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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 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 we consider potentials x^{2n} ($n = 2,3,4$) and $m^2x^2 + gx^4$ in one-dimensional space.

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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 this or that potential. Sometimes it is necessary to consider very sophisticated potentials, and as a rule the eigenvalues and eigenfunctions can not be found exactly. One has to turn to approximate methods. Two of them are commonly used: the numerical integration with the help of computers and the Rayleigh-Schrödinger perturbation theory (see e.g. [1]). Both methods have certain drawbacks. The former is applicable actually to one dimensional problems only, and practically does not work in two or more dimensions. 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 to be ineffective.

In this paper I construct a new iteration scheme which permits to determine eigenvalues and eigenfunctions of the k - dimensional Schrödinger equation with arbitrary potential.

Unlike the ordinary perturbation theory, the series emerging within the scheme proposed are expected to be convergent. Physical arguments demonstrating the convergence are presented. As an attempt of a more rigorous consideration I formulate also a simple theorem which gives a necessary condition for the convergence of the procedure.

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

The general consideration is supplemented by a few examples. We deal with one-dimensional potentials, which are rather often encountered in various applications, namely X^{2n} (n = 2, 3, 4) and quartic anharmonic oscillator.

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

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

into a nonlinear one. The nonlinearization transformation I mean has the form

$$\vec{y} = -\frac{\vec{\nabla}\psi}{\psi} = -\vec{\nabla}(\ln\psi) \qquad (2)$$

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

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

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

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

is satisfied.

The potential V can be always decomposed into two pieces $V = V_0 + \lambda V_1$ such that the equation

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

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

$$\vec{\gamma} = \sum_{n=0}^{\infty} \lambda^n \vec{\gamma}_n \qquad (6)$$

$$E = \sum_{n=0}^{\infty} \lambda^n E_n \qquad (7)$$

Then the values of E_n and functions $\vec{\gamma}_n$ are determined by the following of linear equations:

$$div\,\vec{\gamma}_n - 2\vec{\gamma}_0\vec{\gamma}_n = E_n - Q_n \qquad (8)$$

(Besides, each of the function $\vec{\gamma}_n$ must satisfy eq.(4).) Here

$$Q_1 = V_1\,,\quad Q_n = -\sum_{i=1}^{n-1} \vec{\gamma}_i \vec{\gamma}_{n-i} \quad at\ n \geq 2 \qquad (9)$$

Multiplying both the right and left-hand sides of eq.(8) by ψ_0^2 we come to

$$div\,(\psi_0^2 \vec{\gamma}_n) = (E_n - Q_n)\psi_0^2 \qquad (10)$$

The latter relation is the usual k - dimensional electrostatics law, ψ_0^2 and $\vec{\gamma}_n$ 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 $\vec{\gamma}_n$ we get an obvious relation:

$$\left| \vec{g}_n \psi_0^2 \right| \to 0 \quad \text{at} \quad |x| \to \infty .$$

This relation can be immediately converted into information about E_n. Really integrating both sides of eq.(10) over the whole space and transforming the volume integral in the left-hand side into the surface integral (with the help of the Gauss theorem) we find

$$E_n = \frac{\int dV \, \psi_0^2 \, Q_n}{\int dV \, \psi_0^2} \qquad (11)$$

This expression gives the value of the n - th correction to the energy level of theunperturbed potential. It is worth noting that the first correction ($n = 1$) coincides with that of conventional Rayleigh-Schrödinger perturbation theory [1]. To determine other corrections E_n it is necessary to solve the electrostatical problem (10), with various right-hand-sides expressions, which is equivalent to solution of the general elliptic equation

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

where $\vec{g}_n = \vec{\nabla} \varphi_n$ and E_n is given by Eq.(11). This is not an eigenvalue problem, since E_n is assumed to be know from lower-order iterations (see eq.(11)). Thus, from the numerical point of view a computer integration of eq.(12) is a much simpler problem than that of eq.(1).

Now as to the convergence of the procedure proposed.*) It is a complicated and difficult question. I 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

*) I restrict myself in following consideration by rising potentials only.

λV_1 is less singular than V_0 and is small as compared to V_0 at $|x| \to \infty$, then the series (6), (7) are convergent. Really, a true reason which lies behind divergencies in ordinary perturbation theory is a singular nature of the perturbation. Consider the analytic structure of, say the ground level energy, E, as a function of the coupling constant λ in the complex λ plane. If $\lambda V_1/V_0 \to \infty$ at $|x| \to \infty$ 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 tunnelings. This signale the divergence of λ series in this case. If the potential V_1 were less singular than V_0, then no reasons would exist for appearing of singularities. At least, such reasons are not on the surface. Thus, one can expect that this situation of all the quantities are nonsingular in λ in the whole complex plane, which automatically means that λ series are factorially convergent. I 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. As to the rigorous result, let us mention the following theorem for one-dimensional case:

If y_0 grows at infinity, $|x| \to \infty$, and $y_n(x)$ are unbounded functions *), then the series (6) - (7) are divergent.

Now let us discuss how to realize the idea concretely. The central point is an optimal choice of the zeroth-order approximation which must guarantee the most rapid convergence

*) For excited states unboundness is required for regular parts of $y_n(x)$.

of the procedure. It is clear that any function from $L_2(R^k)$ serves in fact as the wave function 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 to be just a bound level wave function 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 asymptotic behavior and number of zeroes of the genuine wave function ψ . Such an 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 as compared to V_0 everywhere, and hence the perturbation theory in $(V - V_0)$ must be convergent.

Let us give a few examples. Consider the Schrödinger equation in one dimension *). Ther eq.(4) represents in fact a well-know Ricatti equation, and eq.(8) can be readily solved exactly,

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*) k - dimensional radially symmetric equation reduces to the one-dimensional one. In these cases a similar perturbation theory was proposed for anharmonic oscillator problem [2] . General formulas were obtained in paper [3] .

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

where Q_n are defined in eq.(10) and the n - th correction to the level energy E_n is given in eq.(11).

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 wave function can be chosen in the following form

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

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

I limit the consideration by the zeroth and first levels, an extension to higher excitations being trivial. These wave functions eqs.(14a,b) satisfy the Schrödinger equation with the followings potentials:

ground state (eq.(14a))

$$V_0^{(0)}(x) = -\left[\sqrt{g}\,n\,x^{n-1} - 2m\sqrt{g}\,x^{n+1}\right] + m^2x^2 + gx^4;\ E_0^{(0)} = m \qquad (15a)$$

first excited state (eq.(14b))

$$V_0^{(1)}(x) = -\left[\sqrt{g}\,(n+2)\,x^{n-1} - 2m\sqrt{g}\,x^{n+1}\right] + m^2x^2 + gx^4;\ E_0^{(1)} = 3m \qquad (15b)$$

(A). Potential $V(x) = x^{2n}$. In this case in eqs.(14a,b), (15a,b) I put m = 1 and g = 1. Then $V_1(x) = V(x) - V_0(x) = -x^2 + \left[nx^{n-1} - 2x^{n+1}\right]$ (for ground state) and $V_1(x) = V(x) - V_0(x) = -x^2 + \left[(n+2)x^{n-1} - 2x^{n+1}\right]$ (for the first exitation), and just these expressions will be treated as perturbations. Substituting them as well as $\psi_0^{(0)} = \exp\left\{-x^2/2 - x^{n+1}/n+1\right\}$

and $\psi_0^{(1)} = x \exp\left\{-x^2/2 - x^{n+1}/(n+1)\right\}$ into eqs.(11), (13) one finds the first corrections to the energy levels. The results are given in Table 1. It is worth emphasizing the rapid convergence of our methods already the second correction contribution does not exceed a few percents.

(B). Quartic anharmonic oscillator $V = m^2x^2 + gx^4$. 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 $\psi_0^{(0)}(x) = \exp\left\{-mx^2/2 - \sqrt{g}x^3/3\right\}$ into eqs.(11), (13) one finds the first corrections to the ground state energy. For example, the first-order correction has a form

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

(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 $g \to \infty$ asymptotics 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. [4,5]), which is known to be correct at $g \to -0$. This deviation from the WKB result is certainly a drawback of the method, but, luckily enough, it does not invalidates it as a whole. Realls, if one could sum the emerging series, the WKB formula would be restored. The latter statement can be proven quite rigourously (at least for examples discussed in (A) and (B)).

Table 2 confronts my results containing two first iterations with numerical calculations [6]. The agreement is excellent in the whole range of g investigated.

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

$$\psi = \sum_{n=0}^{\infty} \lambda^n \psi_n \qquad (17)$$

where the n - th correction ψ_n is determined by a sum over all intermediate states of unperturbed potential. For example, for the first correction we have

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

where the superscripts $(n), (\ell)$ label the number of the level. On the other hand, within the approach proposed the correction $\psi_1^{(\ell)}$ may be obtained from the definition (2) and eq.(13). Then, the following sum rule is obtained

$$\psi_1^{(\ell)} = \left\{\psi_0^{(\ell)}\right\}^2 \left\{-\int_0^x \psi_1 \, dx' + C_1\right\} = \sum_{n=0}^{\infty}{}' \frac{V_{n\ell}}{E_0^{(\ell)} - E_0^{(n)}} \psi_0^{(n)} \qquad (18)$$

Here the constant C_1 is determined by requiring that the first-order perturbed wave function is normalized to unity In general case make the interrelation explicit let us invoke the definition (2) and consider series (6), (7) as formal ones. By comparing two alternative expressions for

coefficients of various powers λ^n in the ψ and E expansions many attractive sum rules can be found. These sum rules give the information about the spectrum of unperturbed potential.

To summarize, I managed to construct the 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 expression 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 electrostatics equation (12). From the numerical point of view such an integration is much more simple than the solution of the eigenvalue problem.

A few points remained to be investigated yet. The rigorous proof of the convergence conditions is still lacking in general case. The orthogonality of the excited states as given by subsequent iterations is questionable. If they are not orthogonal, then what is the optimal way to orthogonalize them?

I conclude with a some remark on literature. In the paper [2] a version of convergent perturbation theory for ground and first states of anharmonic oscillator to one dimension was proposed. With some effort one can show that the technique of Ref. 2 is a particular case of the approach developed here to one dimension, when $\psi_0(x)=[V(x)]^{1/2}$ and unperturbed potential $V_0(x)=V(x)-V'(x)/2\sqrt{V(x)}$. Moreover, this recipe applicable directly to a narrow class of one-dimensional problems. One-dimensional Schrödinger equation was considered also in a recent paper [7] which I learnt about after the completion of

present work. There is a certain overlap between the results of paper [7] and the part of my work which treats one-dimensional potentials.

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Table 1. Ground-state and first excited energy levels in potentials X^{2n}. Values ΔE characterize the corresponding term of our perturbation theory. In brackets the relative deviations from exact values are contained. E_{exact} from Ref. 8.

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	1.13359(6,9%)	3.94939(4%)	1.15841(1,2%)	4.35903(0,5%)	1.23476(0,73%)	4.87684(2,5%)
	ΔE	0.13359	0.94939	0.15841	1.35903	0.23476	1.87684
2	E	1.09519(2,3%)	3.84482(1,2%)	1.14747(0,2%)	4.33976(0,03%)	1.225595(0,02%)	4.75414(0,36%)
	ΔE	0.04841	0.10458	0.01094	0.01927	0.009165	0.122696
3	E	1.06976(0,9%)	-	-	-	-	-
	ΔE	0.01542	-	-	-	-	-
E_{exact}		1.06036211	3.79967315	1.14480246	4.33859882	1.22582010	4.75587451

Table 2. Ground-state energy level of anharmonic oscillator with quartic anharmonicity (two approximations). ($E' = E/2$, $g' = g/2$, see eq.(I5a)). E'_{exact} from Ref. 6

g'	E'	E'_{exact}
0.1	0.561658	0.559146
0.2	0.604862	0.602405
0.3	0.640163	0.637992
0.4	0.670641	0.668773
0.5	0.697772	0.696176
0.6	0.722399	0.721039
0.7	0.745055	0.743904
0.8	0.766125	0.765144
0.9	0.785861	0.785032
1	0.804468	0.803771
10	1.50463	1.50497
50	2.49734	2.49971
100	3.12582	3.13138
500	5.29675	5.31989
1000	6.65739	6.69422

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