A general argument predicting an asymptotic series starts by noting that a finite (non-zero) radius of convergence would mean the behavior should not abruptly change from $+|\lambda|$ to $-|\lambda|$ for small enough $|\lambda|$.

- zero radius of convergence means nonanalyticity at $\lambda = 0$ (pole or branch point)
- The picture of $V(\xi)$ completely changes behavior of the physics: goes from localized to unconfined.
- This shows up by inspection, as the integral diverges for $\lambda < 0$, converges for $\lambda > 0$.
  $\Rightarrow$ nonanalytic at $\lambda = 0$
- This argument can be applied in relativistic quantum field theory: Dyson used it in the 50's to argue that QED perturbation theory is asymptotic (changing the sign of e^2 - not e - leads to a vacuum unstable to decay into e^+e^- pairs, since like particles attract and unlike repel).

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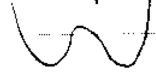
- This is not a problem in QED, where $\alpha = \frac{e^2}{4\pi} \sim \frac{1}{137}$ is small enough so that the error decreases for all terms that have been calculated. (Minimum is expected at $n \sim 137$!)

- So perturbation theory may be ok but what if it isn't? Waste of time?
  - No, because it organizes how we attack the problem and identifies or isolates different parts of the physics (such as short-range correlations from repulsive short-range potentials or long-range correlations from particles moving collectively, like vibrations)
    - It can lead to partial resummations of the series including a subset of terms to all orders $\Rightarrow$ non perturbative.

- Alternative approaches are also suggested by the integral:
  - strong coupling – treat the quadratic part as a perturbation to the quartic potential
  - for case c):  do a stationary phase (saddle point) approximation to expand about the minima of the potential. Note that we expect tunneling in the quantum mechanics case – this is very naturally accommodated in path integrals.

- So let's look at how we will do perturbation theory in practice when we can't generate the series in closed form.
  - The alternative starts with the observation that we can do Gaussian integrals
$$\Rightarrow \boxed{\int_{-\infty}^{\infty} d\xi \; e^{-\frac{a\xi^2}{2}} = \sqrt{\frac{2\pi}{a}}}$$
even in the more general case where $a\xi^2 \to \xi_i A_{ij} \xi_j$ and we extend to consider complex and Grassmann (non-commuting) variables.

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· The idea is to add a "source term" to the exponent:

$$\boxed{Z_\lambda \to Z_\lambda[j] = N\int_{-\infty}^{\infty} d\xi\, e^{-\frac{a\xi^2}{2} - \frac{\lambda\xi^4}{4} + j\xi}}$$

so that

$$\boxed{Z_\lambda = Z_\lambda[j]\big|_{j=0}}$$

· we've switched to an unspecified normalization constant N (so it is not distracting and we can see clearly when it drops out of a calculation)

· The idea is to recover Z_λ after any j manipulations (such as derivatives wrt j) by setting $j=0$ at the end.

[· In a slight abuse of notation, we write $Z_\lambda[j]$ instead of $Z_\lambda(j)$ because we will generalize j to be a function (say of space and time) in our path integrals, so that Z_λ is a functional of $j(x)$. This is conventionally indicated by using square brackets [ ] instead of ( )'s as for functions. Not like mathematica!]

· You might think of adding j as being a mathematical trick but we'll adopt a more physical interpretation: think of it as generalizing the Hamiltonian as when you have an external magnetic field under your control — by changing that field and seeing how Z changes.

· In particular, because $\frac{\partial}{\partial j} e^{j\xi} = \xi e^{j\xi}$, we can replace functions of ξ by functions of j (and take them out of the integral):

$$f(\xi)\, e^{j\xi} = f\!\left(\frac{\partial}{\partial j}\right) e^{j\xi}$$

where $f\!\left(\frac{\partial}{\partial j}\right)$ means to replace ξ by $\frac{\partial}{\partial j}$ in the (assumed) Taylor series of $f(\xi)$ and to act with them to the right.

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$$\Rightarrow \boxed{Z_\lambda[j] = N e^{-\frac{\lambda}{4}\left(\frac{\partial}{\partial j}\right)^4} \int_{-\infty}^{\infty} d\xi \, e^{-\frac{a}{2}\xi^2 + j\xi}}$$

Now complete the square in the exponent

$$Z_\lambda[j] = N e^{-\frac{\lambda}{4}\left(\frac{\partial}{\partial j}\right)^4} \int_{-\infty}^{\infty} d\xi \, e^{-\frac{a}{2}\left(\xi^2 + \frac{2j}{a}\xi\right)}$$

$$= N e^{-\frac{\lambda}{4}\left(\frac{\partial}{\partial j}\right)^4} \int_{-\infty}^{\infty} d\xi \, e^{-\frac{a}{2}\underbrace{\left(\xi^2 + \frac{2j\xi}{a} + \frac{j^2}{a^2}\right)}_{(x+\frac{j}{a})^2}} e^{+\frac{a}{2}\frac{j^2}{a^2}}$$

switch to $x' = x + j/a$, $dx' = dx$

$$= \left[e^{-\frac{\lambda}{4}\left(\frac{\partial}{\partial j}\right)^4} e^{\frac{1}{2} j a^{-1} j}\right] \underbrace{N \int_{-\infty}^{\infty} d\xi' \, e^{-\frac{a}{2}\xi'^2}}_{Z_{\lambda=0} \equiv Z_0}$$ ← independent of j

$$\Rightarrow \boxed{Z_\lambda[j] = Z_0 \, e^{-\frac{\lambda}{4}\left(\frac{\partial}{\partial j}\right)^4} e^{\frac{1}{2} j a^{-1} j}}$$

and $$\boxed{\frac{Z_\lambda}{Z_0} = \left[e^{-\frac{\lambda}{4}\left(\frac{\partial}{\partial j}\right)^4} e^{\frac{1}{2} j a^{-1} j}\right]\Bigg|_{j=0}}$$

- Z_0 is the non interacting ($\lambda = 0$) partition function. If we can calculate it by other means, then all of the constant factors (N) drop out.
- If we take $\ln Z/Z_0$ we get $\Omega - \Omega_0$, the interacting thermodynamic potential, which is often all we need.

- In the Zinn-Justin Chap 1 excerpt, we have the generalization to j being a discretized function:

$$\boxed{\begin{aligned} \int_{-\infty}^{\infty} d\xi_1 d\xi_2 \cdots d\xi_n \, e^{-\frac{1}{2}\xi_i A_{ij}\xi_j + j_i \xi_i} &= \int_{-\infty}^{\infty} d\xi_1 \cdots d\xi_n \, e^{-\frac{1}{2}\underline{\xi}^T \underline{\underline{A}}\, \underline{\xi} + \underline{j}^T \underline{\xi}} \\ = (2\pi)^{n/2} (\det \underline{\underline{A}})^{-1/2} e^{\frac{1}{2} j_i (A^{-1})_{ik} j_k} &= (2\pi)^{n/2} (\det \underline{\underline{A}})^{-1/2} e^{\frac{1}{2}\underline{j}^T \underline{\underline{A}}^{-1} \underline{j}} \end{aligned}}$$

- Note how $\frac{1}{a} \to \underline{\underline{A}}^{-1}$, so we'll be able to generalize, with $\frac{\partial}{\partial j} \to \frac{\partial}{\partial j_i} \xrightarrow[\text{limit}]{\text{continuous}} \frac{\delta}{\delta j(x)}$

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- Suppose we want an expectation value, such as $\langle \xi^2 \rangle$:

$$\boxed{\langle \xi^2 \rangle = \frac{N\int_{-\infty}^{\infty} d\xi\, \xi^2 e^{-\frac{a}{2}\xi^2-\frac{\lambda}{4}\xi^4}}{N\int_{-\infty}^{\infty} d\xi\, e^{-\frac{a}{2}\xi^2-\frac{\lambda}{4}\xi^4}} = \frac{\left(\frac{\partial}{\partial j}\frac{\partial}{\partial j} Z_\lambda[j]\right)\Big|_{j=0}}{Z_\lambda[j]\big|_{j=0}} = \frac{\left[\left(\frac{\partial}{\partial j}\frac{\partial}{\partial j}\right) e^{-\frac{\lambda}{4}\left(\frac{\partial}{\partial j}\right)^4} e^{\frac{1}{2}ja^{-1}j}\right]_{j=0}}{\left(e^{-\frac{\lambda}{4}\left(\frac{\partial}{\partial j}\right)^4} e^{\frac{1}{2}ja^{-1}j}\right)_{j=0}}}$$

← first the derivatives, then set $j=0$

notice cancellation of factors N

- $\langle \xi^2 \rangle$ is analogous to a Green's function or correlation function in our real theories.
- Note: no "path integral" left, just derivatives.

- To generate a perturbative expansion for Z_λ or $\langle \xi^2 \rangle$ in powers of λ, expand $e^{-\frac{\lambda}{4}\left(\frac{\partial}{\partial j}\right)^4}$ to the relevant power of λ and expand $e^{\frac{1}{2}ja^{-1}j}$ so there are just enough j's for the $\left(\frac{\partial}{\partial j}\right)$'s to kill $\Rightarrow$ since we set $j=0$ at the end, any terms with left over j's will vanish!

$$\Rightarrow \frac{Z_\lambda}{Z_0} = \left[1 - \frac{1}{4}\lambda\left(\frac{\partial}{\partial j}\right)^4 + \frac{1}{2!}\left(\frac{\lambda}{4}\right)^2\left(\frac{\partial}{\partial j}\right)^4\left(\frac{\partial}{\partial j}\right)^4 + \frac{1}{3!}\left(\frac{\lambda}{4}\right)^3\left(\frac{\partial}{\partial j}\right)^4\left(\frac{\partial}{\partial j}\right)^4\left(\frac{\partial}{\partial j}\right)^4 + \dots\right] \times \left[1 + \frac{1}{2}\left(ja^{-1}j\right) + \frac{1}{2!}\left(\frac{1}{2}ja^{-1}j\right)\left(\frac{1}{2}ja^{-1}j\right) + \dots\right]$$

- Let's do λ^1 and λ^2. We know the answer in our case that $\boxed{\frac{Z_\lambda}{Z_0} = \sum_{n=0}^{\infty} Z_n \lambda^n}$ with $\boxed{Z_n = \frac{(-1)^n}{n!}\frac{(4n-1)!!}{4^n}\frac{1}{a^{2n}}}$ $\Rightarrow$ $\boxed{Z_1\lambda = -\frac{3}{4}\frac{\lambda}{a^2}}$ and $\boxed{Z_2\lambda^2 = \frac{105}{32}\frac{\lambda^2}{a^4}}$

$$\lambda^1: -\frac{1}{4}\lambda\left(\frac{\partial}{\partial j}\right)^4 \frac{1}{2!}\left(\frac{1}{2}ja^{-1}j\right)\left(\frac{1}{2}ja^{-1}j\right) = -\frac{\lambda}{a^2}\frac{1}{32}\left(\frac{\partial}{\partial j}\right)^4(jjjj) = -\frac{\lambda}{a^2}\frac{1}{32}4! = -\frac{3\lambda}{4a^2} \checkmark$$

- we've kept the only term that survives when $j \to 0$.
- Note the 4!, which comes from all the ways $\left(\frac{\partial}{\partial j}\frac{\partial}{\partial j}\frac{\partial}{\partial j}\frac{\partial}{\partial j}\right)$ can annihilate $j \times j \times j \times j$
[check: $=\left(\frac{\partial}{\partial j}\frac{\partial}{\partial j}\frac{\partial}{\partial j}\right)[jjj+jjj+jjj+jjj] = 4\times\frac{\partial}{\partial j}\frac{\partial}{\partial j}(jj+jj+jj) = 4\times3\times\frac{\partial}{\partial j}\{j+j\} = 4\times3\times2\times1 = 4!$]

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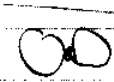
- The basic calculation is $\frac{\partial}{\partial j}(j) = 1$. In the path integral generalization it will almost be as simple!

- If we associate the a^{-1} in $\frac{1}{2} j a^{-1} j$ with a line ——— and the "interaction" $\frac{\lambda}{4}$ with a •, we can represent our result with a Feynman (-like) diagram!

- Try the next order:

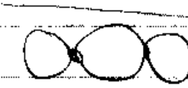
$$\lambda^2: \ \frac{1}{2}\left(\frac{\lambda}{4}\right)^2 \left(\frac{\partial}{\partial j}\right)^4 \left(\frac{\partial}{\partial j}\right)^4 \frac{1}{4!}\left(\frac{1}{2}\right)^4 \frac{1}{a^4}(jj)(jj)(jj)(jj) = \frac{1}{2}\cdot\frac{1}{16}\cdot\frac{1}{16}\cdot\frac{1}{4!}\cdot 8! \frac{\lambda^2}{a^4} = \frac{105}{32}\frac{\lambda^2}{a^4} \checkmark$$

- Lots of combinatoric factors, but we can organize it according to how the $\left(\frac{\partial}{\partial j}\right)^4$ attacks the $j a^{-1} j$ terms, as represented by diagrams:

 × 

each $\left(\frac{\partial}{\partial j}\right)^4$ hits two separate $\frac{1}{2} j a^{-1} j$ terms

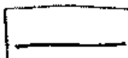
each $\frac{\partial}{\partial j}$ in $\left(\frac{\partial}{\partial j}\right)^4$ picks up one j from each $\frac{1}{2} j a^{-1} j$ term



for each $\left(\frac{\partial}{\partial j}\right)^4$, two $\frac{\partial}{\partial j}$'s hit one $j a^{-1} j$ term and the other two hit different $j a^{-1} j$'s

cf.  same!

- We can do the same thing for $\langle \xi^2 \rangle$, where we find out that

$\boxed{\text{———} \Rightarrow \frac{1}{a}}$  and $\boxed{\times \rightarrow -\frac{\lambda}{4} 4!}$  except for some additional combinatoric rules, called a symmetry factor.

[we'll do this explicitly later]
$\Rightarrow$ "Feynman rules"

Using the Feynman rules we'll be able to just write down diagrams rather than explicitly carrying out the derivatives (which are tedious, even if trivial).

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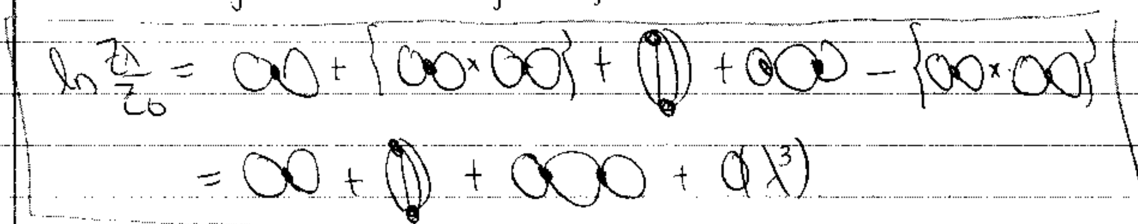
- Now recall that we really don't want Z_λ but $\ln Z_\lambda$, which is proportional to the thermodynamic functions of interest.
  - To find $\ln Z_\lambda$ or $\ln Z_\lambda/Z_0$ in perturbation theory, just do the Taylor series expansion:

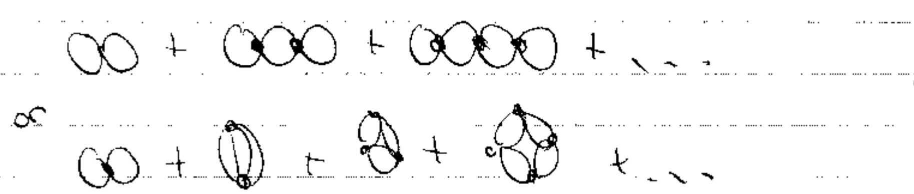
$$\boxed{\begin{aligned} \ln \frac{Z_\lambda}{Z_0} &= \ln\left[1 - \frac{3\lambda}{4a^2} + \frac{105}{32}\frac{\lambda^2}{a^4} + O(\lambda^3)\right] \\ &= -\frac{3\lambda}{4a^2} + \frac{3\lambda^2}{a^4} + \ldots \end{aligned}}$$

- There are two parts at $O(\lambda^2)$: the $\frac{105}{32}\frac{\lambda^2}{a^4}$ appearing once and $-\frac{3\lambda}{4a^2}$ appearing twice in the Taylor expansion.
- If we go back to diagrams, we find that



and the "disconnected" parts cancel when we take the logarithm.
  - This is not convincing yet, because we don't know that the factors multiplying the cancelling terms are really the same.
  - But, in fact, we can prove the result in general (which is called the "linked cluster theorem") using a very elegant technique called the "replica method." (later!)

- We will look at more examples later, but just note that the idea of infinite partial summations can be expressed as summing a class of diagrams. E.g., for $\ln \frac{Z_\lambda}{Z_0}$,



are either of these good approximations?

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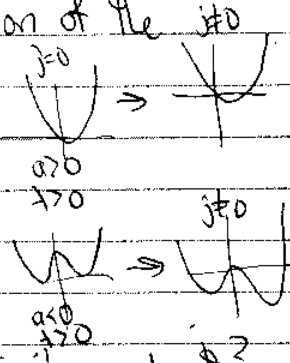
- What is the analog of the Legendre transformation of the thermodynamic potential $\ln Z_\lambda(j)$?

- Start again with

$$\boxed{Z_\lambda[j] = N\int_{-\infty}^{\infty} d\xi \, e^{-\frac{a\xi^2}{2} - \frac{\lambda\xi^4}{4} + j\xi}}$$

$j \neq 0$



and treat j as a thermodynamic variable. What is it paired with?
Should be $\frac{\partial}{\partial j}\ln Z_\lambda[j] = \frac{1}{Z_\lambda}\frac{\partial Z_\lambda}{\partial j} = \langle \xi \rangle$, which makes sense.

$$\text{So} \quad \langle \xi \rangle \equiv \bar{\xi}(j) = \frac{\partial}{\partial j}\ln Z_\lambda[j] \equiv \frac{\partial}{\partial j} F_\lambda[j]$$

(F_λ is the "free energy")

is a function of the independent variable j. So $\bar{\xi}(j)$ tells us what the expectation value of ξ is as a function of j.
- It should be (why?) an <u>invertible</u> function $\Rightarrow$ find $j(\bar{\xi})$

- Then find $\Gamma_\lambda[\bar{\xi}]$ by

$$\boxed{\Gamma_\lambda[\bar{\xi}] = F_\lambda[j(\bar{\xi})] - j(\bar{\xi}) \times \bar{\xi}}$$

- When j is a source <u>function</u>, this will be called the effective action. $\Gamma_\lambda[\bar{\xi}]$ should tell us what j we will need to produce a desired $\bar{\xi}$.
- Check the thermodynamic relation we expect:

$$\frac{\partial \Gamma_\lambda}{\partial \bar{\xi}} = \cancel{\frac{\partial F_\lambda}{\partial j}\frac{\partial j}{\partial \bar{\xi}}} - \cancel{\frac{\partial j}{\partial \bar{\xi}}\cdot \bar{\xi}} - j(\bar{\xi}) = -j(\bar{\xi}) \quad \text{as expected.}$$

- What does the expansion of Γ_λ in powers of λ look like in diagrams?

- What good is Γ_λ? (To be addressed!)

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Teaser: Saddle point evaluations of integrals (the other curves on the handout)

· Let's set up some of the basic ideas.

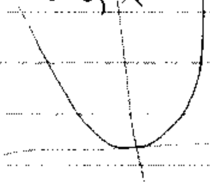
Consider yet again Z_λ but now try a variable change from ξ to $y = \sqrt{\lambda}\,\xi$. Then (putting back the normalization)

$$\boxed{Z_\lambda = \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi\lambda/a}}\, e^{-\frac{1}{\lambda}\left(\frac{ay^2}{2} + \frac{1}{4}y^4\right)}}$$

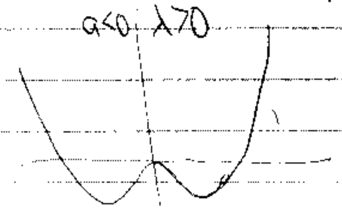
What happens when $\frac{1}{\lambda}$ gets large (i.e. λ is small)?

(under certain conditions) $\Rightarrow$ more and more of the contribution to Z_λ comes from the region in the integrand near stationary points of the exponent (where the derivative of the exponent vanishes).

$a>0,\ \lambda>0$



$a<0,\ \lambda>0$



$\Rightarrow$ an asymptotic expansion in $1/\lambda$.

"Review" the general theory (you may not have seen this before!) (Next time).

· The bottom line is that we derive a new expansion

$$\boxed{Z_\lambda \doteq \underbrace{\underbrace{\frac{e^{(\sqrt{1+4\lambda}-1)^2/16\lambda}}{(1+4\lambda)^{1/4}}}_{\text{LO}}\left(1 + \frac{12\lambda^2}{2(1+4\lambda)(1+\sqrt{1+4\lambda})^2} + \ldots\right)}_{\text{NLO}}}$$

$\Rightarrow$ look at how well it does!