ANHARMONIC OSCILLATOR*

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The study of anharmonic oscillator does reveal many interesting aspects of various branches of physics. To give you an example let me mention the use of anharmonic contribution to explain the vibrational spectra of the diatomic molecules in chemical physics. Another example in classical physics is the understanding of thermal expansion by considering the presence of a term βx^3 in the one-dimensional anharmonic oscillator Hamiltonian. The main reason why I am motivated to investigate the problem of anharmonic oscillator is the fact that some one-dimensional model field theory of the $\lambda \phi^4$ type can be easily understood through a study of quantum mechanical anharmonic oscillator problem.

To be exact let us consider a model Hamiltonian given by

$$H = \frac{1}{2}\dot{\phi}^2 + \frac{1}{2}m\phi^2 + g\phi^4$$

when ϕ is a field variable and it is only a function of time alone and of no space-dimension. Obviously, then, we have a particle situated at a particular point and interacting with itself through a ϕ^4 self-interaction. Since the asymptotic field does not exist, we have no scattering. We, then, are only interested in solving the equation

$$H | \psi \rangle = E | \psi \rangle$$
.

An exact knowledge of E in this one-dimension would give us a complete understanding of the exact mass shift in this model field theory. It is hoped that such knowledge would in future give a lead to discuss the real 4-dimensional field theory of nature. To see the connection of the one-dimensional field theory with wave-mechanical anharmonic oscillator in one-dimension we use interaction representation and set

$$\phi = \frac{1}{\sqrt{2m}} \left[ae^{-imt} + a^+e^{imt} \right]$$

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and

$$\dot{\phi} = \sqrt{\frac{m}{2}} \left[-iae^{-imt} + ia^{+}e^{imt} \right].$$

This immediately reduces the Hamiltonian H into

$$H = m(a^{+}a + \frac{1}{2}) + \frac{g}{4m^{2}}(a + a^{+}).^{4}$$

To solve the mass-shift equation we put

$$|\psi\rangle = \sum_{n} C_{n} (a^{+})^{n} |0\rangle$$

in $H | \psi \rangle = E | \psi \rangle$. This gives the following difference equation for C_n

$$EC_{n} = (n + \frac{1}{2}) C_{n} + g/4 [C_{n-4} + 4 (n - 2) a_{n-2} + 6n (n - 1) C_{n} + 4n (n + 1) (n + 2) C_{n+2} + (n + 1) (n + 2) (n + 3) \times (n + 4) C_{n+4}].$$
(1)

Write the one-dimensional anharmonic oscillator Hamiltonian in the form

$$H = -\frac{d^2}{dx^2} + m^2x^2 + \lambda x^4; \quad \lambda = 2g.$$

We now see that this Hamiltonian equation $H\psi = E\psi$ is again leading to the difference equation (1) if we solve this by making the ansatz

$$\psi = \sum_{n} C_{n} He_{n}(x)$$

where $He_n(x)$ are the standard hermite polynomials. I need not elaborate this further here. This identification is, however, of immense help. For we now can have Feynman diagram techniques available to us for the evaluation of many physical processes. For example, for a vertex we put a factor of λ , and for a propagator we write the expression $(E^2 - m^2 + i\epsilon)^{-1}$ while for a loop integration we should perform an integration $\int_{-\infty}^{\infty} dE/2\pi i$. Using these tricks we can easily calculate the ground state energy shift ΔE for the anharmonic oscillator problem by noting that ΔE receives contribution from all connected closed loop diagrams. The result of this is the following:

$$\triangle E = \frac{1}{2} + \frac{3}{4}\lambda - \frac{21}{8}\lambda^2 + \frac{333}{16}\lambda^3 - \dots$$

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It is interesting to note that the above perturbation series (in the anharmonic strength) is a divergent one although every term is finite. Bender and Wu¹ have calculated the first 75 terms and showed that, in fact, the n-th term behaves as $3^n \Gamma(n)$. Thus this one-dimensional problem teaches a very interesting thing, namely, that, in one-dimension model field theory, there is no finite mass-shift. This also implies that perturbation series calculation of the energy shift of the harmonic oscillator by λx^4 anharmonic perturbation leads to a divergent expression. Question then immediately occurs, how then one can use this for description of physical phenomena even at the quantum mechanical level? The next-half of the talk would be devoted to this. To make physical processes understandable we first look if at all one can find a way to give meaning to this divergent expansion. Some people have used the Pade-approximation techniques to sum such divergent series. The method consists of approximating a series by a series of rational functions. That is, by replacing $\phi(Z) = \sum_{n} a_{n}Z^{n}$ in terms of $P_{m}(Z)/Q_{m}(Z)$ where P_m and Q_m are polynomials of degree m. The m may be 1, 2, 3 ... K. The various K-values lead to [K, K]-diagonal Pade approximants. The hope is that [K, K]-approximant in the limit of large K would give the correct value of $\phi(Z)$ beyond points where ϕ is not ordinarily defined. Thus Pade approximation provides a way of analytic continuation of a series, outside its radius of convergence. In general the [N, M] Pade approximant for

$$f = \sum_{n} a_{n} x^{n}$$
 is
$$f = \frac{P^{(M)}}{Q^{(N)}}$$

where

$$P^{(M)} = \begin{bmatrix} a_{M-N+1} & a_{M-N+2} & \dots & a_{M+1} \\ \vdots & & & & & \\ a_{M} & a_{M+1} & \dots & a_{M+N} \\ \sum_{j=N}^{M} a_{j-N}x^{j} & \sum_{j=N-1}^{M} a_{j-N+1}x^{j} & \dots & \sum_{j=0}^{M} a_{j}x^{j} \end{bmatrix}$$

and

$$\mathbf{Q^{(N)}} = \begin{bmatrix} a_{\mathbf{M}-\mathbf{N}+\mathbf{1}} & \dots & a_{\mathbf{M}+\mathbf{1}} \\ \vdots & \vdots & \ddots & \vdots \\ a_{\mathbf{M}} & \dots & a_{\mathbf{M}+\mathbf{N}} \\ x^{\mathbf{N}} & \dots & 1 \end{bmatrix}$$

This approximation scheme for analytic continuation reminds us of the associated technique of continued fraction method of analytic continuation. For example, let $C_N(x)$ be the N-th convergent for $f(x) = \sum b_n x^n$.

That is

$$C_{N}(x) = \frac{f(x_{1})}{1 + a_{1}(x - x_{1})}$$

$$1 + a_{2}(x - x_{2})$$

$$1 + a_{N}$$

where $x_1, x_2 f \dots x_N$ are N-points for which we have

$$C_N(x_i) = f(x_i); i = 1, ... N.$$

If $f(x_i)$ (i = 1, ..., N) are known, then the coefficients $a_1, a_2, ...,$ etc., are all known. For example we have

$$f(x_2) = \frac{f(x_1)}{1 + a_1(x_2 - x_1)}$$

$$f(x_3) = \frac{f(x_1)}{1 + a_1(x_3 - x_1)}$$

These then determine, a_1 , a_2 , etc.,

$$a_1(x_2 - x_1) = -1 + \frac{f(x_1)}{f(x_2)}$$

$$a_2(x_3 - x_2) = -1 + \frac{a_1(x_3 - x_1)}{-1 + f(x_1)}$$

$$f(x_2), \quad \text{etc.}$$

The various convergents are nothing but the various Pade approximants: The continued fraction method requires the knowledge of f(x) at some points like $x = x_1, x_2 \cdots x_N$. This is particularly useful when one knows in advance that the series is an asymptotic one, in that case, the values of f(x) is known for many sufficiently small values of the parameter which in turn enable one to obtain the value of f(x) at points beyond $(x_1 \cdots x_N)$ through the various convergents of the continued fraction.

As an interesting application of continued fraction² in physics let me point out how one can obtain various bound state solutions of Schrodinger equation. Consider the differential equation for f(x) when $\psi = e^{-x^2/2} f(x)$ and ψ is the solution of the Hamiltonian equation $H\psi = E\psi$, with H standing for the harmonic oscillator problem namely

$$p^2/2m + \frac{1}{2}m\omega^2x^2.$$

With

$$\xi = \sqrt{m\omega/\hbar}; \quad \epsilon = 2E/\hbar\omega$$

we have for f(x)

$$f'' - 2\xi f' + (\epsilon - 1)f = 0,$$

which gives the following continued fraction for f'/f;

gives the following continued fraction
$$\frac{f'}{f} = \frac{1 - \epsilon}{-2\xi + 3 - \epsilon} - \frac{1 - \epsilon}{-2\xi + 5 - \epsilon}$$

Putting $\epsilon = 1$, $\epsilon = 3$, etc., one easily discovers the various Hermite polynomials as solutions.

Another interesting method known as Borel transform has become very useful in connection with the summation of a divergent perturbation series. This has recently found interesting application not only in perturbation expansion but also in non-polynomial field theory. Let me illustrate the powerfulness of the method in connection with non-polynomial theory. we consider a Lagrangian

$$-L = \bar{\psi}\psi u(x)$$

where

$$u(x) = G \frac{1}{1 + g\phi(x)}$$

and we are particularly interested in calculating the propagator for the field U(x) it being given that $\phi(x)$ is a mass-less scalar field. Our method, however, is quite straightforward, to generalize the massive ϕ , field. For simplicity we put G = g = 1; and write to calculate

$$\langle : U(x) : : U(x') : \rangle_{T}$$

i.e., the vacuum expectation value of the time ordered product of the super-field U(x) and U(x'). We consider the normal ordered fields, namely: U(x): and U(x'): This is to avoid the divergences which occur in $\phi^2(x)$, that is

$$\phi^{2}(x) = :\phi^{2}(x): + \triangle(0).$$

Noting

$$\frac{1}{1+\phi} = \int_{0}^{\infty} e^{-t (1+\phi)} dt$$

we can easily write

$$\langle : \mathbf{U}(x) : : \mathbf{U}(x') : \rangle_{\mathbf{T}} = \int_{0}^{\infty} \int_{0}^{\infty} e^{-t} e^{-t'} dt dt' \langle : e^{-t\phi} : : e^{-t'\phi(x')} : \rangle_{\mathbf{T}}$$

Using

$$\langle : e^{-t\phi} \colon : e^{-t'\phi(x')} \colon \rangle = e^{-tt} \vartriangle_{\mathbb{F}}(x-x')$$

we find for

$$F(x - x') = \langle : U(x) : : U(x') : \rangle_{T}$$

the following,

$$F(x-x') = \sum_{n=0}^{\infty} n! \triangle_F^n(x-x');$$

we can sum this series by taking Borel transform.

So we re-write

$$F(x - x') = \sum_{n} \int_{0}^{\infty} e^{-\xi} (\xi \triangle_{F})^{n} d\xi$$
$$= \int_{0}^{\infty} e^{-\xi} f(x - x') d\xi$$

where

$$f(x-x') = \sum_{n} (\xi \triangle_{\mathbf{F}}(x-x'))^{n}.$$

From now on we take x' = 0, so that we have

$$f(x) = \sum_{n} \xi^{n} \triangle_{F}^{n}(x),$$

Many ways have now been suggested to sum this and then to take its fourier transform. This is necessary as the physical problems require handling in momentum space for correct interpretation. We do like to consider the f.t. of f(x) here because we would then discover an interesting physical consequence regarding non-polynomial theory. For example, write

$$f(x) = 1 + \xi \triangle_{\mathbf{F}}(x) f(x)$$

going over to momentum space we have

$$f(p) = (2\pi)^4 \,\delta^4(p) + \frac{\xi}{(2\pi)^4 i} \int \frac{f(p-p')}{(p-p')^2} d^4p'.$$

where we used ϕ for a massless scalar field. The above integral equation has an immediate solution. Hence $\tilde{F}(p)$ can be easily written down. For example it is equal to

$$\int_{0}^{\infty} f(p) e^{-\xi} d\xi.$$

Without going into detail we find that

$$\tilde{F}(p) = \frac{1}{p^2} + \int_{0}^{\infty} \frac{\sigma(t)}{p^2 + t} dt$$

where

$$\sigma(t) = (t-2) e^{-t}; \quad 0 < t < \infty$$

Thus the spectral function $\sigma(t)$ is indefinite showing the presence of a state with negative norm, since we can identify

$$(t-2) e^{-t} = \sigma(t) = \sum_{n} |\langle 0 | v | n \rangle|^{2}.$$

Thus the present example of the superfield U(x) produces a ghost state through Borel transform, etc. I need only mention that Borel technique and a combination of Borel-Pade technique have been of good use in producing $\triangle E$ for the anharmonic oscillator case. To complete my talk I consider a purely non-perturbative technique in connection with anharmonic oscillator case. This has been investigated by Datta, Saxena, Srivastava, Varma and myself for the last few years. This is the Hill determinant approach. We consider the equation:

$$\left(-\frac{d^2}{dx^2}+x^2+\lambda x^4\right)\psi=\epsilon\psi.$$

Assume that

$$\psi = \sum_{n} C_n e^{-x^2 2} x^{2n}$$

be the solution for even-parity case. In that case C_n 's should satisfy the following difference equation.

$$2(n+1)(2n+1)C_{n+1} + (\epsilon - 1 - 4n)C_n = \lambda C_{n-2}$$

The eigenvalue condition now emerges from this if we demand under what condition the above difference equation has a solution. The condition is the vanishing of an infinite determinant

To accelerate the determination of the eigenvalues we note that if D_n stands for $n \times n$ approximant of this determinant then

$$D_{n} = (\epsilon - 1 - 4n) D_{n-1} - 16\lambda n (n-1) (n-\frac{1}{2}) (n-3/2) D_{n-3}.$$

From a simple knowledge of a few lower-order D's one can recussively determine various higher order D_n 's. The zeros of D_n 's for $n \to \infty$ on the eigen-

values. Obviously the lowest root will correspond to the ground state energy shift. We have calculated these eigenvalues. Our results are in remarkable agreement with those obtained by Pade or Borel-Pade methods. We find that for sufficiently small values of λ the exact result is just obtained from a sum of a first few terms of the perturbation series, showing that the perturbation series for the anharmonic oscillator is just an asymptotic series in the sense of Watson. A rigorous demonstration of this fact has recently been shown by Simon. We are now carrying out to obtain some criteria to normalize the respective eigen functions. We hope to discuss many applications of our result in the near future.

REFERENCES

- 1. Bender, C. and Wu, T. .. Phys. Rev., 1969, 184, 1231.
- 2. Biswas, S. N. and Vidhani, T. J. Phys., A 6, 1973, p. 468.
- 3. —, Malik, G. P. and Phys. Rev. (Dec. 1972). Sudarshan, E. C. G.
- 4. Sudarshan, E. C. G. .. Fundamental Problems in El. Part. Phys., New York, 1968; Phys. Rev., 1970, D1, 474.
- 5. Biswas, S. N., Datta, K.,
 Saxena, R. P.,
 Srivastava, P. K.
 and Varma, V. S.
- Phys. Rev., 1971, D4, 3617; J. Math. Phys, 1973; Phys. Rev., 1973.

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