AN ALTERNATIVE PERTURBATIVE EXPANSION IN QUANTUM MECHANICS.
SCALING AND CUT-OFF RESUMMATION *

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Abstract

An alternative perturbative expansion in quantum mechanics which allows a full expression of the scaling arbitrariness is introduced. This expansion is examined in the case of the anharmonic oscillator and is conveniently resummed using a method which consists in introducing an energy cut-off that is carefully removed as the order of the expansion is increased. We illustrate this technique numerically by computing the asymptotic behavior of the ground state energy of the anharmonic oscillator for large couplings, and show how the exploitation of the scaling arbitrariness substantially improves the convergence of this perturbative expansion.

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1. Introduction

Perturbation theory, as everybody knows, consists of calculating the quantities associated to a Hamiltonian $H(g)$ as Taylor expansions in the coupling $g$ around $g = 0$, which corresponds to an exactly solvable Hamiltonian. In systems like the anharmonic oscillator, however, these series fail to converge. This problem is generally addressed by resumming the series with the Padé or Borel methods. In cases like the double well potential or physically interesting field theories like QCD, however, these methods are inapplicable due to the existence of instantons.

In this paper, we alternatively look at perturbation theory in a different, very physical way. The central idea is the realization that all the energy scales of the unperturbed Hamiltonian participate in the calculation of an observable (an eigenstate, for instance) of the perturbed system at a certain energy. This view naturally leads us to investigate two aspects of perturbation theory. On one hand we investigate how every energy scale contributes to the perturbed eigenstate and how the calculation of these contributions can be optimized using energy-dependent scaling transformations. This leads us to introduce a perturbative expansion that exploits the scaling arbitrariness to a maximum. On the other hand, we identify the divergences in the anharmonic oscillator as due to the fact that the contributions calculated in perturbation theory from arbitrarily high energies are unbounded. From this realization we propose a resummation technique based on the introduction of an energy cut-off.

The optimization of perturbation theory using scaling properties is accomplished in Quantum Field Theory (QFT) by the Renormalization Group (RG)\(^\text{1,2}\). In the process of renormalization a new mass scale $\mu$ needs to be introduced and we get vertex functions expressed in terms of more parameters than the physically independent ones. This parameter redundancy is exploited by the RG: we can suitably change the scale $\mu$ and the rest of parameters in such a way that we always remain in the same physical theory. Although these changes do not affect the theory, they do modify its perturbation expansions order by order. Thus, depending on the energy scale at which we are working, we can select the appropriate $\mu$ scale which optimizes this perturbative expansion. As is well known, this technique has proved to be extremely fruitful in QFT, its most important achievement being, perhaps, the discovery of asymptotic freedom in non Abelian Gauge Theories\(^\text{3,4}\).

However, it is not clear to us that the conventional use of the RG fully exploits the scaling properties of the theory. In the computation of vertex functions at a certain energy, we will obviously use a $\mu$ scale of that same energy. In that computation, however, all scales are involved since we perform loop integrals over the full range of virtual momenta; the effect of the perturbation on these other scales should, nevertheless, be optimally computed using a different $\mu$.

In a recent paper\(^\text{5}\), we showed how the RG in a 4-dimensional $\phi^4$ theory could be extended to provide improved perturbation expansions free of infrared divergences in the massless case. There, we computed higher order vertex functions ($n > 4$) using skeleton expansions in which full propagators and 4-point functions are inserted respectively at each line and vertex of the skeleton diagrams. In this way, depending on the momenta running through a line or reaching a vertex of a diagram, the propagators and couplings conveniently adjust themselves to those particular scales. This would take care of the objection of the previous paragraph for higher order vertex functions. Unfortunately, the equivalent treatment for the primitive divergences would imply solving the Schwinger-Dyson integral equations\(^\text{6}\), which is a highly non-trivial matter.

In this paper we provide, for the simple case of one-dimensional Field Theory (i.e., Quantum Mechanics), a perturbative expansion that maximally exploits the arbitrariness of scaling in the sense stated above. That is, we describe a perturbative expansion in which, in the computation at
a certain energy, the effect of the interaction on all the other energies involved is suitably computed using the optimal scale for every energy.

Consider the Hamiltonian \( H(g) = P^2/2m + V(g, x) \) where \( g = 0 \) corresponds to the exactly solvable system and \( g = g_f \) to the perturbed one. We shall consider the eigenvectors and eigenvalues of \( H(g) \) as functions of \( g \). However, instead of doing the usual Taylor expansion in \( g \), we will use another expansion which is much more convenient for visualizing how the various energy scales contribute to the calculation and for exploiting the scaling arbitrariness. We will divide the interval \( g \in [0, g_f] \) into \( N \) equal segments by introducing \( N - 1 \) intermediate points and will transport all eigenvectors and eigenvalues from one point to the next using first order perturbation theory. \( N \) is here the order of our expansion; when \( N \) is increased, the intermediate segments become smaller and smaller and first order of perturbation more and more accurate.

In this framework, scaling can be easily implemented to improve perturbation theory at every step for each energy level. If \( g_1 \) and \( g_2 \) are the initial and final points of a certain elementary step, for every given energy level we appropriately rescale \( H(g_2) (U^{-1}(\lambda)H(g_2)U(\lambda) = \lambda^2 \tilde{H}(g_2)) \), where \( U(\lambda) \) is the scaling operator given in coordinate representation by \( U(\lambda)\Psi(x) = \sqrt{\lambda}\Psi(\lambda x) \) in such a way that \( H(g_1) \) and \( \tilde{H}(g_2) \) are as similar as possible at that particular energy. This requirement can be expressed by demanding that the classical turning points of the two potentials coincide at that energy, since this ensures that the corresponding wave functions will be essentially confined to the same space interval, minimizing their difference. We then compute the eigenvector \( \tilde{\Psi} \) of \( \tilde{H}(g_2) \) using first order perturbation theory and finally determine the eigenvector \( \Psi \) of \( H(g_2) \) applying the scaling operator to \( \tilde{\Psi} \) (\( \Psi = U(\lambda)\tilde{\Psi} \)).

We are essentially dividing the interaction introduced at each step into two parts: an interaction that does not change the natural scale of the eigenvectors and which is computed in first order of perturbation theory, and a pure change of scale which is computed exactly by applying the appropriate scaling transformation. In this way, we remove from perturbation theory the burden of having to express the changes of scale introduced by the interaction, and it can thus be more accurate. It is important to recognize that these changes of scale introduced by the interaction strongly depend on the energy and, therefore, the scaling transformation \( U(\lambda) \) will vary from eigenvector to eigenvector.

Having introduced our alternative expansion and its optimization by scaling in section 2, we turn in section 3 to the discussion of the divergences of perturbation theory, particularizing for the anharmonic oscillator.

As is well known, the divergence of the Taylor expansions for the energy levels of the anharmonic oscillator is attributed to the fact that for negative couplings the potential is unbounded from below and the system becomes unstable. This instability manifests itself in the form of singularities in the second and third sheets of the Riemann surface associated to the analytic continuation of the eigenvalues for complex couplings\(^7,8\). These singularities have \( g = 0 \) as accumulation point and hence, the perturbation expansions for the energy levels have a null radius of convergence. The knowledge of the analytic properties of the eigenvalues\(^7,8\) and of the asymptotic behavior of the Taylor coefficients\(^9\) enables us to use the powerful machinery of the Borel Transformation\(^10,11\) to resum the series.

In the framework of the perturbation expansion presented in this paper, we look at the divergence in a different way. For large \( N \), one would expect that the errors made by first order of perturbation theory in an elementary step are of order \((\Delta g)^2 = (g_f/N)^2\); thus, the total error for the \( N \) steps would go like \( 1/N \) making the series converge to the right result. However, this is not true for the anharmonic oscillator. In this case, the perturbation changes the asymptotic behavior
of the potential for large $x$ and, consequently, the perturbation becomes arbitrarily large for high energy states (which are sensitive to the potential at large $x$). Thus, the errors made by first order of perturbation theory in an elementary step cannot be uniformly bounded with respect to energy by increasing $N$. The divergence in the low energy states then arises because these big errors at high energy are propagated down to the lower energy states in the subsequent elementary steps.

The use of the optimizing rescalings explained above ameliorates this problem reducing substantially the errors at high energy. Nevertheless, although the difference between the perturbed and unperturbed potentials effective at each energy is greatly reduced by making their classical turning points coincide, this difference is still arbitrarily large at high energies and the divergence persists.

We show how this problem can be overcome introducing an energy cut-off by, for example, limiting the number of states of the system. In this way, we can reduce the errors of first order of perturbation theory for all states as much as we want by increasing the number of elementary steps. The theory can then be resummed by carefully removing this cut-off as we increase the order of perturbation.

Thus, we regard our technique as a double expansion: in the number of elementary steps (the order) and in the number of eigenstates that we take around the energy at which we are computing (the cut-off). The way in which we calculate the double limit of this expansion is crucial: it can lead to the correct result or to a divergence. We provide a criterion to find the suitable order of perturbation associated to every value of the cut-off and show how, as expected, this order is substantially lower for the expansion that fully exploits the scaling arbitrariness.

2. An alternative perturbative expansion and scaling

In this section we will introduce the mentioned alternative expansion and will show how to fully exploit the scaling arbitrariness to optimize it. We have in mind its application to the anharmonic oscillator, but the formalism can be presented in a general way: we will consider a Hamiltonian of the form $H(g) = P^2/2m + V(g, X)$ where the potential satisfies $V(g, -x) = V(g, x)$, $V(g, x) < V(g, x')$ if $|x| < |x'|$ and $\lim_{|x| \to \infty} V(g, x) = \infty$.

If $\Psi_n(g)$, $E_n(g)$ are respectively the eigenvectors and eigenvalues of $H(g)$, we will first determine the expressions of their derivatives with respect to $g$ in terms of them. The defining equations are:

$$H(g)\Psi_n(g) = E_n(g)\Psi_n(g) \quad (1)$$

$$(\Psi_n(g), \Psi_n(g)) = 1 \quad (2)$$

The eigenvectors are completely determined up to a global phase factor. This phase can be conveniently chosen to satisfy the equation $(\Psi_n(g), \dot{\Psi}_n(g)) = 0$ (3). Differentiating (1) with respect to $g$ yields:

$$\dot{H}(g)\Psi_n(g) + H(g)\dot{\Psi}_n(g) = \dot{E}_n(g)\Psi_n(g) + E_n(g)\dot{\Psi}_n(g) \quad (4)$$
And using (3) and the projection of (4) on $\Psi_k(g)$ $\forall k$, we get the desired expressions:

$$\dot{E}_n(g) = (\Psi_n(g), \dot{H}(g)\Psi_n(g))$$

$$\dot{\Psi}_n(g) = \sum_{k \neq n} \frac{(\Psi_k(g), \dot{H}(g)\Psi_n(g))}{E_n(g) - E_k(g)} \Psi_k(g)$$

By repeatedly differentiating these equations with respect to $g$ and setting $g = 0$, we obtain the ordinary perturbation theory. As we pointed out in the introduction, we will use here a different strategy which is much more convenient for later introducing the scaling arbitrariness. We shall alternatively expand in the number of intermediate points in which we divide the interval $g \in [0, g_f]$ (the ‘order of perturbation’) and eigenvectors and eigenvalues will be propagated from one point to the next using a first order approximation. In view of (5)-(6), this first order approximation should be:

$$\Psi_n(g + \Delta g) \simeq \Psi_n(g) + \sum_{k \neq n} \frac{(\Psi_k(g), (H(g + \Delta g) - H(g))\Psi_n(g))}{E_n(g) - E_k(g)} \Psi_k(g)$$

$$E_n(g + \Delta g) \simeq E_n(g) + (\Psi_n(g), (H(g + \Delta g) - H(g))\Psi_n(g))$$

but it is, nevertheless, more convenient to replace (7)-(8) by

$$\Psi_n(g + \Delta g) \simeq (\Psi_n(g) + \delta \Psi_n(g))/\|\Psi_n(g) + \delta \Psi_n(g)\|$$

where

$$\delta \Psi_n(g) = \sum_{k \neq n} \frac{(\Psi_k(g), (H(g + \Delta g) - H(g))\Psi_n(g))}{E_n(g) - E_k(g)} \Psi_k(g)$$

$$E_n(g + \Delta g) \simeq (\Psi_n(g + \Delta g), H(g + \Delta g)\Psi_n(g + \Delta g))$$

because, although these formulas coincide with (7)-(8) at first order, they have the advantage of yielding exactly normalized states and the exact energies corresponding to the (approximate) eigenstates for finite values of $\Delta g$.

No scaling properties have yet been introduced; so far we have just changed the way in which we do our expansions. The different philosophies underlying each of these two expansions, can probably be best illustrated in the more familiar context of expanding a function around a point.

Suppose that we want to solve the equation

$$\frac{\partial g}{\partial x}(x, y) = O_y g(x, y)$$

with the boundary condition $g(0, y) = f(y)$, ($O_y$ is an operator that acts on the y variable only). Here are the two strategies:

i) Differentiating (9) with respect to $x$ and setting $x = 0$, we get:

$$\frac{\partial^n g}{\partial x^n}(0, y) = O_y^n g(0, y) = O_y^n f(y)$$
and we can build the Taylor expansion

\[
g(x, y) = \lim_{N \to \infty} \sum_{n=0}^{N} \frac{x^n}{n!} O_y^n f(y)
\]  

(10)

ii) We divide the interval \([0, x]\) into \(N\) parts and transport \(g(\xi, y)\) from one point to the next using the first order approximation

\[
g(\xi + \epsilon, y) \simeq g(\xi, y) + \epsilon O_y g(\xi, y) \quad (\epsilon = x/N)
\]

By repeatedly doing this, we get:

\[
g(\epsilon, y) \simeq f(y) + \epsilon O_y f(y)
\]

\[
g(2\epsilon, y) \simeq g(\epsilon, y) + 2\epsilon O_y f(y) + \epsilon^2 O_y^2 f(y)
\]

\[\vdots\]

\[
g(N\epsilon, y) \simeq g((N-1)\epsilon, y) + N\epsilon O_y g((N-1)\epsilon, y) = \sum_{n=0}^{N} \binom{N}{n} \epsilon^n O_y^n f(y)
\]

Thus, using this approach we get the expansion

\[
g(x, y) = \lim_{N \to \infty} \sum_{n=0}^{N} \frac{N!}{(N-n)! N^n} \frac{x^n}{n!} O_y^n f(y)
\]

(11)

To apply this to the expansion of a function around a point, we just need to realize that the function \(g(x, y) \equiv f(x + y)\) is determined by the equations

\[
\frac{\partial g}{\partial x}(x, y) = \frac{\partial g}{\partial y}(x, y) ; \quad g(0, y) = f(y)
\]

which is the former situation with \(O_y = \partial / \partial y\). Substituting \(x\) by \(x - x_0\) and \(y\) by \(x_0\) in (10) and (11) we get the expressions

\[
i) \quad f(x) = \lim_{N \to \infty} \sum_{n=0}^{N} \frac{f^{(n)}(x_0)}{n!} (x - x_0)^n
\]

(12)

\[
ii) \quad f(x) = \lim_{N \to \infty} \sum_{n=0}^{N} \frac{N!}{(N-n)! N^n} \frac{f^{(n)}(x_0)}{n!} (x - x_0)^n
\]

(13)

Term by term, (12) and (13) coincide as \(N \to \infty\), but not uniformly so, and as a result (13) has certain advantages over (12); for example, for the function \(f(x) = 1/(1 + x)\), (12) converges in the interval \([0, 1]\) while (13) converges in \([0, a]\) where \(a\) is the solution of \(\log(a) - 1/a = 1\), \((a \simeq 3.59)\). We therefore may wonder whether our expansion based on (7′), (8′) already has improved convergence properties over conventional perturbation theory.

However, let us go further to improve our expansion by the exploitation of the scaling arbitrariness. As is well known, the eigenfunction corresponding to a given energy level, quickly vanishes outside the classically allowed region. Thus, the distance between the classical turning
points of the potential is a measure of the length scale characteristic of that eigenstate. This scale can be preserved for all couplings by doing a scaling transformation which depends on \( g \).

The scaling operator is given in the coordinate representation by

\[
U(\lambda)\Psi(x) = \sqrt{\lambda}\Psi(\lambda x)
\]

and transforms the position and momentum operators in this way:

\[
U^{-1}(\lambda)XU(\lambda) = X/\lambda \quad U^{-1}(\lambda)PU(\lambda) = \lambda P
\]

The Hamiltonian transformed by the operators \( U(\lambda(g)) \) is then

\[
\tilde{H}(g) = \lambda^{-2}(g)U^{-1}(\lambda(g))H(g)U(\lambda(g)) = \frac{P^2}{2m} + \lambda^{-2}(g)V(g, X/\lambda(g))
\]

and \( \lambda(g) \) can then be chosen to maintain the scale corresponding to the \( n \)th eigenstate by solving the equations

\[
E_n(0) = V(0, x_0) \quad E_n(0) = \lambda^{-2}(g)V(g, x_0/\lambda(g))
\]

The first equation determines the classical turning point \( x_0 \) of the unperturbed potential for the energy \( E_n(0) \) and the second equation says that \( \lambda(g) \) should be chosen by demanding that the classical turning point for the perturbed potential at the same energy \( E_n(0) \) is again \( x_0 \). The coupling \( g \) can, of course, be conveniently reparameterized to make sure that equal increments of the coupling correspond to similar increases of the interaction in the rescaled Hamiltonian \( \tilde{H} \).

The perturbative expansion for the \( n \)th state associated to \( \tilde{H}(g) \) will clearly be better than that associated to \( H(g) \): \( \tilde{\Psi}_n(g_f) \) and \( \tilde{\Psi}_n(0) \) have the same number of nodes and are confined to the same region. In this way \( (\tilde{\Psi}_n(0), \tilde{\Psi}_n(g_f)) \) is maximized and the terms \( (\tilde{\Psi}_k(0), \tilde{\Psi}_n(g_f)) \) \( (k \neq n) \), which express the strength of the perturbation, are minimized. The eigenvector and eigenvalue corresponding to \( \tilde{H}(g_f) \) can then be immediately obtained from \( \tilde{\Psi}_n(g_f) \) by

\[
\Psi_n(g_f) = U(\lambda(g_f))\tilde{\Psi}_n(g_f) \quad E_n(g_f) = \lambda^2(g_f)\tilde{E}_n(g_f)
\]

as follows from (16).

What it has been done so far is just setting the appropriate scale for the \( n \)th eigenstate. This would correspond in Field Theory to set the \( \mu \) scale equal to the energy at which we are calculating. At this stage, both the ordinary Taylor expansion and our alternative expansion could be applied to the rescaled Hamiltonian \( \tilde{H}(g) \). From here on, we will suppose that we are studying a particular eigenstate and that we have already done the mentioned global rescaling of the Hamiltonian and dropped the tildes from the rescaled quantities.

As one can see in (7) or (7'), all energy scales participate in the calculation of a certain eigenstate and the effect of the perturbation on each of these energies, should be calculated at their appropriate scales. It is in taking care of this fact where our alternative perturbative expansion is much more convenient. Its advantage is that it merely consists in repeating many times a very simple routine: first order of perturbation theory. Thus, the scaling arbitrariness can be expressed in a single step very simply, and this new algorithm repeated for every step. Instead, in a Taylor expansion, the \( N \)th order is something very difficult to interpret.
Obviously, the way to exploit the scaling arbitrariness at a single step is just to do, for every eigenstate and for the elementary increment of the coupling, the global rescaling that we carried out for our selected state and the entire range of the coupling.

To be more precise, suppose that $g_1$ and $g_2$ are the initial and final points of a certain elementary step and that we know $\Psi_l(g_1), E_l(g_1) \forall l$. The appropriate rescaling of $H(g_2)$ for the $k$th state is

$$\tilde{H}(g_2) = \lambda_k^{-2}U^{-1}(\lambda_k)H(g_2)U(\lambda_k)$$

where, in analogy with (17), $\lambda_k$ is determined by

$$E_k(g_1) = V(g_1, x_k) \quad E_k(g_1) = \lambda_k^{-2}V(g_2, x_k/\lambda_k)$$

We now use a first order approximation between $H(g_1)$ and $\tilde{H}(g_2)$ followed by a scaling transformation between $\tilde{H}(g_2)$ and $H(g_2)$. Using (7) and (8) we have the approximations

$$\tilde{\Psi}_k(g_2) \simeq \Psi_k(g_1) + \delta\tilde{\Psi}_k(g_1)$$

where

$$\delta\tilde{\Psi}_k(g_1) = \sum_{l \neq k} \frac{(\Psi_l(g_1), (\tilde{H}(g_2) - H(g_1))\Psi_k(g_1))}{E_k(g_1) - E_l(g_1)}\Psi_l(g_1)$$

$$\tilde{E}_k(g_2) \simeq E_k(g_1) + (\Psi_k(g_1), (\tilde{H}(g_2) - H(g_1))\Psi_k(g_1))$$

which will then be inserted in

$$\Psi_k(g_2) = U(\lambda_k)\tilde{\Psi}_k(g_2)$$

$$E_k(g_2) = \lambda_k^2\tilde{E}_k(g_2)$$

In the spirit of the more convenient formulas (7') and (8') we have

$$\tilde{\Psi}_k(g_2) \simeq (\Psi_k(g_1) + \delta\tilde{\Psi}_k(g_1))/\|\Psi_k(g_1) + \delta\tilde{\Psi}_k(g_1)\|$$

which we then substitute in

$$\Psi_k(g_2) = U(\lambda_k)\tilde{\Psi}_k(g_2)$$

$$E_k(g_2) = (\Psi_k(g_2), H(g_2)\Psi_k(g_2))$$

Since $U(\lambda_k)$ is unitary, $\Psi_k(g_2)$ is exactly normalized.

Thus, for each state, the approximations are applied to an interaction that maintains the scale at that particular energy and the change of scale is carried out by an exact scaling transformation. We have, therefore, accomplished our goal: in this perturbative expansion, the effect of the interaction at every energy is calculated at its appropriate scale.
3. The anharmonic oscillator: cut-off resummation and scaling.

In this section, we will investigate the improvements in the perturbation theory of the anharmonic oscillator when the scaling arbitrariness is exploited as described in the former section. An additional difficulty is, however, present in this case: the instability of the system for negative couplings gives rise to a singularity at \( g = 0 \). We will show that this singularity is not overcome by the exploitation of scaling and that can be interpreted as due to the fact that for any order, the perturbative approximations are inadequate at very high energies. To overcome this problem, we will introduce a cut-off by limiting the number of states considered and will provide a criterion for finding the appropriate order of perturbation that should be associated to every value of the cut-off to conveniently resum the series. We will finally show how this order is substantially lower in the case in which the scaling arbitrariness is fully exploited.

We will choose the ground state to carry out all the numerical analysis. An analogous development could be done for any eigenstate. We first perform the global rescaling appropriate for the ground state explained in section 2.

\[
H(g) = P^2 + X^2 + gX^4 \quad ([X, P] = i) \quad (28)
\]

\[
\tilde{H}(g) = \lambda^{-2}(g)U^{-1}(\lambda(g))H(g)U(\lambda(g))
= P^2 + \frac{X^2}{\lambda^3(g)} + g\frac{X^4}{\lambda^6(g)} \equiv P^2 + \alpha X^2 + \beta X^4 \quad (16)
\]

Using equation (17), we can immediately find that the relationship between \( \alpha \) and \( \beta \) is

\[
\alpha = 1 - \beta \quad (29)
\]

Then, the rescaled Hamiltonian (which is naturally parameterized with \( \beta \)) is

\[
\tilde{H}(\beta) = P^2 + (1 - \beta)X^2 + \beta X^4 \quad (30)
\]

\( \beta(g) \) and \( \lambda(g) \) are the solutions of

\[
\beta = g/\lambda^6 \quad \Rightarrow \quad \beta^3 + (g^{-2} - 3)\beta^2 + 3\beta - 1 = 0
\]

\[
1 - \beta = 1/\lambda^4 \quad \Rightarrow \quad \lambda = (1 - \beta)^{-1/4} \quad (31)
\]

and \( E_0(g) \) is finally determined by

\[
E_0(g) = \lambda^2(g)\tilde{E}_0(\beta(g)) \quad (32)
\]

where \( \tilde{E}_0(\beta) \) is the eigenvalue of the rescaled Hamiltonian (30), which will be calculated perturbatively. It should be noted that while \( g \) ranges from zero to infinity, \( \beta(g) \) goes from zero to one. This fact illustrates very clearly the importance of this rescaling of the Hamiltonian in calculations for large couplings. From (31), we have that, for large \( g \)

\[
\beta(g) = 1 - \frac{1}{g^{2/3}} + \frac{2}{3g^{4/3}} + O\left(\frac{1}{g^2}\right) \quad (33)
\]

\[
\lambda^2(g) = g^{1/3}(1 + \frac{1}{3g^{2/3}} + O\left(\frac{1}{g^{4/3}}\right)) \quad (34)
\]
By inserting these equations in (32) we can determine the asymptotic behavior of \( E_0(g) \):

\[
E_0(g) = g^{1/3} \left\{ \tilde{E}_0(1) + \frac{\tilde{E}_0(1)}{3} - \frac{d\tilde{E}_0}{d\beta}(1) \frac{1}{g^{2/3}} + O\left( \frac{1}{g^{4/3}} \right) \right\}
\]  

(35)

We will later on calculate the coefficient \( \tilde{E}_0(1) \). This is obviously the most unfavorable quantity to calculate in a perturbative expansion since it is the most removed from the non interacting theory.

We will study our alternative perturbative expansion for the Hamiltonian (30) in the two versions presented in section 2. Expansion I will be the one that does not take advantage of scaling; eigenvectors and eigenvalues are propagated from one point to the next using (7)-(8) or (7')-(8'). Expansion II will be the one that fully exploits the scaling arbitrariness, propagating each eigenvector and eigenvalue using the (step and energy dependent) optimal rescalings described in (22)-(27).

As we pointed out at the beginning of this section, we will need to limit the number of states of the system in order to resum the series. By limiting the number of states, we mean that we consider the projection of the Hamiltonian on the space generated by a finite number of the eigenstates of the harmonic oscillator. Since the Hamiltonian is invariant under parity, the parts corresponding to the even and odd states are uncoupled. Thus, only even states will need to be considered in the calculation of the ground state energy.

Expansion I can be readily applied to this truncated Hamiltonian. In fact, it is easy to see that only a finite number of states contribute to a given order of perturbation and, therefore, beyond this number, the truncated expansion gives the exact result at that order. For example, only 8 states contribute at 3rd order and 26 at 4th order.

The limitation of the number of states, brings about a slight inconvenience in expansion II because the scaling operator does not map our finite dimensional subspaces into themselves. To overcome this difficulty it should be noted that everything after equation (20) in the last section, formally holds if we substitute \( U(\lambda_k) \) by an arbitrary unitary operator. Thus, the obvious thing to do is to replace \( U(\lambda_k) \) by unitary operators that leave invariant our finite dimensional spaces and coincide with \( U(\lambda_k) \) when the number of states is taken to infinity. Such operators can be obtained by taking the projection of \( U(\lambda_k) \) on the finite dimensional spaces in the basis formed by our finite number of (even) eigenstates of the harmonic oscillator and unitarizing it by orthonormalizing Gramm-Schmidt the columns of this projection starting from the one corresponding to the lowest eigenstate up.

For a large number of states (large cut-off), these operators will virtually coincide with \( U(\lambda_k) \) at low energy. There will be, however, some differences for the highest energy states which are necessary to accommodate the cut-off. Fortunately, as it will be shown, this boundary effect introduced by the cut-off does not spoil the scaling optimization.

The two different ways of carrying out the first order approximations in both expansions I and II that were presented in section 2, give rise to two versions of each expansion. We will denote by A those expansions in which the states are not exactly normalized at each step (eqs. (7)-(8) and (22)-(25)) and by B those in which they are (eqs. (7')-(8') and (26),(24),(27)).

The even eigenstates of the harmonic oscillator will be denoted by \(| l \rangle\). In coordinate representation are given by

\[
| l \rangle = \left( \frac{1}{\sqrt{\pi 2^{2l} (2l)!}} \right)^{1/2} H_{2l}(x) e^{-x^2/2} \quad l = 0, 1, 2, \ldots \quad ((P^2 + X^2) | l \rangle = (4l + 1) | l \rangle)
\]

(36)
We will say that the cut-off is equal to $n$ when we limit the number of states to the set $|0\rangle, |1\rangle, \ldots, |n\rangle$.

The numerical calculations that follow were done using ‘Mathematica’ on a NeXT computer. The programs involved are quite simple: one just needs to write the algorithm for transporting eigenvectors and eigenvalues from one intermediate point to the next, and ask the machine to repeat this algorithm $N$ times.

In tables I and II, we list the values of $E_0(g=1)$ computed respectively with the A versions of expansions I and II as functions of the order of perturbation and the cut-off. The exact value is $1.3923512$.

**Table I** (expansion I(A))

| ↓cut-off/order→ | 1   | 2   | 3   | 4   | 5   | 6   |
|----------------|-----|-----|-----|-----|-----|-----|
| 2              | 1.4671 | 1.4177 | 1.4060 | 1.4025 | 1.4009 | 1.4000 |
| 4              | 1.4671 | 1.4177 | 1.4102 | 1.4003 | 1.3957 | 1.3950 |
| 6              | 1.4671 | 1.4177 | 1.4482 | 796.31 | $3.0 \times 10^9$ | $9.3 \times 10^{20}$ |
| 8              | 1.4671 | 1.4177 | 1.4556 | $3.3 \times 10^4$ | $7.7 \times 10^{16}$ | $5.7 \times 10^{46}$ |
| 10             | 1.4671 | 1.4177 | 1.4556 | $4.0 \times 10^6$ | $3.5 \times 10^{25}$ | $1.0 \times 10^{58}$ |

**Table II** (expansion II(A))

| ↓cut-off/order→ | 1   | 2   | 3   | 4   | 5   | 6   |
|----------------|-----|-----|-----|-----|-----|-----|
| 2              | 1.4671 | 1.4178 | 1.4061 | 1.4025 | 1.4009 | 1.3999 |
| 4              | 1.4671 | 1.4175 | 1.4035 | 1.3994 | 1.3976 | 1.3965 |
| 6              | 1.4671 | 1.4175 | 1.4038 | 1.3995 | 1.3976 | 1.3965 |
| 8              | 1.4671 | 1.4175 | 1.4039 | 1.4087 | 1.3982 | 1.3965 |
| 10             | 1.4671 | 1.4175 | 1.4038 | 1.8093 | $4.9 \times 10^8$ | $3.5 \times 10^{14}$ |
| 12             | 1.4671 | 1.4175 | 1.4037 | 7.3734 | $1.2 \times 10^{10}$ | $-5 \times 10^{27}$ |

It is clear that when we remove the cut-off by taking it to infinity, we get divergent series in both cases. Thus, the exploitation of scaling in expansion II is not enough to overcome the divergence although, as one can see by comparing tables I and II, it tames it considerably.

To better understand this divergence and the effects of exploiting scaling, we have listed in tables III and IV (for expansions I and II respectively) the energies and norms of all states at every intermediate point for the case cut – off = 6, order = 5, $g = 1$ ($\beta = 0.43015\ldots$).
Let us look at the first point. The amount in which the norm of the states differ from 1 is a measure of the errors made by perturbation theory in the first step. These errors increase with energy and are substantially smaller for expansion II showing very clearly the remarkable improvement introduced by scaling.

As one can see in table III, the divergence in expansion I occurs because the big errors at high energy are amplified and propagated to the lower energy states in the subsequent steps, finally reaching the ground state. The same thing happens in expansion II but for a larger value of the cut-off ($\simeq 10$). The errors of perturbation theory at a given energy are reduced by increasing the

| points→ | 0  | 1      | 2      | 3       | 4       | 5       |
|---------|----|--------|--------|---------|---------|---------|
| energy(0) | 1  | 1.021  | 1.034  | 1.043   | 7.710   | $2.2 \times 10^9$ |
| norm(0)   | 1  | 1.0005 | 1.0008 | 1.183   | 1.1 $\times 10^4$ | 5.4 $\times 10^{12}$ |
| energy(1) | 5  | 5.623  | 5.991  | 6.448   | 2.224   | 7.3 $\times 10^{11}$ |
| norm(1)   | 1  | 1.026  | 1.047  | 11.71   | 2.0 $\times 10^9$   | 3.4 $\times 10^{13}$ |
| energy(2) | 9  | 11.25  | 13.27  | 27.73   | 5.346   | 1.9 $\times 10^{11}$ |
| norm(2)   | 1  | 1.187  | 1.844  | 24.59   | 1.0 $\times 10^9$   | 1.3 $\times 10^{13}$ |
| energy(3) | 13 | 17.92  | 29.19  | 573.7   | 8.8 $\times 10^9$   | 7.9 $\times 10^{13}$ |
| norm(3)   | 1  | 1.629  | 7.237  | 716.3   | 2.2 $\times 10^9$   | 1.7 $\times 10^{14}$ |
| energy(4) | 17 | 25.62  | 75.17  | 7013    | 4.6 $\times 10^9$   | 3.6 $\times 10^{14}$ |
| norm(4)   | 1  | 2.395  | 20.52  | 557.1   | 4.7 $\times 10^9$   | 1.0 $\times 10^{14}$ |
| energy(5) | 21 | 34.35  | 166.4  | 1791    | 4.1 $\times 10^9$   | 5.7 $\times 10^{12}$ |
| norm(5)   | 1  | 3.434  | 10.65  | 152.9   | 5.6 $\times 10^9$   | 5.5 $\times 10^{13}$ |
| energy(6) | 25 | 44.12  | 234.8  | 5697    | 1.0 $\times 10^9$   | 3.3 $\times 10^{13}$ |
| norm(6)   | 1  | 2.911  | 18.36  | 812.2   | 1.6 $\times 10^9$   | 1.2 $\times 10^{14}$ |

| points→ | 0  | 1      | 2      | 3       | 4       | 5       |
|---------|----|--------|--------|---------|---------|---------|
| energy(0) | 1  | 1.021  | 1.034  | 1.043   | 7.710   | $2.2 \times 10^9$ |
| norm(0)   | 1  | 1.0005 | 1.0008 | 1.183   | 1.1 $\times 10^4$   | 5.4 $\times 10^{12}$ |
| energy(1) | 5  | 5.501  | 5.843  | 6.115   | 6.344   | 6.542   |
| norm(1)   | 1  | 1.002  | 1.002  | 1.002   | 1.003   | 1.003   |
| energy(2) | 9  | 10.61  | 11.63  | 12.42   | 13.08   | 13.65   |
| norm(2)   | 1  | 1.004  | 1.005  | 1.005   | 1.005   | 1.005   |
| energy(3) | 13 | 16.21  | 18.11  | 19.67   | 21.12   | 22.56   |
| norm(3)   | 1  | 1.007  | 1.009  | 1.012   | 1.015   | 1.019   |
| energy(4) | 17 | 22.38  | 26.80  | 30.27   | 34.00   | 37.96   |
| norm(4)   | 1  | 1.019  | 1.062  | 1.076   | 1.091   | 1.112   |
| energy(5) | 21 | 32.41  | 43.00  | 51.39   | 60.50   | 71.54   |
| norm(5)   | 1  | 1.217  | 1.418  | 1.458   | 1.495   | 1.530   |
| energy(6) | 25 | 51.09  | 98.46  | 166.1   | 233.3   | 295.5   |
| norm(6)   | 1  | 1.300  | 1.521  | 1.541   | 1.538   | 1.528   |
order but then, we have more steps and the errors from higher energy states better propagate down to the ground state. Thus, the obvious thing to do is to keep the cut-off fixed while we increase the order to reduce all errors as much as we want.

Table V lists the values of $E_0(g = 1)$ calculated with expansion I(A) for a cut-off equal to 6 as we increase the order of perturbation.

**Table V (expansion I(A))**

| order | $E_0(g = 1)$ | order | $E_0(g = 1)$ | order | $E_0(g = 1)$ |
|-------|-------------|-------|-------------|-------|-------------|
| 1     | 1.4671      | 7     | $1.0 \times 10^{32}$ | 13    | 1.3934      |
| 2     | 1.4177      | 8     | $4.7 \times 10^{38}$ | 14    | 1.3933      |
| 3     | 1.4482      | 9     | $5.2 \times 10^{36}$ | 15    | 1.3933      |
| 4     | 796.3       | 10    | 1.3937      | 20    | 1.3930      |
| 5     | $3.0 \times 10^9$ | 11    | 1.3936      | 25    | 1.3929      |
| 6     | $9.3 \times 10^{20}$ | 12    | 1.3935      | 30    | 1.3928      |

At low orders, as we already pointed out, only the lowest energy states give substantial contributions to $E_0$ and we get decent approximations. From orders 4 to 9 there are enough steps to let the big errors at high energy propagate down to the ground state: the numbers take off. Finally, beyond 10, the order is high enough to curb the errors at all energies originating excellent approximations.

As we pointed out in the introduction, we are considering a double expansion: in the cut-off and in the order; and the way in which we take these quantities to infinity is crucial. If we first remove the cut-off we get a divergence, while by taking the order to infinity first and then the cut-off, such divergences are avoided.

Table III shows how the norms of the intermediate states grow very rapidly causing the energies (which are given by eq. (8)) to take off as well. Thus, the exact normalization of the states in the B versions of the expansions should represent a significant improvement. Table VI lists the values of $E_0(g = 1)$ at order 6 as we increase the cut-off, calculated with expansion I(B) and seems to indicate that there is no divergence in this case.

**Table VI (expansion I(B))**

| cut-off | $E_0(g = 1)$ | cut-off | $E_0(g = 1)$ |
|---------|-------------|---------|-------------|
| 1       | 1.39819     | 7       | 1.39323     |
| 2       | 1.39654     | 8       | 1.39333     |
| 3       | 1.39351     | 9       | 1.39339     |
| 4       | 1.39299     | 10      | 1.39337     |
| 5       | 1.39312     | 11      | 1.39340     |
| 6       | 1.39338     | 12      | 1.39339     |

Whether the B series without cut-off are in fact convergent or not is somewhat irrelevant because, as one can see in table VI, the best approximation is obtained for a finite cut-off (4 in this case). This is due to the fact that for a fixed order, the approximations of perturbation theory at each step, even though greatly improved and curbed by normalization, are not valid for high energy states.
As we said, the resummation procedure that we are proposing is to change the order in which we take the limits in our double expansion: first take the order to infinity and next the cut-off. However, for a fixed cut-off, it is only worth increasing the order until the precision obtained is of the order of the error made by the fact that we are limiting the number of states. Next, we will give a criterion to determine when we should stop increasing the order for a fixed cut-off.

In order to do that, we should first know how fast the series for fixed cut-offs tend to their limits when we increase the order \( N \). In the A expansions, both the states and energies are propagated at each step with first order of perturbation theory; thus, the error at each step is of order \((\Delta g)^2 \propto 1/N^2\) and the total error will go like \(1/N\). The same applies, in the B expansions, to the eigenstates, but not to the ground state energy. This is calculated with the formula \( E_0 = (\Psi, H\Psi) \). The (approximate) ground state \( \Psi \) can be written as \( \Psi = \Psi_0 + \chi(1/N)/N \), where \( \Psi_0 \) is the exact ground state and \( \chi(1/N) \) has a finite limit when \( N \to \infty \). Thus,

\[
E_0 = (\Psi_0, H\Psi_0) + \frac{1}{N} \{(\Psi_0, H\chi(0)) + (\chi(0), H\Psi_0)\} + O(1/N^2) \tag{37}
\]

Since \( \Psi_0 \) minimizes \( E_0 \), the term proportional to \( 1/N \) in (37) must vanish and we get that the errors in the B expansions go like \( 1/N^2 \) for large \( N \). This fact shows once again the superiority of the B expansions.

If \( E_0(N) - E_0(\infty) \) goes like \( 1/N \) for the A expansions and like \( 1/N^2 \) for the B ones, then \( Q_0(N) \equiv (E_0(N) - E_0(2N))/(E_0(2N) - E_0(4N)) \) must respectively tend to 2 and 4 for large \( N \). In tables VII and VIII we numerically verify this behavior in the particular case cut-off=4, \( g = 1 \). Something completely analogous is found for the A and B versions of expansion II since the use of scaling does not modify the arguments presented.

| Table VII (expansion I(A)) |
|-----------------------------|
| order(N) | \( E_0(N) \) | \( Q_0(N) \) |
| 50        | 1.392672024 | 1.98   |
| 100       | 1.392527424 | 1.99   |
| 200       | 1.392454389 |        |
| 400       | 1.392417667 |        |

| Table VIII (expansion I(B)) |
|-----------------------------|
| order(N) | \( E_0(N) \) | \( Q_0(N) \) |
| 50        | 1.392387789 | 4.10   |
| 100       | 1.392382513 | 4.04   |
| 200       | 1.392381227 |        |
| 400       | 1.392380909 |        |

We can now give a criterion for when we should stop increasing the order for a given cut-off. As we said, this should be that the precision obtained with that order is about the error made by the fact that we are limiting the number of states.
Let $E_0(n, N, g)$ be the $N$th order approximation to $E_0(g)$ when the cut-off is set equal to $n$. From the knowledge of the asymptotic behavior we can estimate the precision obtained. For the B versions of the expansions it will be

$$\epsilon = E_0(n, N, g) - E_0(n, \infty, g) \simeq \frac{4}{3}(E_0(n, N, g) - E_0(n, 2N, g))$$

(38)

On the other hand, a good estimate of the error made by the fact that we have a finite cut-off is the difference $\Delta = E_0(n - 1, N, g) - E_0(n, N, g)$ (39). Thus, a sensible criterion would be, for example $\epsilon < \Delta/2$, i.e.

$$E_0(n - 1, N, g) - E_0(n, N, g) > \frac{8}{3}(E_0(n, N, g) - E_0(n, 2N, g))$$

(40)

and the appropriate approximation for a cut-off equal to $n$ would finally be:

$$E_0(n, \infty, g) = E_0(n, N, g) - \epsilon \simeq \frac{1}{3}(4E_0(n, 2N, g) - E_0(n, N, g))$$

(41)

where $N$ is an order that satisfies (40).

As an example, we will apply this technique to compute the coefficient $\tilde{E}_0(1)$ of equation (35) that determines the asymptotic behavior of the ground state energy for large $g$ and which, as we mentioned, is the most unfavorable quantity of the anharmonic oscillator to calculate perturbatively. In table IX we list the smallest order $N$ for which (40) is satisfied and the corresponding approximation $\tilde{E}_0(n, 1) \equiv (4\tilde{E}_0(n, 2N, 1) - \tilde{E}_0(n, N, 1))/3$ for a cut-off ranging from 3 to 6 and for both expansions I and II (B versions).

| $n$ | $N$ | $\tilde{E}_0(n, 1)$ | $N$ | $\tilde{E}_0(n, 1)$ |
|-----|-----|---------------------|-----|---------------------|
| 3   | 6   | 1.0650              | 6   | 1.0648              |
| 4   | 7   | 1.0614              | 8   | 1.0612              |
| 5   | 19  | 1.06046             | 13  | 1.06044             |
| 6   | 100 | 1.060389            | 42  | 1.060389            |

Table IX

The coefficient $\tilde{E}_0(1)$ has been computed by variational methods\(^8\), the result being $1.060362\ldots$. It is remarkable the high degree of accuracy that is obtained for a relatively low cut-off. For instance, for $n = 6$ the error made is about $3 \times 10^{-5}$. This is because we have taken advantage of scaling: the free and interacting ground states have the same scale and are, therefore, very similar; the small difference between them can then be very well approximated by a linear combination of a few higher energy harmonic states.

Finally, it should be noted how, as expected, expansion II (which makes full use of scaling) is much more efficient than expansion I. This is more notable the higher the cut-off is, since it is at high energies where the optimizing rescalings are larger. As an example, we compare in Table X the values of $\tilde{E}_0(8, N, 1)$ for expansions I and II. For instance, we only need to calculate to order 40 in expansion II to get the same precision as with order 100 in expansion I.
Summary

We have introduced an alternative perturbative expansion which is very convenient for investigating the contributions of the various energy scales in the calculation of an eigenvalue and which can be very naturally improved by carrying out energy-dependent rescalings. We have identified the divergences in the expansions for the anharmonic oscillator as due to the fact that the errors made by perturbation theory in this case cannot be uniformly bounded for all energies. To overcome this problem, we have introduced an energy cut-off giving rise to a double expansion in both the order and the range of energies considered. Finally, we have provided a criterion for how this limit should be taken in order to get the correct physical results.

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References

1M. Gell-Mann and F.E. Low, Phys. Rev. 95, 1300 (1954).
2P. Ramond, Field Theory: A Modern Primer, Addison-Wesley, 1989.
3D.J. Gross and F. Wilczek, Phys. Rev. Lett. 30, 1343 (1973).
4H.D. Politzer, Phys. Rev. Lett. 30, 1346 (1973).
5J.M. Prats, Nucl. Phys. B387, 97 (1992).
6J.D. Bjorken and S.D. Drell, Relativistic Quantum Fields, McGraw-Hill, 1965.
7C.M. Bender and T.T. Wu, Phys. Rev. 184, 1231 (1969).
8B. Simon, Annals of Phys. 58, 76 (1970).
9C.M. Bender and T.T. Wu, Phys. Rev. D7, 1620 (1973).
10S. Graffi, V. Grecchi and B. Simon, Phys. Lett. 32B, 631 (1970).
11J. Zinn-Justin, Phys. Rep. 70, 2 (1981).
12A. Galindo and P. Pascual, Mecanica Cuantica, Alhambra, 1978.