объединенный
институт
ядерных
исследований
дубна

E5-92-202

E.P.Yukalova, V.I.Yukalov

CALCULATION OF EIGENVALUES OF SCHRÖDINGER OPERATORS FOR ARBITRARY COUPLING

Submitted to "International Workshop on "Polarons and Applications", May 1992, Pushchino, Russia

1992

1. Introduction

The calculation of eigenvalues of Schrödinger operators is a standard problem of quantum mechanics and statistical mechanics. In the majority of realistic cases this problem cannot be solved exactly, and one invokes perturbation theory. Usually, perturbation theory yields the series in powers of a parameter called the coupling constant. In many cases, such a series can be shown to diverge [1] for any finite value of the coupling constant. The situation becomes even more dramatic when, because of the complexity of a problem, one is not able to find a number of terms of perturbation theory, thus being unable to resort to a resummation technique [2]. How then one could find a solution of the problem characterized by an arbitrary value of the coupling constant, if one can calculate only a few first terms of perturbation theory?

An answer to this question has been done by the method of self - similar approximations [3]. The method has been formulated in a general form being applicable to any sequences. Different variants of the method have been considered [4,5]. Here, we adapt this method for calculating the eigenvalues of Schrödinger operators.

2. Self - Similar Approximation

Let a Hamiltonian H be given parametrically depending on the variable $g \in R$ called the coupling constant. Our aim is to find the eigenvalues E_n of the Hamiltonian; n being a parameter (multiparameter) enumerating the energy levels.

It is convenient to use the dimensionless quantities for the operators and their eigenvalues,

$$H(g) \equiv \frac{H}{\omega}, \qquad e(n,g) \equiv \frac{E_n}{\omega}, \tag{1}$$

where ω is an appropriate constant in energy units. The approximate terms of perturbation theory will be denoted by

$$e_k(n,g) \equiv \frac{E_n^{(k)}}{\omega}; \qquad k = 0, 1, 2, \ldots \tag{2}$$

Perturbation theory in powers of the coupling constant is, as a rule, divergent. To make it convergent, we need to construct a renormalized perturbation theory [6]. For doing this, take as an initial approximation a Hamiltonian $H_0(g,z)$ containing a trial parameter z. The generalization to the case of a set of parameters $z = \{z^\alpha; \alpha = 1, 2, 3, \ldots\}$ is straightforward. Use the Rayleigh - Schrödinger perturbation theory with respect to

$$\Delta H \equiv H(g) - H_0(g,z), \tag{3}$$

which gives the sequence of approximations $e_k(n,g,z)$. Change the trial parameter z for a set of functions,

$$z \to \{z_k(n,g)\}, \tag{4}$$

whose role is to govern the convergence of the sequence of approximations

$$e_k(n,g) \equiv e_k(n,g,z_k(n,g)); \tag{5}$$

this is why $z_k(n,g)$ are called the governing functions. The concrete forms of defining the latter will be examined below.

Following the general way of the method of self - similar approximations [3], introduce the coupling function $g(n,f)$ by the equation

$$e_0(n,g,z(n,g)) = f; \qquad g = g(n,f), \tag{6}$$

in which

$$z(n,g) \equiv z_1(n,g). \tag{7}$$

Define the relative fixed - point distance

$$\delta_{sk} \equiv (k_* - k)/(s - k), \tag{8}$$

where k_* is the number corresponding to the self - similar approximation being a fixed - point of a self - similar mapping [3], and s is the number of the senior approximation. For brevity, k_* can be called the fixed - point number; and s, the senior number.

Write the finite difference

$$\Delta_{sk}(n,f) \equiv e_s(n,g,z_k) - e_k(n,g,z_k) + (z_s - z_k)\frac{\partial}{\partial z_k} e_k(n,g,z_k), \tag{9}$$

in which

$$g = g(n,f), \qquad z_k = z_k(n,g(n,f)); \quad k < s,$$

and the function

$$y_{sk}(n,f) \equiv \{\delta_{sk}\Delta_{sk}(n,f)\}^{-1}. \tag{10}$$

Function (10) is normalized by the integral

$$\int_{e_k(n,g)}^{e_*(n,g)} y_{sk}(n,f)df = 1, \tag{11}$$

where the upper limit is the sought self - similar approximation for the eigenvalue of the Hamiltonian $H(g)$. Integral (11) resembles the normalization condition for a distribution, because of which the function (10) could be called the distribution of approximations. However, this similarity is purely formal since the function (10) is not, in general, non-negative.

The self - similar approximation $e_*(n,g)$ is a fixed - point of a self - similar mapping [3]. To define a convergent procedure, the fixed point is to be stable. The stability is characterized by the mapping multipliers

$$M_k(n,g) \equiv \lim_{f\to e_*(n,g)} \left| \frac{\partial}{\partial f} \bar{e}_k(n,f) \right|, \tag{12}$$

in which

$$\bar{e}_k(n,f) \equiv e_k(n,g(n,f)), \tag{13}$$

and by the Lyapunov exponents

$$\Lambda_{sk}(n,g) \equiv \lim_{f\to e_*(n,g)} \frac{\partial}{\partial f}\Delta_{sk}(n,f). \tag{14}$$

The stability conditions read

$$M_k(n,g) < 1, \qquad \Lambda_{sk}(n,g) < 0. \tag{15}$$

Conditions (15) for the method of self - similar approximations have been established in Ref.[7].

The accuracy of the renormalized approximations (5) is characterized by the quantity

$$\epsilon_k(n,g) \equiv \left| \frac{e_k(n,g)}{e(n,g)} - 1 \right| \tag{16}$$

showing the error of (5) with respect to the exact value $e(n,g)$. The corresponding error for the self - similar approximation is

$$\epsilon_*(n,g) \equiv \left| \frac{e_*(n,g)}{e(n,g)} - 1 \right| . \tag{17}$$

It is instructive to define the maximal errors,

$$\epsilon_k \equiv \sup_{n,g} \epsilon_k(n,g) \tag{18}$$

and

$$\epsilon_* \equiv \sup_{n,g} \epsilon_*(n,g). \tag{19}$$

The accuracy of a method, as a whole, must be defined just by its maximal error. Provided the stability conditions (15) are true, it should be

$$\epsilon_* \leq \inf_k \epsilon_k. \tag{20}$$

3. Anharmonic Oscillator

To illustrate the method, let us consider the one - dimensional anharmonic oscillator with the Hamiltonian

$$H = -\frac{1}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2}{2}x^2 + \lambda m^2 x^4, \tag{21}$$

in which $m, \omega, \lambda > 0$ and $x \in (-\infty, +\infty)$. Introduce the dimensionless coupling constant g and the space variable ξ ,

$$g \equiv \frac{\lambda}{\omega^3}, \qquad \xi \equiv (m\omega)^{1/2}x. \tag{22}$$

Then, the Hamiltonian (21) transforms into the dimensionless form

$$H(g) = -\frac{1}{2}\frac{d^2}{d\xi^2} + \frac{1}{2}\xi^2 + g\xi^4. \tag{23}$$

As an initial Hamiltonian we choose

$$H_0(g,z) = -\frac{1}{2}\frac{d^2}{d\xi^2} + \frac{z^2}{2}\xi^2. \tag{24}$$

Applying the Rayleigh - Schrödinger perturbation theory with respect to (3), we can find the corresponding approximate terms. To simplify the illustration, we shall write down only the expressions related to the ground - state level, although the same procedure and results hold true for the whole spectrum [8]. The abreviated notation will be used below:

$$e_k(g,z) \equiv e_k(o,g,z), \qquad e_k(g) \equiv e_k(o,g),$$

$$e_*(g) \equiv e_*(0,g), \qquad e(g) \equiv e(0,g). \tag{25}$$

In this way, starting from the initial approximation

$$e_0(n,g) = \frac{1}{2}z, \tag{26}$$

we get the first and second approximations:

$$e_1(g,z) = e_0(g,z) + \frac{3g + z - z^3}{4z^2}, \tag{27}$$

$$e_2(g,z) = e_1(g,z) - \frac{6g^2 + (6g + z - z^3)^2}{16z^5}. \tag{28}$$

The relative fixed - point distance (8) can be defined in one of the following ways. The first possibility is to claim, as is usually done in the

renormalization - group calculations, that the senior approximation of the renormalized perturbation theory is equivalent to the fixed - point. More precisely, this means that the number of the senior approximation s coincides with the fixed - point number k_*. Under this assumption, we have

$$\delta_{21} = 1; \qquad s = k_*. \tag{29}$$

The second possibility is to treat δ_{sk} as a fitting parameter to be defined from ad additional condition. In many cases, it is not too difficult to find the strong coupling limit of the spectrum. For instance, in the considered situation

$$e(g) \simeq 0.667986 g^{1/3}; \qquad g \to \infty.$$

Then the fixed - point distance δ_{21} can be found from the asymptotic constraint condition

$$\lim_{g\to\infty} \frac{e_*(g)}{e(g)} = 1. \tag{30}$$

Below, we shall analyse both these possibilities.

4. Minimal Sensitivity

Another choice to be made is to opt for a particular kind of the fixed - point conditions defining the governing functions [3,7]. Two main types of these conditions are known, the principle of minimal difference [6] and the principle of minimal sensitivity [9]. To understand their comparative peculiarities, we consider them separately.

Begin with the principle of minimal sensitivity which in our case defines the governing function by the equation

$$\frac{\partial}{\partial z} e_1(g, z) = 0; \qquad z = z(g) \equiv z(0, g). \tag{31}$$

This, together with (27), gives

$$z^3 - z - 6g = 0. \tag{32}$$

The positive solution to (32) is

$$z(g) = \begin{cases} (2/\sqrt{3}) \cos(\alpha/3); & g \leq g_0, \\ A^+ + A^-; & g \geq g_0, \end{cases}$$

in which

$$\alpha = \arccos(g/g_0),$$

$$A^{\pm} = (3g)^{1/3} \left\{ 1 \pm \left[1 - \left(\frac{g_0}{g} \right)^2 \right]^{1/2} \right\}^{1/3},$$

$$g_0 = \frac{1}{9\sqrt{3}} = 0.064150.$$

For function (10) we have

$$y_{21}(f) = -\frac{768 f^3}{\delta_{21}(4f^2 - 1)^2}. \tag{33}$$

Substituting (33) into integral (11), we obtain the equation

$$\frac{4e_*^2(g) - 1}{4e_1^2(g) - 1} = \exp\left\{ \frac{1}{4e_*^2(g) - 1} - \frac{1}{4e_1^2(g) - 1} - \frac{\delta_{21}}{24} \right\} \tag{34}$$

for the self - similar approximation $e_*(g)$. Here

$$e_1(g) = \frac{3z^2 + 1}{8z}; \qquad z = z(g).$$

To check whether the fixed - point $e_*(g)$ is stable, we need to calculate the mapping multipliers (12) and the Lyapunov exponent (14). Dealing with the ground - state level, we shall again simplify the notation by writing

$$M_k(g) \equiv M_k(0, g), \qquad \Lambda_{sk}(g) \equiv \Lambda_{sk}(0, g).$$

For these quantities we find

$$M_1(g) = \frac{12e_*^2(g) - 1}{16e_*^2(g)}, \qquad M_2(g) = M_1(g) + \Lambda_{21}(g),$$

$$\Lambda_{21}(g) = -\frac{[4e_*^2(g) - 1][4e_*^2(g) + 3]}{768 e_*^4(g)}.$$

The latter expressions satisfy the stability condition (15).

The maximal errors (18) for the renormalized approximants (5) are $\epsilon_1 \approx 2\%$ and $\epsilon_2 \approx 1\%$. the exact values $e(g)$ are given by numerical calculations [10].

To find the accuracy of the self - similar approximation $e_*(g)$ defined by equation (34), we have to opt for a particular choice of the fixed - point distance δ_{21} . If we take (29) , then the maximal error of (34) is $\epsilon_* \approx 0.3\%$ at $g \approx 1$. If we assume (30), then

$$\delta_{21} = 0.955774. \tag{35}$$

The maximal error of (34) with the fixed - point distance (35) is again $\epsilon_* \approx 0.3\%$ at $g \approx 1$. A more detailed comparison of these two variants of taking the fixed - point distance either from assumption (29) or from(35) is presented in Table 1.

5. Minimal Difference

Try now to define the governing function from the principle of minimal difference [6] taking it in the from

$$e_1(g,z) - e_0(g,z) = 0; \quad z = z(g). \tag{36}$$

The latter leads to the equation

$$z^3 - z - 3g = 0, \tag{37}$$

whose positive solution is

$$z(g) = \begin{cases} (2/\sqrt{3})\cos(\beta/3); & g \leq g_0', \\ \\ B^+ + B^-; & g \geq g_0', \end{cases}$$

where

$$\beta = \arccos(g/g_0'),$$

$$B^{\pm} = \left(\frac{3g}{2}\right)^{1/3} \left\{ 1 \pm \left[1 - \left(\frac{g_0'}{g}\right)^2 \right]^{1/2} \right\}^{1/3},$$

$$g_0' = \frac{2}{9\sqrt{3}} = 0.1283.$$

Function (10) becomes

$$y_{21}(f) = -\frac{384 f^3}{5\delta_{21}(4f^2-1)^2}, \tag{38}$$

and the integral (11) yields

$$\frac{4e_*^2(g)-1}{4e_1^2(g)-1} = \exp\left\{ \frac{1}{4e_*^2(g)-1} - \frac{1}{4e_1^2(g)-1} - \frac{5}{12}\delta_{21} \right\} \tag{39}$$

with

$$e_1(g) = \frac{1}{2}z(g).$$

For the mapping multipliers and the Lyapunov exponent we get

$$M_1(g) = 1, \qquad M_2(g) = 1 + \Lambda_{21}(g),$$

$$\Lambda_{21}(g) = -\frac{5[4e_*^2(g)-1][4e_*^2(g)+3]}{384 e_*^4(g)}.$$

The stability conditions (15) are fulfilled for $M_2(g)$ and $\Lambda_{21}(g)$. However, the multiplier $M_1(g)$ does not satisfy (15).

The maximal errors of the renormalized approximants (27) and (28), with the governing function given by (36), are $\epsilon_1 \approx 8\%$ and $\epsilon_2 \approx 15\%$ at $g \to \infty$.

Equation (39) containing the fixed - point distance (29) leads to the maximal error $\epsilon_* \approx 12\%$ at $g \to \infty$. The accuracy of (39) can be essentially improved if we extract δ_{21} from the constraint condition (30), which gives

$$\delta_{21} = 0.367416. \tag{40}$$

Then, the maximal error of (39) with the fixed- point distance (40) is $\epsilon_* \approx 0.9\%$ at $g \approx 1$. In the latter case, the errors for different coupling constants are shown in Table 2.

Comparing the obtained results we come to the following conclusion. The accuracy of the method of self - similar approximations strongly depends on the validity of stability conditions (15). The fixed - point condition defining the governing functions can be written either as the principle of minimal sensitivity or as the principle of minimal difference. The former provides the stability of the method while the latter does not. This is why the principle of minimal sensitivity yields much more accurate results than the principle of minimal difference.

Table 1

Self - similar approximations for the ground - state energy of the one - dimensional anharmonic oscillator, given by Eq.(34), with the governing function defined by the principle of minimal sensitivity

g	$e(g)$	$e_*(g)$	$e_*(g)$	$\epsilon_*(g)$	$\epsilon_*(g)$
		Eq.(29)	Eq.(35)	Eq.(29)	Eq.(35)
0.01	0.50726	0.50728	0.50728	0.004%	0.004%
0.30	0.63799	0.63959	0.63968	0.25%	0.28%
1	0.80377	0.80606	0.80634	0.28%	0.32%
200	3.9309	3.9284	3.9319	0.06%	0.03%
20000	18.137	18.121	18.137	0.09%	0%

Table 2

Self - similar approximations given by Eqs.(39), (40) with the governing function defined by the principle of minimal difference

g	$e(g)$	$e_*(g)$	$\epsilon_*(g)$
0.01	0.50726	0.50731	0.01%
0.30	0.63799	0.64239	0.69 %
1	0.80377	0.81076	0.87%
200	3.9309	3.9337	0.07%
20000	18.137	18.138	0.006%

References

1. B.Simon, Bull. Am. Math. Soc. **24**, 303 (1991).
2. P.M.Stevenson, Nucl. Phys. **B231**, 65 (1984).
3. V.I.Yukalov, J. Math. Phys. **32**, 1235 (1991).
4. V.I.Yukalov, Int. J. Mod. Phys. **B3**, 1691 (1989).

5. V.I.Yukalov, Physica **A167**, 833 (1990).

6. V.I.Yukalov, Mosc. Univ. Phys. Bull. **31**, 10 (1976).

7. V.I.Yukalov, JINR Preprint **E5-92-153** (Dubna, 1992).

8. E.P.Kadantseva and V.I.Yukalov, JINR Preprint **E5-91-466** (Dubna, 1991).

9. P.M.Stevenson, Phys. Rev. **D23**, 2916 (1981).

10. F.T.Hioe and E.W.Montroll, J.Math. Phys. **16**, 1945 (1975).

Received by Publishing Department
on May 8, 1992.

Юкалова Е.П., Юкалов В.И. E5-92-202

Вычисление собственных значений шредингеровских операторов при произвольной константе связи

Метод автомодельных приближений применен для вычисления собственных значений шредингеровских операторов. В этом методе автомодельное приближение трактуется как неподвижная точка автомодельного отображения. Процедура сходится, если неподвижная точка устойчива, для чего требуется выполнение соответствующих условий устойчивости. Для того чтобы последовательность приближений сходилась, необходимо ввести управляющие функции, определяемые из условий на неподвижную точку. Проанализированы два варианта таких условий: принцип минимальной чувствительности и принцип минимальной разности. В качестве иллюстрации рассмотрен одномерный ангармонический осциллятор.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна 1992

Yukalova E.P., Yukalov V.I. E5-92-202

Calculation of Eigenvalues of Schrödinger Operators for Arbitrary Coupling

The method of self-similar approximations is applied for calculating the eigenvalues of Schrödinger operators. In this method the self-similar approximation is treated to be a fixed-point of a self-similar mapping. The procedure is convergent if the fixed point is stable, which requires the validity of the corresponding stability conditions. To make the sequence of approximations convergent, one has to introduce the governing functions defined by the fixed-point conditions. Two variants of these conditions are analysed: the principle of minimal sensitivity and the principle of minimal difference. The illustration is given by the one-dimensional anharmonic oscillator.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

Preprint of the Joint Institute for Nuclear Research. Dubna 1992