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A new approach to the eigenvalue problem in quantum mechanics: convergent perturbation theory for rising potentials

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Abstract. A new iteration procedure for solution of the Schrödinger equation with arbitrary local potential is proposed. Both the eigenvalues and eigenfunctions are represented in the form of a series which is well convergent under certain conditions. The solution of the k-dimensional Schrödinger equation within the proposed scheme reduces to a problem of the k-dimensional electrostatics. As an example potentials x^{2n} $(n = 2, 3, 4)$ and $m^2x^2 + gx^4$ in one-dimensional space are considered.

1. Introduction

The Schrödinger equation is the basis for solution of many physical problems. Various phenomena, both well known and discovered recently, are described by this equation with some potential. Sometimes it is necessary to consider very sophisticated potentials, and as a rule the eigenvalues and eigenfunctions cannot be found exactly. One has to turn to approximate methods. Two are commonly used: the variational method and the Rayleigh–Schrödinger (RS) perturbation theory (see e.g. Landau and Lifshitz 1963). Both methods have certain drawbacks. The former requires a separate investigation of the question about its accuracy. The latter as a rule yields a divergent series which is sensible only at small values of the coupling constant. It has nothing to say about the strong coupling regime. Moreover, often it is necessary to investigate the analytical structure of the solution. In this case both methods turn out to be ineffective. There also exists numerical integration with the help of computers. However, this is applicable only to one-dimensional problems, and practically does not work in two or more dimensions.

In this paper we construct a new iteration scheme for determination of the eigenvalues and eigenfunctions of the k-dimensional Schrödinger equation with arbitrary local potential (§ 2).

Unlike the standard treatment of RS perturbation theory (Landau and Lifshitz 1963), our procedure does not require the knowledge of the whole spectrum of the unperturbed potential. The only information needed is that referring to the level of the unperturbed potential we are interested in. It gives us the possibility of choosing the unperturbed potential as we want. In particular, the emerging series can be made convergent. In these cases, the RS series will be convergent as well. Physical arguments demonstrating the convergence are presented. As an attempt at a more rigorous

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consideration we formulate also a simple theorem which gives a sufficient condition for the convergence of the procedure (§ 3).

Besides practical usefulness the approach possesses a certain elegance. For example, constructing successive iterations reduces to the solution of k-dimensional electrostatics with varying (coordinate-dependent) dielectric permeability. In one-dimensional space the answer is written out in closed form.

The general consideration is supplemented by a few examples (§ 4). We deal with one-dimensional potentials, which are rather often encountered in various applications, namely x^{2n} $(n = 2, 3, 4)$ and the quartic anharmonic oscillator. The question of the relation between traditional perturbation theory and that described here is discussed in § 5. In this section a remark on literature is given too. The subject of this paper is restricted to the case of the ground state and the cases of excited states if node positions are known precisely. In the general case of excited states our procedure is somewhat modified. This problem is considered elsewhere (Turbiner 1979b).

2. Description of method

Let us proceed to a systematic description of the method. We start with a certain transformation of the Schrödinger equation, which converts the standard linear equation

$$\Delta\psi + (E - V)\psi = 0 \tag{1}$$

into a nonlinear one. Here V is a multiplicative operator. *The nonlinearisation* transformation we mean has the form

$$\boldsymbol{y} = -(\boldsymbol{\nabla}\psi)/\psi = -\boldsymbol{\nabla}(\ln \psi) \tag{2}$$

where Δ and $\boldsymbol{\nabla}$ are ordinary k-dimensional Laplace and gradient operators. Using equations (1) and (2) it is a trivial matter to obtain a new nonlinear relation

$$\operatorname{div} \boldsymbol{y} - \boldsymbol{y}^2 = E - V \tag{3}$$

which is completely equivalent to the original Schrödinger equation provided that the additional condition

$$\boldsymbol{y} = \boldsymbol{\nabla} \text{ (scalar function)} \tag{4}$$

is satisfied.

The potential V can always be decomposed into two pieces $V = V_0 + \lambda V_1$ where λ is a formal parameter such that the equation

$$\Delta\psi_0 + (E_0 - V_0)\psi_0 = 0 \tag{5}$$

can be solved exactly. Then $\boldsymbol{y}_0 = -(\boldsymbol{\nabla}\psi_0)/\psi_0$. We delay discussion of the question as to how to choose V_0 in each particular case and will now develop a perturbation theory with respect to λ. In a standard way write

$$\boldsymbol{y} = \sum_{n=0}^{\infty} \lambda^n \boldsymbol{y}_n, \tag{6}$$

$$E = \sum_{n=0}^{\infty} \lambda^n E_n. \tag{7}$$

Then the values of E_n and the functions $\mathbf{y}_n$ are determined by the linear equations

$$\operatorname{div} \mathbf{y}_n - 2\mathbf{y}_0 \mathbf{y}_n = E_n - Q_n \tag{8}$$

where each of the functions $\mathbf{y}_n$ must satisfy equation (4). Here

$$Q_1 = V_1, \qquad Q_n = -\sum_{i=1}^{n-1} \mathbf{y}_i \mathbf{y}_{n-i} \qquad \text{for } n \geqslant 2. \tag{9}$$

Multiplying both the right- and left-hand sides of equation (8) by ψ_0^2, we obtain

$$\operatorname{div}(\mathbf{y}_n \psi_0^2) = (E_n - Q_n)\psi_0^2. \tag{10}$$

The latter relation is the usual k-dimensional electrostatics law, ψ_0^2 and $\mathbf{y}_n$ playing the role of the dielectric permeability and the field strength respectively. To specify it completely one needs a boundary condition. Invoking the definitions of ψ_0 and $\mathbf{y}_n$, an obvious relation holds:

$$|\mathbf{y}_n \psi_0^2| \to 0 \qquad \text{for } |x| \to \infty,$$

which can be treated as a boundary condition. This relation can immediately be converted into information about E_n. Indeed, integrating both sides of equation (10) over the whole space and transforming the volume integral on the left-hand side into the surface integral (with the help of the Gauss theorem), we find

$$E_n = \int \mathrm{d}V \psi_0^2 Q_n \Big/ \int \mathrm{d}V \psi_0^2. \tag{11}$$

This expression gives the value of the nth correction to the energy level of the unperturbed potential. It is worth noting that the first correction E_1 coincides with that of conventional Rayleigh–Schrödinger perturbation theory (Landau and Lifshitz 1963). To determine other corrections E_n, it is necessary to solve the electrostatical problem (10), with various right-hand-side expressions, which is equivalent to solution of the general elliptical equation

$$\Delta\varphi_n - 2(\mathbf{y}_0 \nabla \varphi_n) = E_n - Q_n \tag{12}$$

where $\mathbf{y}_n = \nabla\varphi_n$ and E_n is given by equation (11). This is not an eigenvalue problem, since E_n is assumed to be known from lower-order iterations (see equation (11)). Thus, from the numerical point of view a computer integration of equation (12) is a much simpler problem than that of equation (1). Besides for some cases it may be solved exactly. It will be discussed elsewhere.

3. Recipe of convergence

The convergence of the procedure proposed† is a complicated and difficult question. We plan to return to its detailed discussion elsewhere. However, a remark which seems physically justified is in order here. It is almost obvious that if the perturbing term λV_1 is less singular than V_0 and is small compared with V_0 for $|x| \to \infty$, then the series (6) and (7) are convergent. A reason which lies behind divergencies in ordinary perturbation theory is the singular nature of the perturbation. Consider the analytic structure of, say,

† We restrict ourselves in the following to consideration of rising potentials only. The results obtained below are valid also in the standard RS perturbation theory.

the ground level energy, E, as a function of the coupling constant λ in the complex λ plane. If $\lambda V_1/V_0 \to \infty$ for $|x| \to \infty$, then changing the sign of λ, $\lambda \to -\lambda$, results in an instability, and, in particular, in E there emerges an imaginary part due to tunnellings. This signals the divergence of the λ series in this case†. If the potential V_1 were less singular than V_0, then no reasons would exist for the appearance of singularities. At least, such reasons are not on the surface. Thus, one can expect that in this situation all the quantities are non-singular in λ in the whole complex plane, which automatically means that λ series are factorially convergent. We did not manage to find a rigorous proof of this statement. However, in numerical examples which will be discussed below the convergence is extremely rapid. We think the following theorem must hold‡.

Theorem. If y_1 is a bounded vector function, then the series (6)–(7) are convergent.

Now let us discuss how to realise the idea concretely. The central point is an optimal choice of the zeroth-order approximation which must guarantee the most rapid convergence of the procedure. It is clear that any function from $\mathscr{L}_2(\mathbb{R}^k)$ series is in fact the wavefunction of some level of some potential. In other words, given any function ψ_0 one can fit a potential

$$V_0 = E_0 + \Delta\psi_0/\psi_0$$

in such a way that the given function ψ_0 turns out to be just a bound level wavefunction in this potential. It is obviously expedient to take ψ_0 in such a way that V_0 would be close to the original potential V, and in particular, would contain all the singularities which are present in V. This is automatically achieved if one puts in ψ_0 the information concerning the behaviour near potential singularities and asymptotics, and nodes of the genuine wavefunction ψ. Such information is easily available in each particular case, at least in one-dimensional and radially symmetrical problems.

Since $V_0(x)$ almost follows $V(x)$ by construction and reproduces all its singularities, their difference, $V_1 = V - V_0$, is small compared with V_0 everywhere, and hence the perturbation theory in $(V - V_0)$ must be convergent.

4. Examples

Let us give a few examples. Consider the Schrödinger equation in one dimension§. Then equation (4) represents a well known Ricatti equation, and equation (8) can be solved exactly‖,

$$y_n(x) = \psi_0^{-2} \int_{-\infty}^{x} (E_n - Q_n)\psi_0^2 \, dx', \tag{13}$$

where Q_n are defined in equation (10) and the nth correction to the energy level E_n is given in equation (11).

† In fact, the above reasoning is the well known 'Dyson argument'.

‡ We know the proof of this theorem in a weaker form. It will be published elsewhere. The question of convergence is considered also by Reed and Simon (1978).

§ The k-dimensional radially symmetric equation reduces to the one-dimensional one. All relations given below after trivial modifications can be used in the k-dimensional symmetric case. A more detailed discussion of the procedure as applied to one-dimensional problems can be found in Turbiner (1979a).

‖ In other words, the Green function of the Schrödinger equation for V_0 at E_0 may be found exactly. From the point of view of second-order ordinary differential equations this is obvious.

For the potentials $V(x)=x^{2n}$ $(n=2, 3, 4)$ and $V(x)=m^2x^2+gx^4$, which are often encountered in various applications, the zeroth-order wavefunction can be chosen in the following form:

$$\psi_0^{(0)}(x)=\exp\left(-\frac{mx^2}{2}-\frac{\sqrt{g}}{n+1}|x|^{n+1}\right), \tag{14a}$$

$$\psi_0^{(1)}(x)=x\exp\left(-\frac{mx^2}{2}-\frac{\sqrt{g}}{n+1}|x|^{n+1}\right). \tag{14b}$$

We limit consideration to the zeroth and first levels. These wavefunctions (14*a*, *b*) satisfy the Schrödinger equation with the following potentials:

Ground state (equation (14*a*))

$$V_0^{(0)}(x)=-(\sqrt{g}n|x|^{n-1}-2m\sqrt{g}|x|^{n+1})+m^2x^2+gx^{2n}, \qquad E_0^{(0)}=m. \tag{15a}$$

First excited state (equation (14*b*))

$$V_0^{(1)}(x)=-[\sqrt{g}(n+2)|x|^{n-1}-2m\sqrt{g}|x|^{n+1}]+m^2x^2+gx^{2n}, \qquad E_0^{(1)}=3m. \tag{15b}$$

4.1. Potential $V(x)=x^{2n}$

In this case in equations (14*a*, *b*), (15*a*, *b*), we put $m=1$ and $g=1$. Then $V_1(x)=V(x)-V_0(x)=-x^2+(n|x|^{n-1}-2|x|^{n+1})$ (for the ground state) and $V_1(x)=V-V_0=-x^2+[(n+2)|x|^{n-1}-2|x|^{n+1}]$ (for the first excitation), and just these expressions will be treated as perturbations. Substituting them as well as $\psi_0^{(0)}(x)=\exp(-x^2/2-|x|^{n+1}/(n+1))$ and $\psi_0^{(1)}(x)=x\exp[-x^2/2-|x|^{n+1}/(n+1)]$ into equations (11) and (13), one find the first corrections to the energy levels. The results are given in table 1. It is worth emphasising the rapid convergence of our method: already the second correction contribution does not exceed a few per cent.

4.2. Quartic anharmonic oscillator $V(x)=m^2x^2+gx^4$

Only the ground state will be considered. Substituting the perturbation $V_1(x)=2\sqrt{g}|x|-2m\sqrt{g}|x|^3$ as well as $\psi_0^{(0)}(x)=\exp(-mx^2/2-\sqrt{g}|x|^3/3)$ into equations (11) and (13), one finds the first corrections to the ground state energy. For example, the first-order correction has the form

$$E_1(g)=2\sqrt{g}\frac{\int_0^\infty (x-mx^3)\exp(-mx^2-\frac{2}{3}\sqrt{g}x^3)\,dx}{\int_0^\infty \exp(-mx^2-\frac{2}{3}\sqrt{g}x^3)\,dx} \tag{16}$$

(we recall that $E_0=m$). A remark concerning the analytic structure of E_1 in the complex g plane is in order here. In fact it reproduces well some of the main features of the behaviour of the genuine energy E, and, unfortunately, fails to reproduce others. Namely, E_1 has a cut $(-\infty, 0]$ and the $g\to\infty$ asymptotic is $\sim g^{1/3}$ as it should be. Moreover, the discontinuity across the cut as $g\to -0$ is exponentially small; however, it does not coincide with the WKB expression (see e.g. Bender and Wu (1969), Simon (1970)), which is known to be correct at $g\to -0$. This deviation from the WKB result is certainly a drawback of the method, but fortunately, it does not invalidate it as a whole. Really, if one could sum the emerging series, the WKB formula would be restored. We think the latter statement can be proved quite rigorously (at least for the example discussed).

Table 1. Ground state and first excited energy levels in potentials x^{2n}. Values ΔE characterise the corresponding term of our perturbation theory. In brackets are the relative deviations from exact values. E_{exact} are the results of numerical calculations (Marinov and Shestopal 1977, unpublished).

Approximation \ Potential		$V(x)=x^4$		$V(x)=x^6$		$V(x)=x^8$	
		Ground level	First level	Ground level	First level	Ground level	First level
0	E	1	3	1	3	1	3
	ΔE	1	3	1	3	1	3
1	E	1.133 59 (6.9%)	3.949 39 (4%)	1.158 41 (1.2%)	4.359 03 (0.5%)	1.234 76 (0.73%)	4.876 84 (2.5%)
	ΔE	0.133 59	0.949 39	0.158 41	1.359 03	0.234 76	1.876 84
2	E	1.095 19 (2.3%)	3.844 82 (1.2%)	1.147 47 (0.2%)	4.339 76 (0.03%)	1.225 595 (0.02%)	4.754 14 (0.36%)
	ΔE	0.048 41	0.104 58	0.010 94	0.019 27	0.009 165	0.122 696
3	E	1.069 76 (0.9%)	—	1.145 44	—	1.225 822	—
	ΔE	0.015 42	—	0.002 03	—	0.000 226	—
E_{exact}		1.060 362 11	3.799 673 15	1.144 802 46	4.338 598 82	1.225 820 10	4.755 874 51

Table 2 presents our results containing the first two iterations and numerical calculations (Hioe *et al* 1978). The agreement is excellent in the whole range of g investigated.

Table 2. Ground state energy level of anharmonic oscillator with quartic anharmonicity (two iterations). ($E' = E/2$, $g' = g/2$, see equation (15a).) E'_{exact} from Hioe *et al* (1978).

g'	E'	E'_{exact}
0.1	0.561 658	0.559 146
0.2	0.604 862	0.602 405
0.3	0.640 163	0.637 992
0.4	0.670 641	0.668 773
0.5	0.697 772	0.696 176
0.6	0.722 399	0.721 039
0.7	0.745 055	0.743 904
0.8	0.766 125	0.765 144
0.9	0.785 861	0.785 032
1	0.804 468	0.803 771
10	1.504 63	1.504 97
50	2.497 34	2.499 71
100	3.125 82	3.131 38
500	5.296 75	5.319 89
1000	6.657 39	6.694 22

5. Conclusion

It is worth noting that the new perturbative procedure proposed here is not only interesting by itself, but yields also information about certain sums encountered in the usual RS perturbation theory†. In fact, there exists an interrelation between our method and that of RS. In the latter the wavefunction is expanded in the following additive way:

$$\psi = \sum_{n=0}^{\infty} \lambda^n \psi_n \tag{17a}$$

where the nth correction ψ_n is determined by a sum over all intermediate states of the unperturbed potential. For example, for the ground state the first wavefunction correction has the form

$$\psi_1^{(0)} = \sum_{n=1}^{\infty}{}' \frac{V_{n0}}{E_0^{(0)} - E_0^{(n)}} \psi_0^{(n)}$$

where the superscript (n) labels the number of the level. On the other hand, we have within the approach proposed the wavefunction expansion in the following multiplicative way,

$$\psi = \psi_0 \prod_{n=1}^{\infty} \exp(-\lambda \mathscr{L}_n), \tag{17b}$$

where $\nabla \mathscr{L}_n = \mathbf{y}_n$. For one dimension the correction $\psi_1^{(0)}$ may be obtained from equation

† We remind the reader that in this paper we restrict ourselves to the case of the ground state and excited states with exactly known node positions.

(13). Then the following sum rule is obtained:

$$\psi_1^{(0)} = \{\psi_0^{(0)}\}\left\{-\int_a^x y_1 \, dx'\right\}. \tag{18}$$

Here the constant a is determined by requiring that the first-order perturbed wavefunction is normalised to unity. In the general case, to make the interrelation explicit let us invoke the definition (2) and consider series (6) and (7) as formal ones. By comparing two alternative expressions for coefficients of various powers λ^n in the ψ and E expressions, many attractive sum rules can be found. These sum rules give the information about the spectrum of the unperturbed potential.

To summarise, we have managed to construct an iterational scheme which does not require the knowledge of the entire spectrum of an unperturbed problem. In one-dimensional and spherically symmetric cases closed analytical expressions for corrections at all orders can be written out. For arbitrary multidimensional potentials, the original eigenvalue problem turns out to be equivalent to integration of the electrostatics equation (12). From the numerical point of view such an integration is much simpler than the solution of the eigenvalue problem.

We conclude with a remark about literature. In the paper by Dolgov and Popov (1978) a convergent iterational scheme for the ground state of an anharmonic oscillator in one dimension was proposed. With some effort one can show that the technique of this paper is a particular case of the approach developed here in one dimension, when $y_0(x) = [V(x)]^{1/2}$ and the unperturbed potential $V_0(X) = V(x) - V'/2\sqrt{V}$. Moreover, it is applicable directly to a narrow class of one-dimensional problems. The one-dimensional Schrödinger equation was considered also in a recent paper by Aharonov and Au (1979) which we learnt about after the completion of the present work. There is a certain overlap between the results of this paper and the part of our work which treats one-dimensional potentials.

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Note added. After the submission of this paper I learned of some new papers and results concerning the issues considered.

(i) One-dimensional case. Perturbation theory (PT) in quadratures, which does not require the knowledge of the whole spectrum (similar to that discussed here), has a long history. It was first proposed by Zel'dovich (1956) and Kirzhnitz (1958). After that it was repeatedly rediscovered by many authors (Polikanov 1967, Pekar 1971, Dolgov and Popov 1978, Aharonov and Au 1979, Turbiner 1979a).

It is worth noting that Polikanov was the first to construct the PT series starting from the Ricatti equation. The possibility of building a convergent PT series by means of this method was mentioned by Dolgov and Popov (1978). The whole issue was elaborated in my recent paper (Turbiner 1979a).

(ii) Multidimensional case. Quite recently there appeared several papers which generalise the approach suggested. Some particular two-dimensional problems were considered; for example, in the paper by Dolgov and Turbiner (1980) the problem of the Stark effect in hydrogen in an *arbitrary* field was solved. Furthermore, in Turbiner (1979b) the approach was generalised to the case of excited states. The relation between the PT and the Ritz variational principle was also discussed ($E_{\text{var}}(\psi_0) = E_0 + E_1$). It was shown that the PT suggested here allows one to estimate the accuracy of variational calculations. As an example, we considered the same problems as in §§ 3.1 and 3.2 above, and the two-dimensional non-symmetric anharmonic oscillator. The details, and in particular some exact solutions of equation (12), are given in a forthcoming publication (*Sov. Phys.-JETP* in press).

(iii) In a quite recent paper by Au and Aharonov (1979) an analogous PT was proposed. However, the possibility of building a convergent perturbative series is not discussed in this paper.

Note added in proof. The method proposed in this paper turned out to be extremely fruitful in the case of the ordinary weak-coupling perturbation theory (V_0 is an exactly soluble potential and V_1 is a polynomial perturbation) (Turbiner A V 1981 *Pisma v Zh. Eksp. Teor. Fiz.* **33** 181–5). In this case the construction of perturbation theory is a purely *algebraic* problem!

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