Universality in an Information-theoretic Motivated Nonlinear Schrodinger Equation

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Abstract

Using perturbative methods, we analyse a nonlinear generalisation of Schrodinger’s equation that had previously been obtained through information-theoretic arguments. We first compute numerically the leading correction, in terms of the nonlinearity scale, to the energy eigenvalues of the linear Schrodinger equation in the presence of some common external potentials and parametrise the results in a simple form. We then study the problem analytically so as to explain the generic features that are observed. In one space dimension these are: (i) For nodeless ground states, the energy shifts are subleading in the nonlinearity parameter compared to the shifts for the excited states, (ii) the shifts for the excited states are due predominantly to contribution from the nodes of the unperturbed wavefunctions and (iii) the energy shifts for excited states are positive for small values of a regulating parameter and negative at large values, vanishing at a universal critical value that is not manifest in the equation. Some of these features hold true for higher dimensional problems. We also study two exactly solved nonlinear Schrodinger equations so as to contrast our observations. Finally, we comment on the possible significance of our results if the nonlinearity is physically realised.

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1 Introduction

Various nonlinear extensions of Schrodinger’s equation have been proposed [1] over the years as possible generalisations of the linear evolution of the original theory. Although several low-energy experiments have placed very small upper bounds [2] on the proposed extensions, there is still the possibility that quantum mechanics might have to be modified at high energies or short distances [3] where the structure of spacetime is expected to be different [4].

However in this paper we remain within the non-relativistic realm so as to explore in more detail the properties of one particular nonlinear extension that was motivated in [5] by maximum uncertainty arguments [6, 7] similar to those used in statistical mechanics [8]. In higher than one space dimension the equation of Ref. [5] was not rotationally invariant, motivating a suggestive link between spacetime symmetries and quantum linearity. Some implications of such a connection for phenomenology were discussed heuristically in [5, 3].

In Ref. [9] some exact nonperturbative solutions of the abovementioned equation were obtained, displaying intriguing and novel features that are probably related to the unusual structure of that equation. Indeed, it was hinted in [9] that the equation might also be interesting as an effective equation in other domains of physics, such as nonlinear optics [10], rather than its original intention in Ref. [9].

Here we investigate how the nonlinearity of that equation perturbs the energy spectrum of the usual linear Schrodinger equation. Since simple estimates already indicate that the size of the nonlinearity scale must be tiny for it to be consistent with phenomenology [5], we shall use standard first order perturbation theory for our study. Our primary aim here is not to confront empirical data but to uncover further properties of the nonlinear equation. As we shall see, even at the perturbative level the equation of Ref. [5] has a rather surprising character. In particular, we find a remarkable universal critical point of the theory that is not at all obvious from the equations of motion.

In the next section we outline our perturbative scheme and present the numerical results in Section (3). The generic features that are observed are then reasoned analytically in Section (4) where we also draw some new conclusions. In Section (5) we contrast the perturbative properties of the nonlinear equation with those of two other exactly solved nonlinear Schrodinger equations. The concluding section summarises the main lessons and discusses some implications. The appendices contain additional technical details.
2 Perturbative framework

Let us focus first on the nonlinear equation for a single particle in one space dimension that was derived in Ref.\[5\],

\[i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi + F(p)\Psi,\]  
(1)

with \(p(x, t) = \Psi^*(x, t)\Psi(x, t)\) the conserved probability density and

\[F(p) \equiv Q_1 - Q,\]  
(2)

where

\[Q_1 = \frac{\hbar^2}{4mL^2\eta^4} \left[ \ln \frac{p}{(1 - \eta)p + \eta p_+} + 1 - \frac{(1 - \eta)p}{(1 - \eta)p + \eta p_+} - \frac{\eta p_-}{(1 - \eta)p_- + \eta p} \right],\]  
(3)

is a regularised nonlinear “quantum potential”. The parameter \(\eta\) takes values \(0 < \eta < 1\), its crucial role being to regulate potential singularities where \(p(x)\) vanishes. We have used the notation

\[p_\pm(x) = p(x \pm \eta L).\]  
(4)

Note that if \(\Psi\) is any solution of the equation, then so is \(\lambda \Psi\) for an arbitrary constant \(\lambda\), so we may re-normalise states freely. The nonlinearity is characterised by the length scale \(L\), in terms of which one may perform a formal expansion of (3),

\[Q_1 \rightarrow Q \equiv \frac{\hbar^2}{2m} \frac{1}{\sqrt{p}} \frac{\partial^2 \sqrt{p}}{\partial x^2},\]  
(5)

with a remainder of \(O(L)\).

Let \(\Psi = e^{-iEt/\hbar}\phi(x)\) be the energy eigenstates of the usual linear Schrodinger equation for a given external potential \(V(x)\). Assuming that the spectrum deforms continuously as the nonlinearity \(F\) is turned on, then to leading order the corrected energies are given by first-order perturbation theory,

\[E_{\text{exact}} = E + \delta E,\]  
\[\delta E = \int_{-\infty}^{\infty} dx \phi^* F(\phi) \phi.\]  
(7)

Note that \(F\) is evaluated using the unperturbed wavefunctions and so from now on \(p\) will refer to \(\phi^*(x)\phi(x)\).
We may trust first-order perturbation theory when the nonlinearity is small. The relevant dimensionless expansion parameter is \( L/a \) where \( a \) is a typical scale in the linear theory, such as the deBroglie wavelength. As equations (3,4) indicate, the expression (7) is actually a complicated function of \( L/a \) from which the leading behaviour must be extracted. We will discard subleading terms from (7) as they will be of the same order as second-order perturbation theory corrections, which we do not study here.

For the problems we will study, the unperturbed wavefunctions \( \phi(x) \) are parity eigenstates so that \( p(x) = p(-x) \). Changing variables \( x \rightarrow -x \) in (7) and using the parity invariance of \( p \) shows that

\[
\delta E(L) = \delta E(-L) .
\]

That is, even though equation (11) is not invariant under \( L \rightarrow -L \), the first-order energy shifts are. Therefore if \( \delta E(L) \) were an analytic function of \( L \), one would have concluded that

\[
\delta E(L) \sim O(L^2) + O(L^4) + ...
\]

as the \( O(L^0) \) term vanishes by construction, see (5). In reality however, \( \delta E(L) \) is generically non-analytic! To see this, consider the naive series expansion of the integrand in (7). It results in the formal expression

\[
\delta E(L) \propto L^2 \eta^2 \int_{-\infty}^{\infty} \frac{dx}{p^2} \left[ 6(2-3\eta)^2(p')^4 - 12(3-8\eta + 6\eta^2)p(p')^2p'' \\
+ 4p^2p'p''' + p^2(3(p'')^2 - 2pp''') \right]
\]

which is ill-defined because of the singularities that occur where \( p(x) \) vanishes, that is where the unperturbed wavefunction has nodes. Thus one may conclude \( \delta E(L) \sim O(L^2) \) only for nodeless states, which are typically only the ground states of a system.

Since excited states of the unperturbed theory have nodes, we cannot use (10) for them. In the next section we perform a numerical investigation of expression (7) and then return in Section (4) to an analytical explanation of the various observed results, such as \( \delta E(L) \sim O(|L|) \) for excited states.

### 3 Numerical Investigation

As convergence near the end-points \( \eta = 0, 1 \) is slow, we integrate (7) numerically at the symmetric point \( \eta = 1/2 \), deferring a discussion of other \( \eta \) values.
to Sect.(4). Although phenomenologically one expects \( L/a \) to be tiny \([5]\), we study much larger values \( \sim 10^{-3} \) for computational efficiency. However we do demand \( \delta E/E \sim 10^{-2} \) or smaller so as to be safely in the perturbative regime. For each \( V(x) \), we obtain the leading dependence of \( \delta E \) on \( L/a \) and the principal quantum number. The numerical results are then parametrised using a best fit to simple analytical power law expressions.

The numerical work was performed with Mathematica \([11]\) and the quoted numbers are accurate to about the last digit.

In the numerical work we have set \( L = 1 \) to define the reference units. Thus \( 1/a \) factors quoted below actually correspond to the dimensionless quantity \( L/a \). We have checked that the numerical results are invariant under \( L \to -L \) as required by the parity invariance argument of Sect.(2).

### 3.1 Infinite Well

The infinite well with walls at \( x = 0 \) and \( x = a \) gives

\[
\phi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n \pi x}{a}
\]  

and unperturbed energies

\[
E_n^0 = \frac{\hbar^2 \pi^2 n^2}{2ma^2}.
\]  

In the presence of the nonlinearity the energies shift and are given to leading order by

\[
E_n = E_n^0 + \delta E_n.
\]  

It is convenient to define dimensionless quantities by dividing the above equation by \( \hbar^2 \pi^2/2ma^2 \),

\[
\tilde{E}_n = n^2 + \delta \tilde{E}_n.
\]  

For various fixed values of \( n, 1 \leq n \leq 50 \), the energy shifts were evaluated numerically for \( 1000 < a < 10,000 \). Fig.(1) shows a log-log plot for the \( n = 1 \) case from which one deduces \( \delta \tilde{E} = -0.99/a \). The other \( n \) values give similar plots, all indicating \( \delta \tilde{E} \propto -1/a \).

On the other hand, for various fixed \( a \), an evaluation over the range \( 5 \leq n \leq 50 \) shows \( \delta \tilde{E} \propto -n^3 \). Fig.(2) is a typical plot. Re-inserting ‘\( L \)’ we find, averaging the best fit for various \( a \) values,

\[
\delta \tilde{E}_n = -1.03 \frac{n^3 |L|}{a} + O(L/a)^2.
\]  

5
In Sect. (4) we will explain this result analytically.

Notice that the correction (11) grows with $n$ and so at some large value of $n$ it is no longer small compared to the unperturbed value. This simply means that one must then go beyond first order perturbation theory. We discuss the possibilities in the concluding section.

3.2 Simple Harmonic Oscillator (SHO)

The potential is now $V(x) = kx^2/2$ giving the usual unperturbed wavefunctions

$$
\phi_n(x) = \frac{1}{\sqrt{n!2^n}} (\pi a^2)^{-1/4} H_n\left(\frac{x}{a}\right) \exp\left(-\frac{x^2}{2a^2}\right)
$$

and unperturbed energies

$$
E_n^0 = (n + \frac{1}{2}) \hbar \sqrt{\frac{k}{m}}.
$$

The linear length scale ‘$a$’ in this problem is the deBroglie length $\hbar^{1/2}/(km)^{1/4}$. We investigated the dimensionless energies shifts

$$
\delta \tilde{E}_n \equiv \frac{\delta E}{\hbar \sqrt{m/k}}
$$

over the range, $0 \leq n \leq 18$ and $100 < a < 1000$.

From Fig.(3) for the ground state, $n = 0$, we find $\delta \tilde{E} \propto -1/a^2$, which is a faster drop than seen for the infinite well. However excited states have a similar behaviour in ‘$a$’ to those of the infinite well, with $\delta \tilde{E} \propto -1/a$ for any fixed $n$, as Fig.(4) shows. The $n$–dependence for fixed $a$ is more complicated as indicated in Fig.(5). In summary we find for the excited states, $n \geq 1$,

$$
\delta \tilde{E}_n = -0.26 \frac{n^{1.41}|L|}{a} + O(L/a)^2.
$$

It must be emphasized that the result (19) is a best fit to an assumed power law over the limited range investigated. However, independent analytical estimates in Appendix B do give a similar result over the same range.
3.3 Hydrogen Atom

We use the standard unperturbed wavefunctions as given, for example, in Ref.\[12\],

$$\psi_{n\ell m}(r, \theta, \phi) = \sqrt{\frac{2}{n \alpha}} \frac{(n-l-1)!}{2n[(n+l)!]} \rho^l e^{-\rho/2} L_{n-l-1}^{2l+1}(\rho) Y_{\ell m}(\theta, \phi),$$  \hspace{1cm} (20)

with \( \rho = 2r/na \), and the corresponding unperturbed energies

$$E_n^0 = -\frac{\hbar^2}{2Ma^2n^2},$$  \hspace{1cm} (21)

where \( M \) is the electron mass.

The three dimensional version of eq.\( (2) \) is \[5\]

$$F(p) \equiv Q_3 - Q,$$  \hspace{1cm} (22)

$$Q_3 = \sum_{i=1}^{3} \frac{\hbar^2}{4ML^2\eta^4} \left[ \ln \frac{p}{(1-\eta)p + \eta p_{+i}} + 1 - \frac{(1-\eta)p}{(1-\eta)p + \eta p_{+i}} - \frac{\eta p_{-i}}{(1-\eta)p_{-i} + \eta p} \right],$$

$$Q = -\frac{\hbar^2}{8M} \left[ \frac{2\partial_i \partial_j p}{p} - \frac{\partial_i p \partial_j p}{p^2} \right],$$  \hspace{1cm} (23)

with \( i = 1, 2, 3 \) and \( p_{\pm1}(x) = p(x_1 \pm \eta L, x_2, x_3) \) and so on. The Bohr radius defines \( a = \hbar^2/Mc^2 \) for this problem and the dimensionless energy shifts are

$$\delta \tilde{E}_n \equiv \frac{\delta E}{\hbar^2}(2Ma^2).$$  \hspace{1cm} (24)

Note that the nonlinearity breaks rotational invariance in the above expression \( (22) \) which is defined in the preferred Cartesian basis as discussed in Ref.\[7\]. Thus the wavefunctions \( (20) \) are first converted to the Cartesian basis for use in \( (22) \) but the final numerical integration was performed after converting back to spherical coordinates. We used the built-in Monte Carlo subroutine in Mathematica for this case and investigated only a very limited range of parameter values due to the time-intensive nature of the three dimensional problem.

Although the pure Coulombic hydrogen atom states have a degenerate spectrum, we still used the simple non-degenerate first order perturbation theory formula for all states as our primary objective is to observe the effects
of the nonlinearity on energy shifts. (Note also that the energy shifts due to the nonlinearity are expected to be much less than other effects, such as relativity, that in reality lift the degeneracy of the unperturbed states.)

Consider first the zero angular momentum, \( l = 0 \) states. For the ground state, \( n = 1 \) we found \( \delta \bar{E} \propto -1/a^2 \) while for the \( n = 2, 3 \) excited states we have \( \delta \bar{E} \propto -1/a \). This dependence on \( a \) is shown in Figs.(6,7) and is similar to that of the SHO. The dependence of the energy shifts on the principal quantum number however appears to be much more complicated than the earlier one-dimensional problems. Fig.(8) plots \( |\delta E/E_0| \) for \( n \geq 2 \).

For higher angular momentum states, there is a clear difference between the \( n = l - 1 \) cases and \( n \neq l - 1 \). For the former case we find \( \delta \bar{E} \propto -1/a^2 \), a behaviour typical of nodeless states, while for latter case we find the expected \( \delta \bar{E} \propto -1/a \) trend. Some plots are in Figs.(9,10,11). We explain the distinction between the two cases in Sect.(4).

As for the dependence on the magnetic quantum number \( m \) we do have the expected invariance under \( m \to -m \), but also find a mild dependence of the energy shift for for different \( m \) corresponding to the same \( n, l \) as a comparison of Figs.(10,11) indicates.

### 4 General Analytical Investigation

Unless otherwise stated, in this section we discuss the nonlinear equation in the presence of a general smooth external potential \( V(x) \).

#### 4.1 Nodeless States

If \( p(x) \) does not vanish in the region of integration, such as the ground state of the SHO, one may use (10) to conclude that \( \delta \bar{E} \sim O(L^2) \). Explicitly, we have for the \( n = 0 \) SHO state,

\[
\delta \bar{E} = \frac{\eta^2(1-\eta)(1-3\eta)}{4} \left( \frac{L}{a} \right)^2 + O(L^4)
\]  

(25)

which for \( \eta = 1/2 \) is in excellent agreement with the leading result extracted numerically from Fig.(3), \( \delta \bar{E} = -0.0156L^2/a^2 \). Equation \( \text{(25)} \) indicates a number of interesting features: It vanishes both as \( \eta \to 0 \), which is the formal linear limit of \( \text{(10)} \) and also as \( L/a \to 0 \) which is the physical linear limit. \( \delta \bar{E} \) also vanishes at \( \eta = 1/3 \) and \( \eta = 1 \) but it is apparent from \( \text{(10)} \)
that unlike the \( \eta \to 0 \) case the other two critical values are dependent on \( V(x) \).

We also note that \( \delta \bar{E} \) in (23) is positive for \( \eta < 1/3 \) and negative for larger values. Such crossing behaviour will also be seen below for excited states but, more remarkably, at a universal (that is, \( V(x) \) independent) value of \( \eta \).

The conclusion \( \delta E \sim O(L^2) \) that we have drawn for nodeless states from (10) is for smooth one-dimensional potentials. For higher dimensions the conclusion is still true because of the form of (22) but now one may encounter some nodes that are integrable, as in the hydrogen atom case to be discussed in Sect.(4.3) below.

### 4.2 Excited States in One Dimension

When the unperturbed wavefunction \( \phi(x) \) vanishes at a number of nodes, the \( L \)-expansion of the quantum potential \( Q_1 \) breaks down. We therefore proceed as follows: Suppose first that \( p(x) \) has exactly one node at \( x = x_1 \). Since there are two widely separated length scales, \( L \ll a \), we may divide the integration region in (7) into three parts, \( (-\infty, x_1 - \frac{\alpha L}{2}) \), \( [x_1 - \frac{\alpha L}{2}, x_1 + \frac{\alpha L}{2}] \) and \( (x_1 + \frac{\alpha L}{2}, \infty) \), where \( \alpha \) is a positive constant tentatively of order one.

In the two nodeless regions the integrand may be expanded safely and it will give a contribution of \( O(L^2) \) to \( \delta E \). In the region including the node one may perform the alternative Taylor expansion \( \phi(x) \approx C^2_1(x - x_1) \) and so \( p(x) \approx C^2_1(x - x_1)^2 \). Thus

\[
\delta E \approx \frac{\hbar^2 C_1^2}{4mL^2\eta^4} \int_{\frac{\alpha L}{2}}^{\frac{\alpha L}{2}} dx x^2 \left[ \ln \frac{x^2}{(1 - \eta)x^2 + \eta(x + \eta L)^2} + 1 \right. \\
- \frac{(1 - \eta)x^2}{(1 - \eta)x^2 + \eta(x + \eta L)^2} - \frac{\eta(x - \eta L)^2}{(1 - \eta)(x - \eta L)^2 + \eta x^2} \\
- \frac{\hbar^2 C_1^2 |L|}{4m\eta^4} \int_{-\alpha/2}^{\alpha/2} dy y^2 \left[ \ln \frac{y^2}{(1 - \eta)y^2 + \eta(y + \eta)^2} + 1 \right. \\
- \frac{(1 - \eta)y^2}{(1 - \eta)y^2 + \eta(y + \eta)^2} - \frac{\eta(y - \eta)^2}{(1 - \eta)(y - \eta)^2 + \eta y^2} + O(L^2). 
\]

(26)
Notice that the $L$-independent $Q$ piece of $F$ in (2) does not contribute to (27) at the leading order. For $\phi(x)$ having nodes at $x = x_1, x_2, \ldots, x_N$ we may repeat the above procedure in the neighbourhood of each node as long as $N|L| << a$ so that the nodes are widely separated. Then

$$\delta E = \frac{\hbar^2 L}{4m\eta^4} J(\eta, \alpha) \sum_{p=1}^{N} C_{np}^2 + O(L^2)$$

(28)

with

$$J(\eta, \alpha) \equiv \int_0^{\frac{\alpha}{2}} dy y^2 [\ln \frac{y^2}{(1-\eta)y^2 + \eta(y+\eta)^2} + 1 - \frac{(1-\eta)y^2}{(1-\eta)y^2 + \eta(y+\eta)^2} - \frac{\eta(y-\eta)^2}{(1-\eta)(y-\eta)^2 + \eta y^2}]$$

(29)

In (28) $n$ refers to the quantum number(s) of the unperturbed state and $p$ labels a node. The expression clearly shows the non-analytic $O(|L|)$ trend observed numerically in the previous section. Notice that the leading $|L|^3$ part of the integral (26) comes already from the $\int dx x^2$ piece after the scaling $x = |L|y$ , and so the expression (28) is exact at the indicated order. Subleading terms in the Taylor expansion of $p_n(x) \approx C_{np}^2(x - x_p)^2 + O(x^3)$ contribute only at $O(L^2)$ to $\delta E$.

The other remarkable aspect of the formula (28) is that the specific dependence on the external potential $V(x)$ has been factorised: it is only in the $C_{np}$ coefficients.

The dominance of the nodes for excited states can be seen from Fig.(12) which shows the integrand $pF(p)$ of (7) for the $n = 2$ state of the SHO. The sharp peaks at the nodes are manifest. Fig.(13) shows an enlarged region of the integrand around one of the nodes.

The integral $J(\eta, \alpha)$ appears to be dependent on the arbitrary cutoff $\alpha$ which we have taken to be independent of $n$ and $p$ (the specific node). We state here some properties of $J(\eta, \alpha)$ which are derived in Appendix A.

- $J(\eta \to 0, \alpha) \to 2\frac{\alpha}{3} \pi \eta^{9/2} + O(\eta^{11/2})$ , so $\delta E \sim J/\eta^4 \to 0$ as $\eta \to 0$ for all excited states. The fractional powers of $\eta$ are another indication of the non-analyticity of the leading energy shifts.
\begin{itemize}
  \item $J(\eta, \alpha \to \infty) \to \frac{\eta^2}{2} \sqrt{1-\eta} \eta^{9/2} (4\eta - 1)\pi + O(1/\alpha)$. Thus for large values of $\alpha$, $J$ varies very slowly leading therefore to a negligible cutoff ambiguity in $\delta E$.
  
  \item For any $\alpha$, $J(\eta, \alpha)$ vanishes at some value of $\eta$. For large $\alpha$, as the previous note shows, $\eta_c \sim 1/4$. From our numerical investigations we found that for the excited states of the infinite well, $\delta E = 0$ for a value of $\eta$ between $(0.24, 0.25)$, in close agreement with the prediction coming from the asymptotic ($\alpha \to \infty$) form of $J$. In practise, we get very good agreement, in the infinite well problem, between the numerical and analytical values for $\eta_c$ if we set $\alpha \geq 10$.
  
  \item We have confirmed numerically that the energy shifts for the excited states of the SHO also vanish at essentially (limited by our numerical precision) the same $\eta_c$. $0.24 - 0.25$ as that for the infinite well. Thus it appears that $\eta_c \sim 0.25$ is a universal, $V(x)$ independent, critical point, as the asymptotic analytical expression for $J$ and (28) also suggest. In summary, we can take $\alpha \geq 10$ for all problems to fix the cutoff ambiguity in (28).
  
  \item $J$ is positive for $\eta$ small and negative for $\eta$ large and so this means that the energy shifts similarly change signs, a fact which we have confirmed for the infinite well and SHO by direct numerical study of the full expression (11). In particular we note that $J(\eta = 1/2, \alpha) < 0$, so explaining the negative sign seen in our results for $\delta E$ in Section(3).
\end{itemize}

### 4.3 Infinite Well Revisited

For the infinite well we may evaluate $\delta E$ explicitly since the $C_{np}$ for these case are easily obtained from the wavefunctions (11),

$$C_{np} = \sqrt{\frac{2}{a}} \frac{n\pi}{a} (-1)^p, \ 0 < p \leq n.$$

Thus the dimensionless energy shift is

$$\tilde{\delta E} = \frac{a^2 |L|}{2\pi^2 \eta^4} \sum_{p=1}^{n} \left[ \frac{2}{a} \left( \frac{n\pi}{a} \right)^2 \right] J(\eta, \alpha)$$

$$= \frac{|L|}{a} \frac{n^3 J(\eta, \alpha)}{\eta^4}.$$
The formula is valid also for the ground state, \( n = 1 \), because the corresponding wavefunction vanishes at the two end points, each of which contributes the equivalent of half of one regular node as can be seen by reviewing the derivation of (28) above. We therefore now have an understanding of the intriguing \( n^3 \) behaviour seen numerically in Sect.(3): each \( C_{np}^2 \) contributes an identical \( n^2 \) piece to the sum over \( n \) terms.

We find at \( \eta = 1/2 \),

\[
\delta \tilde{E}_n = \frac{|L|}{\alpha} 16n^3 J(1/2, \alpha) \tag{33}
\]

\[
\equiv -f(\alpha) \frac{|L|}{\alpha} n^3, \tag{34}
\]

with \( 0.99 < f(\alpha) < 1.05 \) as the cutoff \( \alpha \) ranges over \((10, \infty)\), in good agreement with our numerical study of the infinite well in Sect.(3) which indicated an average value of 1.03 for the numerical factor.

For other potentials an explicit evaluation of the sum in (28) does not appear feasible as the coefficients in general are very complicated functions of \( n \) and \( p \) that are rarely known in closed form. However an asymptotic or numerical evaluation of \( \sum C_{np}^2 \) might be possible if an explicit dependence on \( n \) is required. We illustrate this for the SHO in Appendix B.

We emphasize however that the expression (28) already displays two universal features: \( \delta E \propto |L| \) for unperturbed states with nodes and the shift being negative (positive) for large (small) \( \eta \) values.

### 4.4 Higher Dimensions

For higher dimensions an explicit analysis similar to the preceding subsection is awkward because the nonlinearity is expressed in the preferred Cartesian basis with broken rotational symmetry whereas most potentials, such as the hydrogen atom, have a symmetry and so are better expressed in other coordinate systems. Nevertheless, we can make some general statements.

For nodeless states we have the analog of (10) by expanding (23) and so get \( \delta E \sim O(L^2) \).

For excited states the presence of nodes leads to singularities as before in the naive Taylor expansion. Arguments similar to above then imply that \( \delta E \) will be enhanced to \( O(|L|) \) as each coordinate is treated separately in (23). Thus we expect again the energy shifts to be positive for small \( \eta \) and negative for larger \( \eta \), vanishing at some intermediate value. The numerical results of
Sect.(3.3) for the angular momentum states \( l \neq n - 1 \) are in agreement with these general expectations although we have not checked the expected variation with \( \eta \).

A very interesting situation arises for the \( l = n - 1 \) states of the hydrogen atom for which the radial wavefunction vanishes only at the origin,

\[
\psi_{n,l=\text{n-1}} \sim r^{n-1} Y_{\ell m}(\theta, \phi).
\]

(35)

Although the corresponding probability density \( p(\vec{r}) \) has a node at the origin, the radial integral in the \( O(L^2) \) contribution \( \delta E \sim \int d\Omega \int_0^\infty dr p(r) \ldots \), the three dimensional analog of (10), is nonsingular, as we see by power counting, if \( 2(n-1)+3 > 4 \), that is, for \( n \geq 2 \). This explains the “anomalous”, \( \delta E \sim L^2 \), behaviour of such excited states observed in Sect.(3.3).

5 Exactly solved models

In using perturbation theory we have assumed, as is usually done in physics, that the quantity of interest will deform continuously as the perturbation is turned on. Here we briefly discuss two nonlinear Schrodinger equations for which exact solutions are available so that one can test perturbation theory. In addition, the models will be used to further highlight some of the distinctive features we have observed for the nonlinear equation (1). For simplicity we consider only the one dimensional case here.

5.1 Gross-Pitaevskii (GP) Equation

This classic [10] equation is used as an effective theory in studies of condensed matter. It corresponds to using \( F(p(x,t)) = gp(x,t) \) in (1). To leading order, one has

\[
\delta E = g \int p^2 dx
\]

so that energy shifts are always positive or negative depending on the sign of the coupling \( g \). Explicitly for the infinite well one has

\[
\delta E_n = \frac{3g}{2a},
\]

(37)

a constant shift independent of \( n \), as obtained earlier in Ref.[13] which also showed that this perturbative result was the appropriate limit of the exact solution of this equation with the infinite well potential.
For the SHO potential we are not aware of any exact solutions for the GP equation but (36) gives the leading order correction,
\[
\delta E \approx \frac{g}{a \sqrt{2 \pi n}} n^{-0.31},
\] (38)
for \( n \geq 1 \), showing that it decreases with \( n \). We obtained (38) through a numerical best-fit to an assumed power law: Fig.(14) shows a graph of \( \delta E \) against \( n \) while Fig.(15) is the corresponding log-log plot.

The constant or decreasing dependence of the energy shifts on \( n \), respectively for the above two potentials in the GP equation, should be contrasted with the results for the information-theoretic nonlinearity (2) which showed an increasing dependence on \( n \). As we saw in Sect.(4) that increasing dependence on \( n \) was due to the prominent role played by nodes which by contrast are completely irrelevant in (36).

### 5.2 A Pseudo-nonlinear model

Starting from the usual linear Schrodinger equation
\[
i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi, \tag{39}
\]
we can re-arrange the kinetic term by an amount \( \epsilon \) to obtain
\[
i\hbar \frac{\partial \Psi}{\partial t} = -(1 - \epsilon) \frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi - \frac{\epsilon \hbar^2}{\Psi 2m} \left( \frac{\partial^2 \Psi}{\partial x^2} \right) \Psi, \tag{40}
\]
which corresponds to an equivalent nonlinear Schrodinger equation with mass \( m/(1 - \epsilon) \) in the linear part and a perturbed nonlinearity
\[
F(p) \equiv -\frac{\epsilon \hbar^2}{\Psi 2m} \left( \frac{\partial^2 \Psi}{\partial x^2} \right). \tag{41}
\]

Thus in this case the exact and unperturbed solutions just correspond to a mass renormalisation. For stationary states first order perturbation theory gives
\[
\delta E = -\frac{\epsilon \hbar^2}{2m} \int dx \frac{p}{\sqrt{p}} \frac{\partial^2 \sqrt{p}}{\partial x^2} \tag{42}
\]
\[
= \frac{\epsilon \hbar^2}{2m} \int dx \left( \frac{\partial \sqrt{p}}{\partial x} \right)^2 \tag{43}
\]
so that again the energy shifts are simply correlated in sign with the sign of \( \epsilon \).

As the wavefunctions for the linear Schrödinger equation with an infinite well potential are independent of the mass and so also of \( \epsilon \), the first order correction using \( 43 \) gives an exactly \( \epsilon \) contribution in this case. When that is added to the unperturbed energies which are proportional to \( 1 - \epsilon \), one gets the full answer, that is, first order perturbation theory for this problem is all there is.

For the SHO and other problems the first order correction will generally, by construction, lead to final results correct up to errors of \( O(\epsilon)^2 \).

Thus in this nonlinear model the perturbative corrections to the energy always have the same \( n \) dependence as that for the unperturbed energies. Therefore one may interpret the analogous results for Eq.\( 2 \) as due in some rough sense to higher derivative terms, higher than the second-order kinetic energy terms like \( 11 \). This is indeed what is implied by a formal expansion of \( 2 \) but as we discussed in Sections (2,4), that formal expansion is in general singular and the actual result depends acutely on whether the unperturbed states do or do not have nodes.

### 6 Conclusion

Our main result is Eq.\( 28 \) which gives the leading correction, due to the nonlinearity \( 2 \), to the energy eigenvalues of the usual 1 + 1 dimensional linear Schrödinger equation for cases where the unperturbed states have nodes. The correction is proportional to \( |L|/\alpha \), hence it is non-analytic and an enhancement over the correction for states without nodes for which \( \delta E \propto L^2 \).

The dependence of \( \delta E \) on the external potential is only through the \( C_{np} \) coefficients.

The function \( J(\eta, \alpha) \) in \( 29 \) depends on a cutoff parameter \( \alpha \) used in the analytic derivation of that equation but we have shown that for large \( \alpha \), \( J \) varies very slowly and indeed using \( J(\eta, \infty) \) gives good agreement with various purely numerical computations. Therefore for states with nodes

\[
\delta E \approx \frac{\hbar^2 |L|}{4m\eta^4} J(\eta, \infty) \sum_{p=1}^{N} C_{np}^2
\]

with

\[
J(\eta, \infty) = \frac{-2}{3} \sqrt{1 - \eta \eta^{9/2} (4\eta - 1)} \pi .
\]
Thus independent of $V(x)$, the leading energy correction to states with nodes vanishes at $\eta = 1/4$, something we have verified numerically for both the infinite well and the SHO potential. The existence of such a universal critical point is quite unexpected as neither the equations of motion nor the full expression (7) indicate such a special point.

As eq.(13) shows, $\delta E < 0$ for $\eta > 1/4$, being positive for smaller $\eta$. Since $\eta$ is a free parameter in the nonlinear equation, it means that there is a qualitative difference in the properties of that equation for $\eta$ small or large.

It is interesting to note from (45) that the expression (44) is real precisely in the range $0 < \eta < 1$, which is exactly the explicit condition on $\eta$ we started with. Also, the fractional power on the $\eta^{9/2}$ factor again emphasizes, in addition to the $|L|$ term, the non-analytic character of (44).

For the usual linear Schrodinger equation in one space dimension, states with nodes are the excited states of a system although in some cases, such as that for the infinite well, the ground state also has nodes. For states without nodes, which are typically ground states, such as for the SHO, the leading energy corrections are of order $L^2$ and given by a simple expansion of (7). Thus at $\eta = 1/4$ all the states of system, with or without nodes, have $\delta E \propto L^2$.

For higher dimensions, the qualitative properties are similar to the one dimensional case. That is, nodeless states get $\delta E \propto L^2$ while states with nodes in general have $\delta E \propto L$. We saw an exception in the hydrogen atom example where some excited states with nodes had $\delta E \propto L^2$ because the potential singularities were integrable.

Let us now discuss the validity of perturbation theory for the infinite well and SHO where $\delta E$ increases with $n$, the principal quantum number, faster than the unperturbed states. For example, in the infinite well case we found $\delta E \propto |L|n^3/a$ so that even if $|L|/a << 1$, at large $n$ the correction $\delta E$ would no longer be small. This indicates a breakdown of first order perturbation theory for large $n$ states, requiring one to go to higher orders. Presumably, if $L/a$ is small, the net perturbative correction should be small for all $n$, so one expects the higher order corrections to sum to a reasonable expression. A simple Pade resummation suggests $\delta E \propto n^2/(1 + bn)$ for the infinite well at $\eta = 1/2$, where $b > 0$ is some constant.

Finally, we discuss some physical implications of our result if the non-linearity (2) is a fundamental or effective representation of potential new physics at short distances as suggested in [5]. For a particle in a large box, we may use the infinite well result, generalised via (22) to three independent
dimensions, to see that for $\eta > 1/4$ high energy states have their energies lowered, that is the nonlinearity acts to moderate high energy divergences. One reaches the same conclusion from the SHO results if one thinks of ordinary free quantum field theory modes as SHO states.

Thus the nonlinearity (2), applied here heuristically to field theory, suggests that the usual high energy divergences of quantum field theory might be moderated, if not absolutely eliminated. Now in [3, 5] it was suggested that the nonlinearity (2) might be linked to gravity simply by requiring $L$ to be a universal length scale. Taken together, this then suggests that gravity might moderate ultraviolet divergences of field theory. Interestingly, the suggestion that gravity might regulate ultraviolet divergences has been made several times in the past through different reasoning within the context of usual linear quantum theory, see for example [14] and references therein.

However the above moderation works only for $\eta > 1/4$ where we have $\delta E < 0$ for excited states. What if in reality one has $\eta < 1/4$? Then $\delta E > 0$ and this means that we are quite possibly under-estimating the amount of energy in quantum systems. One wonders if this might be relevant for the dark energy/matter problem in cosmology.

So it appears that knowing the physically relevant value of $\eta$ is quite important for potential phenomenological applications of the nonlinear equation. Perhaps $\eta$ could be fixed theoretically through a renormalisation group study of a discretised version of the nonlinear equation (2). In this regard, the naturally induced discretisation noted in [9] might be useful.
7 Appendix A: The $J(\eta, \alpha)$ function.

In our analytical expression for the leading $O(|L|)$ correction to the excited energy levels we encountered the function.

\[
J(\eta, \alpha) = \int_{-\alpha/2}^{\alpha/2} dy y^2 \left[ \ln \left( \frac{y^2}{(1-\eta)y^2 + \eta(y+\eta)^2} + 1 \right) - \frac{(1-\eta)y^2}{(1-\eta)y^2 + \eta(y+\eta)^2} - \frac{\eta(y-\eta)^2}{(1-\eta)(y-\eta)^2 + \eta y^2} \right].
\] (46)

The integral may be evaluated exactly but the result is long and not very illuminating. So let us first consider a very crude approximation of (46) which reveals some of the key features. Consider a value of $\eta$ away from the end-points 0, 1. Next approximate the integrand by its value near the midpoint of the integration domain, $y \sim 0$, so

\[
J(\eta, \alpha)_{\text{crude}} \sim \int_{-\alpha/2}^{\alpha/2} dy y^2 \left[ \ln y^2 + \frac{(1 - 2\eta)}{(1 - \eta)} - \ln \eta^3 \right].
\] (47)

For $\alpha < 2$ we see immediately that the $\ln y^2$ term is always negative while the $\eta$ dependent piece starts out positive for low $\eta$ values and turns negative at larger values. Thus this crude version of $J$ shows the sign change we expect.

It might interest the reader to note that the logarithmic contribution from (3) to the integral in (7) is well known to be nonnegative, as is easily proven using the inequality $\log z \leq z - 1$. However as we see from (47), at some points of the integration domain the logarithmic contribution can be negative and indeed that is where the nodes dominate.

We now turn to a more precise examination of (46) but in various limits. First,

\[
J(\eta \to 0, \alpha) = \frac{2}{3} \pi \eta^{9/2} - 3 \pi \eta^{11/2} - \frac{18\eta^6}{\alpha} + \frac{5}{4} \pi \eta^{13/2} + O(\eta^7).
\] (48)

Note the $\alpha$ dependence in the third term. Thus $J$ starts out from zero as $\eta$ increases from 0, increases in value to a maximum, and then decreases for larger $\eta$ values, reaching $J = 0$ again at some point. Fig.(16) shows the behaviour of $J$ for $\alpha = 10$. Next,
\[ J(\eta, \alpha \to \infty) \to -\frac{2}{3} \sqrt{1 - \eta} \eta^{9/2} (4\eta - 1)\pi - \frac{2\eta^6(9 - 32\eta + 24\eta^2)}{\alpha} + O(1/\alpha^2). \]

(49)

This shows the mild dependence of \( J \) at large \( \alpha \). Fig.(17) shows the plot for \( \eta = 1/2 \).

One possibility to fix \( \alpha \) theoretically is to choose the point where \( \partial J/\partial \alpha \) vanishes but such a minimum point does not exist for all \( \eta \) values as Fig.(17) for \( \eta = 1/2 \) shows. Thus a better choice seems to be a value of \( \alpha \) where \( J \) varies very slowly. Such a region always exists at large \( \alpha \) as we see from the asymptotic form (49).

Indeed it is the large value \( \alpha \geq 10 \) that gives a value for \( \eta_c \) in (49) that agrees with direct numerical calculations in Sect.(3). With \( \alpha \) fixed this way, at large values, we have \( J \) unambiguously positive for low values of \( \eta \) and negative for large \( \eta \) values.

To summarise some of the features of the \( J(\eta, \alpha) \) function: \( J = 0 \) at \( \eta = 0 \) and \( \eta = \eta_c \) with \( \eta_c \to 1/4 \) as \( \alpha \to \infty \). We have \(-0.0017 < J(1/4, \alpha) < 0\), showing the consistently tiny value for \( J \) for all \( \alpha \) near the point \( \eta = 1/4 \). As \( \eta \to 1 \), \( J \) is negative, approaching zero, from below, only as \( \alpha \to \infty \).

8 Appendix B: Semi-analytical Analysis of SHO Energy Shifts

Recall that our analytical estimates of the energy shifts for the excited states gave

\[ \delta E = \frac{\hbar^2 |L|}{4m\eta^4} J(\eta, \alpha) \sum_{p=1}^{N} C_{np}^2 + O(L^2). \]

For the SHO, we obtain \( C_{np} \) from the wavefunctions

\[ \psi_n(z) = N_n (\pi a^2)^{-1/4} H_n(z) \exp(-z^2/2), \]

where \( z = x/a \), \( N_n = 1/\sqrt{2^n n!} \), and \( H_n(z) \) are the \( n \)-th order Hermite polynomials. Observe that the wavefunction vanishes only when the Hermite polynomial is zero.

What is required is the Taylor expansion of the wavefunction about the nodes. At the nodes,

\[ H_n(z_p^n) = 0 \quad \text{for} \quad p = 1, 2, \ldots n, \quad (50) \]
where \( z^n_p \) refers to the \( p \)-th root of \( H_n(z) \). Therefore near a root we have, to leading order,
\[
\psi_n(z) \approx \psi_n(z^n_p) + \frac{d\psi_n}{dz}(z^n_p)(z - z^n_p)
\]
\[
= \frac{d\psi_n}{dz}(z^n_p)(z - z^n_p).
\]
Reverting to \( x \), one obtains
\[
C_{np} = \frac{d\psi_n}{dx}(z^n_p) = \frac{1}{a} \left( N_n(\pi a^2)^{-1/4} H'_n(z^n_p) \exp \left[ -\left( z^n_p \right)^2 / 2 \right] \right).
\]
Using the identity
\[
H_{n+1}(x) + H'_n(x) = 2xH_n(x)
\]
then gives
\[
H'_n(z^n_p) = -H_{n+1}(z^n_p). \tag{52}
\]
Finally,
\[
C^2_{np} = \frac{1}{a^3} \frac{1}{\sqrt{\pi} 2^n n!} \left[ H_{n+1}(z^n_p) \right]^2 \exp \left( -\left( z^n_p \right)^2 \right). \tag{53}
\]
We evaluate the sum of these \( C^2_{np} \) through a numerical computation of the roots and sums of the Hermite polynomials. Since the \( 'a' \) behaviour is already explicit, we examine the \( n \)-dependence by calculating \( \sum a^3 C^2_{np} \) for \( n = 1 \) to \( n = 23 \). Fig. (18) shows a log-log plot of \( \sum a^3 C^2_{np} \) against \( n \). Furthermore, if one uses \( \eta = 1/2 \) and \( \alpha = 10 \):
\[
\delta \tilde{E} = \frac{a^2 |L|}{\eta^4} \left( \sum C^2_{np} \right) J(1/2, 10) \tag{54}
\]
\[
= -0.25 |L| a n^{-1.40}, \tag{55}
\]
while the limit \( \alpha \to \infty \) would increase the numerical prefactor slightly to 0.27. These results are thus in good agreement with the purely numerical ones quoted in Section (3) (which were actually for relatively low values of \( a \)).
References

    S. Weinberg, Ann. Phys. (NY) 194, 336 (1989);
    (1999);
    For some reviews, see G. Svetlichny, arXiv:quant-ph/0410036; R. Carroll,

    T. Chupp and R. Hoare, Phys. Rev. Lett. 64, 2261, (1990);
    R. Walsworth, et.al, Phys. Rev. Lett. 64, 2599 (1990), and references
    therein.

    2004 workshop held at Piombino, Italy), quant-ph/0412192;
    the 3rd QTRF conference held at Vaxjo, Sweden, June 2005),


    (1999);


    Probability Theory, The Logic of Science (Cambridge University Press,
    2004);
    For a review see R. Balian, Studies in Hist. and Phil. of Mod. Phys.,
    36 (2005) 323.


    and wave collapse (Springer, 1999).


Figure Captions

- Figure 1: Log-log plot of $|\delta \tilde{E}|$ vs. $a$ for the ground state $n = 1$ of the infinite well. The line has slope $0.99985(2)$ and intercept $0.0448(1)$. In this and the other figures the ‘logs’ are natural logarithms.

- Figure 2: Log-log plot of $|\delta \tilde{E}|$ vs. $n$ for $a = 5000$ of the infinite well. The line has slope $2.9984(2)$ and intercept $-8.4680(6)$.

- Figure 3: Log-log plot of $|\delta \tilde{E}|$ vs. $a$ for the ground state $n = 0$ of the SHO. The line has slope $-2.0000(1)$ and intercept $-4.1587(7)$.

- Figure 4: Log-log plot of $|\delta \tilde{E}|$ vs. $a$ for the $n = 12$ state of the SHO. The line has slope $-0.9980(2)$ and intercept $2.156(1)$.

- Figure 5: Log-log plot of $|\delta \tilde{E}|$ vs. $n$ for $a = 1000$ of the SHO. The line has slope $1.413(8)$ and intercept $-8.25(2)$.

- Figure 6: Log-log plot of $|\delta \tilde{E}|$ vs. $a$ for the ground state $n = 1$ of the Hydrogen atom. The line has slope $-1.9987(2)$ and intercept $-2.482(1)$.

- Figure 7: Log-log plot of $|\delta \tilde{E}|$ vs. $a$ for the $n = 2$, $l = 0$ state of the Hydrogen atom. The line has slope $-1.032(9)$ and intercept $-3.49(4)$.

- Figure 8: Plot of $|\delta E/E_0|$ vs. $n \geq 2$ for $l = 0$ states of Hydrogen atom. Curves for different values for $a$ are shown.

- Figure 9: Log-log plot of $|\delta \tilde{E}|$ vs. $a$ for the $n = 2$, $l = 1$, $m = 0$ state of the Hydrogen atom. The line has slope $-2.02(4)$ and intercept $-6.75(24)$.

- Figure 10: Log-log plot of $|\delta \tilde{E}|$ vs. $a$ for the $n = 3$, $l = 2$, $m = 2$ state of the Hydrogen atom. The line has slope $-1.979(7)$ and intercept $-10.14(3)$.

- Figure 11: Log-log plot of $|\delta \tilde{E}|$ vs. $a$ for the $n = 3$, $l = 2$, $m = 1$ state of the Hydrogen atom. The line has slope $-1.986(4)$ and intercept $-9.61(2)$. 

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• Figure 12: Plot of the integrand $pF(p)$ vs. $x$ of (17) of the $n = 2$ state of the SHO. It depicts how the contribution to the energy shift is dominated by the nodes.

• Figure 13: An enlarged portion of Fig.(12) around one of the nodes. It illustrates the significant contribution to (17) of a small interval in the vicinity of the node.

• Figure 14: Plot of $\delta E$ vs $n$ for the GP equation with SHO potential.

• Figure 15: Log-log plot of $\delta E$ vs $n$ for the GP equation with SHO potential. The line has slope $-0.307(5)$ and intercept $-1.15(1)$.

• Figure 16: Plot of $J(\eta, \alpha = 10)$ from $\eta = 0$ to $\eta = 0.28$.

• Figure 17: Plot of $J(\eta = 1/2, \alpha)$ from $\alpha = 0$ to $\alpha = 400$.

• Figure 18: Log-log plot of $\sum a^3C_{np}^2$ vs. $n$ for the SHO. The line has a slope of $1.404(7)$ and intercept $0.03(1)$, matching closely the result $\delta E \propto n^{1.41}$.
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