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Algebraic convergent perturbation theory for quantum systems with strong anharmonicity

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Abstract. A novel perturbative method based on the non-trivial decomposition of the Hamiltonian into the unperturbed part and the perturbation is proposed. The method admits using practically any approximate solution of the Schrödinger equation as a starting point by constructing a perturbative expansion. The resulting series is convergent. The procedure of calculation of its terms is purely algebraic. The method is available for calculations in both the weak- and strong-coupling regimes, and for estimating and increasing the accuracy of variational analysis results.

1. Introduction

The principal trouble with the standard perturbation theory (SPT), which long remains a basic tool in studying quantum mechanical systems with polynomial potentials, lies in the fact that the resulting series diverges. This blocks an extension into a domain of strong anharmonicity.

The origin of this divergence has been studied by Dyson (1952): for a perturbed oscillator and similar systems the perturbation potential increases at large distance more rapidly that the unperturbed one, irrespective of how small the coupling constant is. Therefore the physics of the problem is drastically changed if the sign of the coupling changes: the stable system transforms to an unstable one. This implies a branch-point singularity at the origin of the complex-coupling constant plane, and hence the zero radius of convergence of perturbative expansions. This reasoning, known as 'Dyson's instability argument', can be easily translated into the path integral language, where the instability of the system manifests itself as the divergence of the Euclidean path integral. (For more details see Turbiner (1984) and Ushveridze (1983).)

Since our aim is to solve the strong-coupling problem in the framework of a perturbative approach, it is sensible to try to split the Hamiltonian of interest into the unperturbed part and the perturbation in such a way as to circumvent Dyson's argument. To discuss this possibility consider an arbitrary observable quantity allowing the expression via the Euclidean path integral

$$A \sim \int \mathrm{D}p\, \mathrm{D}q \ldots \exp\left(\mathrm{i} \int p\dot{q}\, \mathrm{d}t - \int H(p, q)\, \mathrm{d}t\right). \tag{1}$$

Here $H = H(p, q)$ is the classical Hamiltonian of the system which is assumed to be

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stable, $H(p, q) > 0$. The stability of the system guarantees the convergence (existence) of integral (1). Evidently, any decomposition of H into the unperturbed part $H_0 = H_0(p, q)$ and the perturbation $H_1 = H - H_0 = H_1(p, q)$ leads to the following perturbative expansion for A:

$$A = \sum_{n=0}^{\infty} A_n. \tag{2}$$

In order to study the convergence properties of this expansion, let us introduce the one-parametric class of 'Hamiltonians' $H(\varepsilon) = H_0 + \varepsilon H_1$ and the corresponding class of 'observables'

$$A(\varepsilon) \sim \int \mathrm{D}p\, \mathrm{D}q \ldots \exp\left(\mathrm{i} \int p\dot{q}\, \mathrm{d}t - \int H_0(p, q)\, \mathrm{d}t - \varepsilon \int H_1(p, q)\, \mathrm{d}t \right). \tag{3}$$

Expanding (3) in powers of ε

$$A(\varepsilon) = \sum_{n=0}^{\infty} \varepsilon^n A_n \tag{4}$$

we note that the radius of convergence of this expansion is determined by the locations of singularities of $A(\varepsilon)$ in a complex ε plane. Examining the system under consideration from the point of view of Dyson-type singularities, we see that they all lie outside (or at the boundary of) the unit radius circle, provided the condition

$$H_0(p, q) \geqslant |H_1(p, q)| \tag{5}$$

is satisfied. Actually, for any $|\varepsilon| < 1$ the system is stable since condition (5) guarantees the existence of integral (3). Thus expression (4) converges for any $|\varepsilon| < 1$. This fact, supplemented by the existence of integral (1), allows us to conclude that the expansion (4) will be convergent for the 'physical' value $\varepsilon = 1$, for which $H(\varepsilon) = H$, $A(\varepsilon) = A$ and (4) coincides with (2). Hence condition (5) is sufficient for the convergence of the perturbative series (2).

Thus our problem is reduced to finding such a splitting of the Hamiltonian H into the unperturbed part and the perturbation that guarantees the sufficient smallness of the perturbation in comparison with the unperturbed part for any p and q. If we wish to construct the perturbation theory converging in both the weak and strong coupling regimes then we must guarantee the fulfilment of (5) for any couplings. However, a straightforward realisation of this idea requires the unperturbed problem to be exactly soluble and we know few exactly soluble problems in quantum mechanics. But fortunately this is a fictitious limitation: one could construct a good perturbative scheme without imposing the simple-minded exact solubility and without requiring that the unperturbed system is of particular physical meaning (Turbiner 1984, Ushveridze 1983, 1984, 1986, Shaverdyan and Ushveridze 1983).

In this paper we formulate the practical realisation of such an approach. We show that a strong-coupling problem in quantum mechanics can be solved in the framework of the non-standard perturbation theory (NPT), based on the non-trivial decomposition of the Hamiltonian into the unperturbed part and the perturbation. In contrast with the SPT, the NPT which is proposed here has the following advantages.

(i) It enables us to use practically any approximate solution of the Schrödinger equations as a starting point by constructing the perturbative expansions.

(ii) It guarantees the necessary smallness of perturbation in comparison with the unperturbed part irrespective of the magnitudes of the coupling constants. This leads to convergence of the resulting series in both the weak- and strong-coupling regimes.

(iii) An effective proximity between the exact and approximate solutions plays the role of the small parameter, determining the rapidity of the NPT series convergence.

(iv) The procedure of calculation of the NPT series terms is purely algebraic.

These properties of NPT enable us to consider it as a convenient instrument for estimating and increasing the accuracy of variational analysis results. It is worth noticing that the early versions of convergent perturbative theory do not simultaneously satisfy the four above-mentioned conditions (see Halliday and Suranyi 1980, Turbiner 1984, Turbiner and Ushveridze 1983, 1984, 1986, Schaverdyan and Ushveridze 1983).

This paper is organised as follows. In § 2 we state the problem and in § 3 we choose the representation in which the Schrödinger equation to be solved assumes an especially simple form. In § 4 we construct the NPT scheme and demonstrate its algebraic nature. In § 5 the convergence of the constructed expansions is proved. Numerical examples are considered in § 6.

2. The problem

Let H be the Hamiltonian of the quantum mechanical system having a discrete spectrum in the Hilbert space W. The degeneracy is allowed.

Consider the Schrödinger equation

$$H\psi = E\psi \tag{6}$$

for the particular state of interest and denote by W_E the set of all its solutions ψ corresponding to the eigenvalue E. Then the non-zeroth approximate solution

$$\psi_0 \in W \qquad E_0 = (\psi_0, H\psi_0)/(\psi_0, \psi_0) \tag{7}$$

of this equation may be obtained by means of the variational method.

Our purpose is to use ψ_0 and E_0 as a starting point (as a zeroth-order approximation) by constructing the perturbative expansions

$$\psi = \psi_0 + \psi_1 + \psi_2 + \ldots \qquad E = E_0 + E_1 + E_2 + \ldots \tag{8}$$

converging to the non-zeroth exact solution ψ and E of equation (1). In order to obtain such expansions it is necessary to decompose the Hamiltonian into the unperturbed part and the perturbation

$$H = H_0 + H_1 \tag{9}$$

in such a way as to guarantee: (i) the sufficient proximity between the exact and the unperturbed Hamiltonians, (ii) the exact solubility of the unperturbed Schrödinger equation, and (iii) the belonging of the approximate solution (7) to the unperturbed Hamiltonian spectrum.

The realisation of this problem requires the choice of an appropriate representation.

3. The Lanczos representation

Let us define W_0 as the set of all elements of W of the form

$$\varphi = f(H)\psi_0 \tag{10}$$

where $f(H)$ are arbitrary functions. This set has the following properties.

Statement 1. W_0 is an invariant subspace of W, i.e. if $\varphi \in W_0$ then $H\varphi \in W_0$ as well.

This statement follows immediately from the definition (10). Being trivial, it is nevertheless very important for us, since it shows that the space W_0 can be treated as the Hilbert space for the operator H. Therefore the question 'what is the spectrum of H in W_0?' is quite a correct one to ask.

In order to investigate this spectrum, consider the Schrödinger equation

$$H\psi = E\psi \qquad \psi \in W_0 \tag{11}$$

and denote by W_{0E} the set of all its solutions ψ corresponding to the eigenvalue E.

Statement 2. If $P_E\psi_0 = 0$, then dim $W_{0E} = 0$. If $P_E\psi_0 \neq 0$, then dim $W_{0E} = 1$.

Indeed, let P_E be the projector onto the eigenspace W_E. Then $W_{0E} = P_E W_0$ and according to the definition (10)

$$W_{0E} = \{F(H)P_E\psi_0\} = \text{constant} \times P_E\psi_0. \tag{12}$$

If $P_E\psi_0 = 0$, then W_{0E} contains only one zero element and therefore dim $W_{0E} = 0$. If $P_E\psi_0 \neq 0$, then any element of W_{0E} is proportional to $P_E\psi_0$, and consequently dim $W_{0E} = 1$. Thus the statement is proved.

This statement shows that the spectrum of H in W_0 is non-degenerate irrespective of the degeneracy of the spectrum of H in the initial space W. Note that this property makes W_0 similar to the Hilbert space for the one-dimensional quantum system. Formula (10) confirms our observation. Indeed, even if the W_0 elements are the functions of many variables (the multidimensional case) there exists a simple correspondence between these elements and the function of one variable.

Now let us introduce the orthonormalised basis in W_0. The basis functions can be chosen as

$$\phi_m = P_m(H)\psi_0 \tag{13}$$

where $P_m(H)$ are the mth order polynomials fixed by the conditions

$$(\phi_m, \phi_l) = \delta_{ml}. \tag{14}$$

Representing ϕ_m in the form

$$\phi_m = \sum_i P_m(E_i)\gamma_i \qquad \psi_i \in W_{E_i} \qquad (\psi_i, \psi_x) = \delta_{ik} \tag{15}$$

and substituting (15) into (14) one finds that the conditions (14) are equivalent to

$$\sum_i P_m(E_i)P_l(E_i)\gamma_i^2 = \delta_{ml} \tag{16}$$

with constants γ_i^2 playing the role of the discrete weight function. This implies that $P_n(H)$ can be considered as orthogonal polynomials of a discrete variable (Bateman and Erdelyi 1953).

Statement 3. (This is very important.) In the basis ϕ_n the Hamiltonian H has a three-diagonal form, i.e.

$$H_{nm} \equiv (\phi_n, H\phi_m) = 0 \qquad \text{if} \qquad |n-m| > 1. \tag{17}$$

This statement, known as a Lanczos theorem, allows a very simple proof. Indeed, from the relations

$$H\phi_m = HP_m(H)\psi_0 = \left(\sum_{l=0}^{m+1} c_{ml}P_l(H)\right)\psi_0 = \sum_{l=0}^{m+1} c_{ml}\phi_l \tag{18}$$

it follows that the equality $H_{lm}=0$ holds for any $l>m+1$. Since H is the Hermitian operator, it should also hold in the case when $l<m-1$. Thus, the statement is proved (Lanczos 1950, Wilkinson 1965).

In what follows we shall use for the basis ϕ_m the term of the Lanczos basis. For the non-vanishing matrix elements of H in the Lanczos basis we have

$$H_{nn}=\frac{B_n}{A_n}-\frac{B_{n-1}}{A_{n-1}} \qquad H_{n,n+1}=\frac{(A_{n-1}A_{n+1})^{1/2}}{A_n} \tag{19}$$

where

$$A_{-1}=1 \qquad A_n=\det\begin{Vmatrix} b_0 & b_1 & \dots & b_n \\ b_1 & b_2 & \dots & b_{n+1} \\ \dots & \dots & & \dots \\ b_n & b_{n+1} & \dots & b_{2n} \end{Vmatrix} \tag{20}$$

$$B_{-1}=0 \qquad B_n=\det\begin{Vmatrix} b_0 & b_1 & \dots & b_{n+1} \\ b_1 & b_2 & \dots & b_{n+2} \\ \dots & \dots & & \dots \\ b_n & b_{n+1} & \dots & b_{2n+1} \end{Vmatrix} \tag{21}$$

$$b_n=(\psi_0 H^n \psi_0). \tag{22}$$

These formulae are the trivial consequences of the general theory of orthogonalisation (Bateman and Erdelyi 1953).

Statements 1-3 enable us to assume that the space W_0 is more convenient for immediate realisation of our programme than the initial one W. Note, however, that the transition from equation (6) to the more simple equation (11), assuming an especially simple form in a Lanczos basis, is available if and only if the exact wavefunction to be found is known to belong to the Lanczos space W_0. The following theorems show when this is possible.

Theorem 1. Let ψ_0 be a good approximation for $\psi \in W_E$ such that

$$\left\| \frac{\psi_0}{\|\psi_0\|}-\frac{\psi}{\|\psi\|} \right\| < \sqrt{2}. \tag{23}$$

Then W_E has a non-zeroth projection on the space W_0 and consequently the eigenvalue E can be found from equation (11).

Proof. From inequality (23) it seems that

$$\left(\frac{\psi_0}{\|\psi_0\|}-\frac{\psi}{\|\psi\|}, \frac{\psi_0}{\|\psi_0\|}-\frac{\psi}{\|\psi\|} \right) = 2-2\frac{(\psi,\psi_0)}{\|\psi\|\|\psi_0\|} < 2 \tag{24}$$

Hence, $P_E\psi_0=0$ and, according to statement 2, we obtain the assertion of this theorem. From this theorem it follows that any sufficiently good variational solution of equation (5) can be used as a zeroth-order approximation in the scheme to be proposed.

Theorem 2. Let ψ_0 be a positive definite trial function. Then the ground-state eigenfunction $\psi \in W_E$ belongs to W_0 and consequently E can be found from equation (11).

Proof. It is known that the ground-state eigenfunction does not have nodes. Hence, it cannot be orthogonal to the function. From the non-degeneracy of the ground state and from statement 2 one obtains the assertion of this theorem.

In what follows we assume the requirements of the theorems 1 and/or 2 to be satisfied.

4. The NPT method

The purpose of this section is to decompose the Hamiltonian H into the unperturbed part H_0 and the perturbation H_1 in such a way as to guarantee the exact solubility of the unperturbed Schrödinger equation and the belonging of the approximate solution (7) to the unperturbed Hamiltonian spectrum.

To construct such a decomposition, recall that in the Lanczos basis ϕ_n the Hamiltonian H has a three-diagonal form and that the zeroth basis function ϕ_0 is proportional to the trial eigenfunction ψ_0. Hence, the simplest way to satisfy both the above-mentioned requirements is to choose as H_0 the diagonal part of H. Thus, we fix the unperturbed Hamiltonian in the diagonal representation, presenting the whole set of its eigenfunctions $\phi_n \in W_0$ and eigenvalues $e_n = (\phi_n, H\phi_n)$. Note that such a choice of H_0 is very natural from the point of view of perturbation theory approach, since the construction of the perturbative corrections requires a knowledge of the unperturbed spectrum only. Therefore, the question 'what is the concrete form of H_0 in coordinate or moment representation?' is not essential for us. Note also, that choosing the unperturbed Hamiltonian in the diagonal Lanczos representation, we circumvent the problem of exact solubility in quantum mechanics. Now there is no need to deal with this problem; we simply present its solution without requiring that the unperturbed system is of particular physical meaning.

Thus we have

$$H_0 = \sum_n H_{nn}\phi_n \otimes \phi_n \tag{25a}$$

$$H_1 = \sum_n H_{n,n+1}(\phi_n \otimes \phi_{n+1} + \phi_{n+1} \otimes \phi_n). \tag{25b}$$

We see that the matrix elements of the perturbation are different from zero for the transitions between the neighbouring states only. Therefore all the sums over intermediate states, appearing when constructing the perturbative corrections, become finite, resulting in the algebraisation of their calculation procedure. In this sense NPT is similar to SPT in which the algebraisation phenomenon has been revealed by Bender and Wu (1969). Repeating the reasoning of their paper we derive the recurrency relations for the NPT series terms.

Substituting expansions (8) and (9) into equation (11) and collecting the terms of the same order, we obtain the equation for the Nth correction

$$\{H_0 - E_0\}\psi_N = -H_1\psi_{N-1} + E_N\psi_0 + \sum_{L=1}^{N-1} E_{N-L}\psi_L \qquad N = 1, 2, \ldots, \infty. \tag{26}$$

Note that the exact eigenfunction ψ is not assumed to be normalised here. Therefore, without loss of generality, all the higher corrections ψ_N can be taken to be orthogonal to ψ_0. This enables us to search the correction ψ_N in the form

$$\psi_N = \sum_{k=1}^{N} F_{Nk}\phi_k \tag{27}$$

where F_{Nk} are certain unknown constants to be found. Substitution of (27) into (26) results in the required recurrency conditions

$$F_{Nk} = (H_{kk} - H_{00})^{-1}\left(\sum_{L=1}^{N-1} E_{N-L}F_{Lk} - F_{N-1,k-1}H_{k-1,k} - F_{N-1,k+1}H_{k,k+1}\right) \tag{28}$$

$$E_N = F_{N-1,1}H_{01}. \tag{29}$$

From formulae (28) and (29) it follows that the constructing of the NPT is an iterative procedure. Moreover, the calculation of Nth correction requires the knowledge of first $2N$ terms of sequence (22) only. This means that the NPT scheme is an extremely economical one from the point of view of its practical realisation.

5. The convergence of the NPT procedure

Note that the proposed choice of the unperturbed problems automatically guarantees the effective proximity between H_0 and H, which is necessary for the series convergence. Indeed, the equality

$$(\phi_n, H\phi_n) = (\phi_n, H_0\phi_n) \tag{30}$$

means that the condition of coincidence of H_0 with H is satisfied for the expectation values. To prove the fact that this actually leads to the convergence of the series, one can use the path integral method.

Let us introduce the raising and lowering operators

$$(a^+)_{nm} = \sqrt{m}\,\delta_{n+1,m} \qquad (a)_{nm} = \sqrt{n}\,\delta_{n,m+1} \tag{31}$$

in the matrix representation. It can be easily proved that

$$[(a^+)^N(a^N)]_{nm} = \frac{\Gamma(n)}{\Gamma(n-N)}\,\delta_{nm} \tag{32a}$$

$$[(a^+)^{N+1}a^N]_{nm} = \frac{\Gamma(m)}{\Gamma(m-N)}\sqrt{m}\,\delta_{m,n+1} \tag{32b}$$

$$[(a^+)^N a^{N+1}]_{nm} = \frac{\Gamma(n)}{\Gamma(n-N)}\sqrt{n}\,\delta_{n,m+1}. \tag{32c}$$

From (32) it follows that the three-diagonal matrix H allows the following representation:

$$H = \sum_N \beta_N (a^+)^N a^N + \sum_N \gamma_N [(a^+)^{N+1}a^N + (a^+)^N a^{N+1}] \tag{33}$$

where the coefficients β_N and γ_N are

$$\beta_N = \frac{1}{N!}\sum_k (-1)^k \frac{N!}{k!(N-k)!}\,H_{kk} \tag{34a}$$

$$\gamma_N = \frac{1}{N!}\sum_k (-1)^k \frac{N!}{k!(N-k)!}\,\frac{H_{k,k+1}}{(k+1)^{1/2}}. \tag{34b}$$

Substituting (34) into (33) and introducing the normal ordering symbol, one can rewrite (33) as

$$H = :\{F(a^+a) + (a^+ + a)Q(a^+a)\}: \tag{35}$$

where

$$F(\rho)=\mathrm{e}^{-\rho}\sum_{n=0}^{\infty}\frac{\rho^n}{n!}H_{nn} \tag{36a}$$

$$Q(\rho)=\mathrm{e}^{-\rho}\sum_{n=0}^{\infty}\frac{\rho^n}{n!(n+1)^{1/2}}H_{n,n+1}. \tag{36b}$$

Recall now that, if the Hamiltonian of the quantum system allows the representation via the normally ordered function of the raising and lowering operators, then any observable quantities in the system can be formally expressed by means of the path integral. The path integral corresponding to the Hamiltonian (35) has a form

$$\int \mathrm{D}p\,\mathrm{D}q\,\exp\left(\mathrm{i}\int p\dot{q}\,\mathrm{d}t-\int\left(F(p^2+q^2)-2qQ(p^2+q^2)\right)\mathrm{d}t\right). \tag{37}$$

The function $F(p^2+q^2)+2qQ(p^2+q^2)$ in (37) is the analogue of the classical Hamiltonian, where the first and second terms play the role of unperturbed part and the perturbation, respectively.

It should be emphasised that in equation (37) the variables q and p do not coincide with the initial coordinates and momenta of the system. Moreover, representation (37) is one dimensional, irrespective of the dimensionality of the initial system. This is one more manifestation of the analogy between the Lanczos space and the Hilbert one for one-dimensional quantum systems.

Note also that due to the evenness of the unperturbed classical Hamiltonian and the oddness of the perturbation, all odd terms of NPT expansion for the energy levels vanish. This assertion can also be obtained immediately from the recurrency relations (27)-(29).

The following estimate plays a central role in our consideration.

Theorem 3. If the Hamiltonian H is a positive definite operator, then the NPT series is a convergent one.

Proof. From the positivity of H it follows that the inequality

$$(\phi, H\phi)/(\phi,\phi)>0 \tag{38}$$

holds for any $\phi\in W_0$. Choosing the function ϕ in the form

$$\phi_{\pm}=\sum_n\left(\frac{\rho^n}{n!}\right)^{1/2}(\pm 1)^n\phi_n \tag{39}$$

and substituting (39) into (38) we obtain

$$F(\rho)>2\sqrt{\rho}\,|Q(\rho)|. \tag{40}$$

Taking $\rho=p^2+q^2$ we see that

$$F(p^2+q^2)>|2qQ(p^2+q^2)|. \tag{41}$$

The last inequality menas that the perturbation Hamiltonian is less than the unperturbed one for any p and q. As was shown in § 1 (for more details see also Ushveridze (1983, 1984)) this is a sufficient condition of the convergence of perturbative expansions for the quantities, allowing the representation via the functional integral. Thus, the theorem is proved.

Once the unperturbed problem is chosen to guarantee the perturbation expansion convergence in the asymptotic, one could try to make use of this convergence for the several first terms as fast as possible. In doing so, one can use the freedom to choose the zeroth-order approximation wavefunction ψ_0. It is natural that the rate of the resulting series convergence strongly depends on the 'goodness' of this approximation. Indeed, first consider two non-vanishing terms of the NPT expansion for a certain eigenvalue E. From formulae obtained in the previous sections it follows that

$$E_0 = \langle H \rangle$$

$$E_2 = \frac{\langle (H - \langle H \rangle)^2 \rangle^2}{\langle (H - \langle H \rangle)^3 \rangle} \qquad \langle \ldots \rangle \equiv (\phi_0 \ldots \phi_0). \tag{42}$$

Now, let us assume that the trial eigenfunction ψ_0 differs slightly from the exact one, ψ:

$$\psi_0 = \psi + \varepsilon f \qquad \varepsilon \to 0. \tag{43}$$

(The function f can be assumed to be orthogonal to ψ without loss of generality.) Substituting (43) into (42) one obtains

$$E_2 / E_0 \sim \varepsilon. \tag{44}$$

This means that the effective proximity between the exact and approximate solutions of equation (6) plays the role of the small parameter of the perturbative expansions: the rate of the NPT series convergence increases if ε approaches zero. From this reasoning it follows that NPT can be used as a good instrument for estimating and increasing the accuracy of variational analysis results.

6. Examples

To demonstrate how NPT works, let us consider the problem of calculation of the ground and first excited states $E^{(0)}$ and $E^{(1)}$ in the simple one-dimensional models of anharmonic oscillators with the Hamiltonian:

$$H = -\frac{\partial^2}{\partial x^2} + x^6. \tag{45}$$

Since the harmonic term in this Hamiltonian is absent, we are dealing with the case of infinitely strong anharmonicity.

Following the proposed NPT method, let us first construct the trial function $\psi_0^{(r)}$. It is reasonable to choose it in one of the two following forms:

$$\psi_0^{(r)} = x^r \exp\left(-\frac{x^4}{4} - \frac{ax^2}{2}\right) \qquad r = 0, 1 \tag{46}$$

and

$$\psi_0^{(r)} = x^r \left(\frac{a}{a + x^2}\right)^{(5+2r)/4} \exp\left(-\frac{x^4}{2}\right) \qquad r = 0, 1 \tag{47}$$

which reproduce these global properties of the exact wavefunctions $\psi^{(r)}$ that can be established without exactly solving the Schrödinger equation. These are: (i) the evenness and oddness of $\psi_0^{(0)}$ and $\psi_0^{(1)}$, respectively, (ii) the true number of the nodes

and (iii) the asymptotic behaviour at infinity. Here a is the auxiliary (variational) parameter. Note however that the two functions in (47) are more suitable for the application of the proposed method, because they reproduce more accurately the asymptotics of exact wavefunctions $\psi^{(r)}$ at large x.

Consider first the case (46). Substituting $\psi_0^{(r)}$ into (22) we obtain

$$b_n^{(r)} = \int dx\, P_n^{(r)}(x^2) x^{2r} \exp(-\tfrac{1}{2}x^4 - ax^2) \tag{48}$$

where $P_n^{(r)}(t)$ are polynomials which can be obtained from the simple recurrence conditions:

$$P_0^{(r)}(t) = 1$$

$$P_{n+1}^{(r)}(t) = -4t\ddot{P}_n^{(r)}(t) + (4t^2 + 4at - 2 - 4r)\dot{P}_n^{(r)}(t)$$
$$+ [a(1+2r) + (3+2r-a^2)t - 2at^2]P_n^{(r)}(t). \tag{49}$$

The integrals (48) are the linear combinations of the well known parabolic cylinder functions and hence they can be calculated without difficulties.

The NPT series terms can be computed by using formulae, (19)-(21), (28) and (29). The results of the summation of these terms up to the sixth order are shown in table 1 where they are compared with the 'exact' values obtained by means of non-perturbative methods (see Hioe *et al* 1978, Turbiner 1984). We can see that the NPT series is really convergent. The accuracy of the results for $E^{(0)}$ and $E^{(1)}$ are of order 10^{-7} and 10^{-5}, respectively.

Table 1.

	$a = 0.37$		$a = 0.66$	
N	$E^{(0)}$ in Nth order of NPT	NPT series terms for $E^{(0)}$	$E^{(1)}$ in Nth order of NPT	NPT series terms for $E^{(1)}$
0	1.227 658 5457	1.227 658 5457	4.445 622 5609	4.445 622 5609
1	1.145 968 0527	−0.081 690 4930	4.348 443 3735	−0.097 179 1875
2	1.144 888 4019	−0.001 079 6509	4.340 158 2927	−0.008 285 0808
3	1.144 810 3902	−0.000 078 0116	4.338 936 3901	−0.001 221 0026
4	1.144 803 3336	−0.000 007 0567	4.338 688 9538	−0.000 247 4363
5	1.144 802 5993	−0.000 000 7343	4.338 625 8093	−0.000 063 1445
6	1.144 802 5048	−0.000 000 0945	4.338 607 3267	−0.000 018 4825
	$E^{(0)}_{\text{exact}} = 1.144\,802\,46$		$E^{(1)}_{\text{exact}} = 4.338\,599$	

In order to increase the rapidity of the NPT series convergence, let us consider the case of the more optimal trial function (47). In this case we have

$$b_n^{(r)} = \int dx\, P_n^{(r)}\left(\frac{a}{a+x^2}\right) x^{2r} \left(\frac{a}{a+x^2}\right)^{(3+2r)/2} \exp -\tfrac{1}{2}x^4 \tag{50}$$

Table 2.

	$a=2$		$a=2$	
N	$E^{(0)}$ in Nth order of NPT	NPT series terms for $E^{(0)}$	$E^{(1)}$ in Nth order of NPT	NPT series terms for $E^{(1)}$
0	1.171 500 9887	1.171 500 9887	4.359 847 5425	4.359 847 5425
1	1.145 088 6410	−0.026 412 3477	4.339 231 3528	−0.020 616 1896
2	1.144 804 7700	−0.000 283 8709	4.338 624 8751	−0.000 606 4777
3	1.144 802 4755	−0.000 002 2945	4.338 600 3329	−0.000 024 5421
4	1.144 802 4560	−0.000 000 0192	4.338 598 9062	−0.000 001 4195
5	1.144 802 4545	−0.000 000 0001		
	$E^{(0)}_{\text{exact}}=1.144\,802\,46$		$E^{(1)}_{\text{exact}}=4.338\,599$	

where the polynomials $P_n^{(r)}(t)$ can be found from the more complex recurrence conditions:

$$P_0^{(r)}(t)=1$$

$$P_{n+1}^{(r)}(t)=-(4/a)t^3(1-t)\ddot{P}_n^{(r)}(t)-(1/a)[4a^2-8a^2t+(12+4a^2)t^2-(14+4r)t^3]\dot{P}_n^{(r)}(t)+(3+2r)\times\{a-[a+(5-2r)/4a]t+[(7+2r)/4a]t^2\}P_n^{(r)}(t). \tag{51}$$

After simple calculations we obtain the NPT series terms. The results are shown in table 2. The accuracy of the results of summation of these terms for $E^{(0)}$ and $E^{(1)}$ up to the fifth order of the NPT are now of 10^{-10} and 10^{-6}, respectively. We see that increasing the accuracy of the zeroth approximation makes it really possible to increase substantially the convergence rate of the series, which is in full accordance with our theoretical predictions.

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