ITEP - 139

INSTITUTE OF THEORETICAL
AND EXPERIMENTAL PHYSICS

A.V.Turbiner

A NEW APPROACH TO THE EIGENVALUE PROBLEMS IN MULTIDIMENSIONAL QUANTUM MECHANICS

MOSCOW 1979

УДК 530.145:539.3 М-16

Abstract

I propose a new perturbation theory for solution of the k-dimensional Schrödinger equation with arbitrary potential. It does not require the knowledge of the entire spectrum of the unperturbed problem and gives closed expressions for the energy shifts. The procedure is a generalization of the variational method and permits to find its accuracy. Two dimensional nonsymmetric anharmonic oscillator is considered as an example.

А.В.Турбинер
Новый подход к проблеме собственных значений в многомерной квантовой механике
Работа поступила в ОНТИ 6/XI-1979г.

Подписано к печати 12/XI-79г. Т-20410. Формат 70x108 1/16.
Печ.л.0.75.Тираж 290 экз.Заказ 139.Цена 5 коп.Индекс 3624.

Отдел научно-технической информации ИТЭФ,117259,Москва

The eigenvalue problem is one of the basic subjects of Quantum mechanics.[1] In numerous applications one often needs to find the bound state energies and wave functions, and usually this is done with the help of a perturbation theory. The standard perturbation theory expresses energy and wave--function corrections in terms of sums over intermediate states or in terms of integrals containing Green's functions. In other words the knowledge of the spectrum and wave functions of the unperturbed problem is presupposed. Such an approach besides purely technical difficulties possesses a principle drawback: the resulting series is as a rule divergent. The reason is simple. In most of the physically interesting cases the perturbation is more singular than the unperturbed potential. Thus, the most interesting strong coupling regime is completely out of the scope of the method. Another widely used approach - variational[1] - is not iterational in nature, and hence the question of its accuracy in each particular case requires a special investigation.

Here I would like to propose a new iterational technique which permits to determine the stationary states of the multidimensional Schrödinger equation with arbitrary potential. It is important that no information about the entire spectrum of the unperturbed problem is needed. The energy shifts to any order are given in quadrature. The computation of the corrections to the wave functions is equivalent to solution of multidimensional electrostatics with variable dielectric permeability. In some particular cases corresponding equations can be solved analytically.

For instance, this is just what happens when the unperturbed wave function is spherically symmetric. In other cases the equations can be readily integrated numerically. It is worth mentioning that the scheme proposed generalizes in a sense develops the well-known variational method. In fact each given trial function within the latter can be considered as a wave function of the zeroth approximation in my scheme. Further iterations yield consequent corrections to the variational-method-based results.

The central point is the freedom in choosing the unperturbed potential. One can always choose it in such a way as to make the procedure convergent. Below the general description of the technique is presented and its application to the two-dimensional nonsymmetric anharmonic oscillator is considered. Other applications and rigorous results concerning the convergence of the method are discussed elsewhere.

The starting point is a certain transformation [2] of the k-dimensional linear Schrödinger equation,

$$\Delta\Psi + (E - V)\Psi = 0 \qquad (1)$$

into a nonlinear equation of a lower order with a right-hand side. (I will use the term "nonlinearization" for this transformation). To integrate the latter a new perturbation theory is developed. After this is done the problem converts again into a linear one. In more detail, the above-mentioned transformation is of the form:

$$\vec{y} = -\vec{\nabla}\Psi/\Psi \qquad (2)$$

where Δ and $\vec{\nabla}$ denote the standard k-dimensio-

nal Laplace and gradient operators. In terms of the new vector field $\vec{y}$ the Schrödinger equation (1) reduces to

$$\vec{\nabla}\vec{y} - \vec{y}^2 = (E-V) \qquad (3)$$

Eq. (3) is equivalent to eq. (1) if the following additional condition holds

$$\vec{y} = \vec{\nabla}(\text{scalar function}) \qquad (4)$$

or, in other words, $\vec{y}$ is a vector field of the potential type,

$$\partial_i y_j - \partial_j y_i = 0 \qquad (4')$$

As to the boundary conditions for eq. (3) they will be discussed a bit later.

One can always represent the potential V as a sum of two terms, $V = V_0 + \lambda V_1$, where V_0 is chosen in such a way that the equation

$$\Delta\psi_0 + (E_0 - V_0)\psi_0 = 0 \qquad (5)$$

can be solved exactly. Here λ is a formal parameter introduced for convenience; V_0 will be referred to as the unperturbed potential. There is no difficulty in decomposing $V = V_0 + \lambda V_1$; actually one simply fixes ψ_0 according to certain rules to be explained below and then constructs V_0 by means of eq. (5). Given ψ_0 one fixes the zeroth order approximation for eq. (3), $\vec{y}_0 = -\vec{\nabla}\psi_0/\psi_0$. Higher order approximations $\vec{y}_1, \vec{y}_2, \ldots$ define the following series:

$$\vec{y} = \vec{y}_0 + \lambda \vec{y}_1 + \lambda^2 \vec{y}_2 + \ldots = \sum \lambda^n \vec{y}_n(\vec{x}) \qquad (6)$$

The bound state energy is also represented in the form of a series

$$E = E_0 + \lambda E_1 + \lambda^2 E_2 + \ldots = \sum \lambda^n E_n \qquad (7)$$

Let us discuss first the ground state. Then ψ_0 has no zeros and all the expressions given below have a precise meaning. In case of excited states complications emerge due to zeros in ψ_0. This case will be considered later.

Substituting (6), (7) into eq. (3) and expanding it in λ we arrive at the following set of linear equations:

$$\vec{\nabla}(\psi_0^2 \vec{y}_n) = (E_n - Q_n)\psi_0^2, \quad \vec{y}_n = \vec{\nabla}(\text{scalar function}) \qquad (8)$$

Here $Q_1 = V_1$ and for $n > 1$

$$Q_n = -\sum_{i=1}^{n-1} \vec{y}_i \vec{y}_{n-i}, \qquad (9)$$

and (8) coincides in fact with the k-dimensional electrostatics law, ψ_0^2 and $\vec{y}_n$ playing the roles of dielectric permeability and field strength respectively.

Let us discuss now the boundary conditions relevant to eq. (8). In this paper I consider only stationary states. For such states invoking the definitions ψ_0 and $\vec{y}_n$ one immediately finds:

$$|\vec{y}_n \psi_0^2| \to 0 \quad \text{for} \quad |x| \to \infty \qquad (10)$$

This condition can be readily converted into information about E_n. To this end integrate eq. (8) over the whole space and transform the volume integral in the left-hand side into the surface one with the help of the Gauss theorem; then

$$E_n = \frac{\int Q_n \psi_0^2 d\bar{x}}{\int \psi_0^2 d\bar{x}} \qquad (11)$$

This expression represents the n-th correction to the unperturbed energy level. Notice, that the first correction ($n = 1$) coincides identically with that in ordinary Schrödinger perturbation theory [1]. To obtain further corrections it is necessary to solve the electrostatics problem (8), which is equivalent, in general, to integration of the following general elliptic equation:

$$\Delta \varphi_n - 2(\vec{\gamma}_0 \cdot \vec{\nabla} \varphi_n) = E_n - Q_n \qquad (12)$$

with the boundary condition (10). Recall that in eq. (12) $\vec{\gamma}_n = \vec{\nabla} \varphi_n$, and E_n is given by eq. (11). It is important that the integration of eq. (12) is <u>not</u> an eigenvalue problem since it is assumed that Q_n is already known from previous iterations (see eq. (9)) and hence E_n is known also. This means that (at least numerically) it is much simpler to solve eq. (12) than the original equation, (1).

Now let us turn to determination of corrections $\vec{\gamma}_n$. In general case the solution of eqs. (8), (10), (4,4') is of the form

$$\psi_0^2 \vec{y}_n = \int \vec{G}(\bar{x}-\bar{x}')(E_n - Q_n)\psi_0^2 d\bar{x}' \qquad (13)$$

where $\vec{G}(\bar{x}-\bar{x}')$ is the relevant Green's function. In the special case of the spherically symmetric zeroth approximation, ψ_0^2, this Green's function is known explicitely

$$\vec{G}_k(\bar{x}) = \frac{1}{\sigma_k} \frac{\vec{x}}{|\bar{x}|^k} \qquad (14)$$

where $\sigma_k = 2\pi^{k/2} / \Gamma(k/2)$ is the square of the k-dimensional unit sphere. Then the solution of eq. (8) is:

$$\psi_0^2 \vec{y}_n = \frac{1}{\sigma_k} \int \frac{\vec{x}-\vec{x}'}{|\bar{x}-\bar{x}'|^k} (E_n - Q_n)\psi_0^2 d\bar{x}' \qquad (15)$$

Notice that the general solution of arbitrary 1-dimensional problem is also given by eq. (15).

A few more remarks about the situation in the 1-dimensional problem (and also in spherically symmetric multidimensional problem which reduces trivially to the 1-dimensional one). In this case the transformation (2) is well known: it converts the Schrödinger equation into the Riccati equation. After the pioneering paper due to Zeldovich [3] many authors emphasized [4-7] that it is extremely important and convenient to proceed from the Schrödinger equation to the Riccati one-the trick allowed to construct easily various versions of the perturbation theory for discrete spectrum. In particular, one of the versions as applied to the problem of 1-dimensional anharmonic oscillator was developed in Ref. [5]. General formulas for ar-

bitrary potentials V_0 and V_1 were proposed independently in Refs. 6 and 7. Besides that Ref. 6 contains also an exhaustive investigation of excited states.

Let us sketch the basic points of the procedure proposed as applied to excited states (recall that the previous consideration refers directly to the ground state only). The main complification which energes for excited states is the presence of zeroes in the wave function. Assume that the positions of these zeroes form a manifold $\mathcal{S}$. For simplicity let us assume $\mathcal{S}$ to be a simply connected, non-self- intersecting surface. Then the wave function can be represented in the form

$$\psi(\vec{x}) = f(\vec{x}) \exp\{-\mathcal{L}(\vec{x})\} \qquad (16)$$

where $f(\vec{x})$ and $\mathcal{L}(\vec{x})$ are nonsingular for finite $\vec{x}$ and $f(\vec{x})$ grows at $|x| \to \infty$ not faster than a power of $|x|$. Besides that $f(\vec{x}) = 0$ and $\vec{\nabla} f(\vec{x}) \neq 0$ when $\vec{x} \in \mathcal{S}$. With these definitions vector $\vec{g}$ (see eq.(2)) takes the form:

$$\vec{y} = \vec{g} - \frac{\vec{\nabla} f}{f} \qquad (17)$$

where $\vec{g} = \vec{\nabla} \mathcal{L}(\vec{x})$. (An analogous notation was introduced in Ref. 6 for 1 -dimensional case). Substituting eq. (17) into (3) and multiplying the resulting relation by f we arrive at

$$f \vec{\nabla} \vec{g} - f \vec{g}^2 - \Delta f + 2 \vec{g} \vec{\nabla} f = (E - V) f \qquad (18)$$

Let $V = V_0 + \lambda V_1$ and ψ_0 denote the solution of

eq. (18) with some E_0 and V_0. Develop now a perturbation theory for E and $\vec{g}$ [6,7], expanding in λ the function f:

$$f = f_0 + \lambda f_1 + \lambda^2 f_2 + \ldots = \sum \lambda^n f_n \qquad (19)$$

To the first order in λ, after some simple algebra one finds

$$\vec{\nabla}\left(\psi_0^2 \vec{g}_1 + e^{-2\mathcal{L}_0}\left(f_1 \vec{\nabla} f_0 - f_0 \vec{\nabla} f_1\right)\right) = \left(E_1 - V_1\right)\psi_0^2 \qquad (20)$$

where the subscript " 0 " lebels the zeroth approximation. Integrating eq. (20) over the whole space and taking into account the boundary condition (10) one obtains an expression for E_1, which coincides with eq. (11) at n=1. The solution (20) has the form

$$\psi_0^2 \vec{g}_1 + e^{-2\mathcal{L}_0}\left(f_1 \vec{\nabla} f_0 - f_0 \vec{\nabla} f_1\right) = \int \vec{G}_{ex}(\bar{x}-\bar{x}')(E_1 - V_1)\psi_0^2 \, d\bar{x}' \qquad (21)$$

where $\vec{G}_{ex}(\bar{x}-\bar{x}')$ is the Green's function for equation (20) (fixed by eq. (10) and the requirement that $\vec{g}_1$ and $\vec{g}_1$ satisfy eq. (4)). One more constraint on the Green's function: it is necessary that the right-hand-side of eq. (21) would be a vector directed along $\vec{\nabla} f_0$ when $\bar{x} \in S_0$. Then some information concerning the deformation of the surface S_0 can be extracted from the condition

$$f_1 = \frac{\vec{\nabla} f_0 \int \vec{G}_{ex}(\bar{x}-\bar{x}')(E_1 - V_1)\psi_0^2 \, d\bar{x}'}{e^{2\mathcal{L}_0}\left(\vec{\nabla} f_0\right)^2}, \quad \bar{x} \in S_0 \qquad (22)$$

A more detailed consideration of the excited states is out

of the scope of the present paper and will be given elsewhere.

Summarizing, it turned possible to construct a perturbation theory which does not require the knowledge of the entire spectrum of the unperturbed problem. An interesting issue is the possibility to make the perturbation theory convergent[5,7,2]. To realize such a possibility one can rely on the freedom in choosing the zeroth approximation, ψ_0. In other words we can decompose the potential V into a sum $V_0 + V_1$ almost arbitrary. It natural to choose ψ_0 and the corresponding potential V_0 ($V_0 = E_0 + \Delta\psi_0/\psi_0$) in a such a way as to incorporate in V_0 and the gross features of V. Just in the same way one would act if one decides to solve the Schrödinger equation using the well-known variational method. This similarity is not accidental. Really, denote by $E_{var.}$ the energy, which one would obtain within the variational method (with the ψ_0 as the trial function). Then it is easy to show that this energy is reproduced by the first two iterations of the procedure described above,

$$E_{var.} = E_0 + E_1 \qquad (23)$$

What is more important is that the procedure proposed goes beyond the variational method. Further iterations (higher order term in the series (7)) give corrections to the variational results. Thus it became possible to find the accuracy of any variational calculation.

Naturally, if one fixes ψ_0 in such a way that $V_0 = E_0 + \Delta\psi_0/\psi_0$ reproduces all the singularities and asymptotic behaviour (at $|\vec{x}| \to \infty$) of the difference $V - V_0 = V_1$ can be considered as a

good small perturbation. Developing the perturbation theory with respect λV_1 one does not encounter singularities in the λ plane, at least for a certain domain of λ. Where the boundary for this domain lies becomes clear from the physical arguments which relate the emergence of the singularities with a drastic rearrangement of the spectrum: for some "critical" values of λ a level either becomes quasistationary or goes into continuum.

As example let us consider the ground state of 2-dimensional anharmonic oscillator with potential

$$V = m(x^2+y^2) + g(x^4+y^4+2cx^2y^2) \qquad (24)$$

Then, one of the simplest trial wave functions has the form

$$\Psi_0 = \exp\left\{-\frac{a}{2}(x^2+y^2) - \frac{\sqrt{g}}{3}(x^2+y^2)^{3/2}\right\} \qquad (25)$$

Function (25) is the ground state wave function in the potential $(E_0 = 2a)$

$$V_0 = -3\sqrt{g}(x^2+y^2)^{1/2} + a^2(x^2+y^2) + 2a\sqrt{g}(x^2+y^2)^{3/2} + g(x^4+y^4+2x^2y^2) \qquad (26)$$

and hence the perturbation is the following

$$V = 3\sqrt{g}(x^2+y^2)^{1/2} - a^2(x^2+y^2) - 2a\sqrt{g}(x^2+y^2)^{3/2} + m(x^2+y^2) + g\left[(c-1)2x^2y^2\right] \qquad (27)$$

Obviously, the ground state energy has a singularity at $C = -1$. Therefore we will change the parameter C from -1 to 1. Besides from that, we will minimize the expression $(E_0 + E_1)$ on parameter a and will calculate the energy shift E_2. Table confronts my re -

sults with numerical calculations [8]. Discussions of details of our calculations will be published elsewhere.

It is pleasure to thank K.G.Boreskov, B.L.Ioffe, A.B.Kaidalov, K.A.Ter-Martirosyan and V.A.Fateyev for useful discussions and I an greatly indebted to Yu.A.Simonov for valuable comments. I want to thank M.A.Shifman for reading of the manuscript and critical remarks.

Table

Ground state energy of the anharmonic oscillator (24) at $g = 2$. Parameter a_{min} realizes the minimum of (E_0+E_1), E_2 gives the first correction to the variational result $(E_0+E_1)_{min}$. E_{exact} from Ref.8. Definition of energy as Ref.8 (at $\lambda = 1$, see p.319).

						$m = 0$					
C	-I	-0,8	-0.6	-0.4	-0.2	0	0.2	0.4	0.6	0.8	I
a_{min}	0.II	0.I8	0.24	0.30	0.35	0.4I	0.46	0.50	0.55	0.59	0.64
E_0+E_I	I.I95	I.23I	I.264	I.296	I.326	I.355	I.383	I.4I0	I.436	I.46I	I.485
$-E_2$	0.039	0.029	0.02I	0.0I6	0.0I2	0.009	0.007	0.005	0.004	0.003	0.003
$E_0+E_I+E_2$	I.I56	I.202	I.243	I.280	I.3I4	I.346	I.376	I.405	I.432	I.458	I.482
E_{exact}	I.I08	I.I72	I.22I	I.264	I.302	I.336	I.368	I.396	I.426	I.452	I.477
						$m = I$					
C	-I	-0.8	-0.6	-04	-0.2	0	0.2	0.4	0.6	0.8	I
a_{min}	0.43	0.48	0.53	0.58	0.63	0.67	0.72	0.76	0.80	0.83	0.87
E_0+E_I	I.498	I.526	I.552	I.578	I.602	I.625	I.648	I.670	I.692	I.7I2	I.733
$-E_2$	0.024	0.0I9	0.0I5	0.0I2	0.009	0.007	0.006	0.005	0.004	0.003	0.003
$E_0+E_I+E_2$	I.474	I.507	I.537	I.566	I.593	I.6I8	I.642	I.665	I.688	I.709	I.730
E_{exact}	I.444	I.484	I.5I9	I.55I	I.580	I.608	I.633	I.658	I.68I	I.703	I.724

References

1. L.D.Landau, E.M.Lifshitz. Quantum Mechanics, Moscow, 1963
2. A.V.Turbiner. Preprint ITEP-117 (1979)
3. Ya.B.Zeldovich. ZhETF 31, 1101 (1956)
4. V.S.Polikanov. ZhETF 52, 1326 (1967); ZhTMF 24, 230 (1975)
   E.P.Sahnovskii. "Atomnaya Energia" 42, 141 (1977)
5. A.D.Dolgov, V.S.Popov. ZhETF 75, 2010 (1978); Phys.Lett., 79B, 403 (1978)
6. Y.Aharonov, C.K.Au. Phys.Rev.Lett., 42, 1582 (1979)
7. A.V.Turbiner. Pisma v ZhETF 30, 379 (1979)
8. F.T.Hioe, Don MacMillen, E.W.Montroll. Phys.Rept. 43C, 306 (1973).

ИНДЕКС 3624