A Variational Pertubation Approach

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ABSTRACT

The paper discusses how the variationally inspired perturbation theory (VIPT) scheme of approximation in quantum mechanics can be improved convergencewise if one uses for variational trial functions the perturbative series with variational parameter, so that one is effectively doing variational calculations directly on the high-order perturbative series for energy. The result optimizes the high-order energy directly and thus represents a significant improvement over the VIPT procedure. When applied to a double potential in which even the VIPT is badly divergent, we saw that the result is still very much convergent.

INTRODUCTION

In a recent article, a new approximation scheme for time-independent problems was presented by You et al. (1998) which improves upon the regular perturbation approach by making use of a variational calculation to obtain a more convergent split up of the Hamiltonian into the unperturbed Hamiltonian and the perturbation. They used this method to get the ground and first excited states of the anharmonic oscillator problem and the ground state of the helium problem. This scheme was called the variationally improved perturbation theory (VIPT) by Aitchison and Dudek (2002), who applied it to the Coulomb plus linear potential

$$V\left(\overset{\text{v}}{r}\right) = -\frac{\alpha}{r} + \beta r \ .$$

The results are very encouraging, especially for large perturbations for which the regular perturbation approach has convergence problems. It is also especially relevant for systems in which a good soluble unperturbed Hamiltonian with a small perturbation

cannot be found. It is to these systems in which the VIPT is divergent that we address the present paper.

In this paper, we shall pursue an alternate way of perturbing the physical system with which we calculate the coefficients of the perturbative series for wave functions by a variational approach. We shall introduce a system for which the VIPT diverges very badly and show that the present technique, called variational perturbation theory (VPT), allows us to calculate a real eigenvalue of energy which is still very close to the correct value.

This paper is organized as follows: In Sec. 2, we introduced the anharmonic oscillator potential with a negative harmonic term so that it represents a double-well potential. The VIPT is then applied to this problem for three different assignments of the strengths of the strengths of the harmonic term, corresponding to different depths of the double well. In Sec. 3, we apply the VPT with three variational parameters corresponding to the strength of the mother Hamiltonian, the harmonic perturbation, and the anharmonic strengths. In Sec. 4, we summarize and comment on what we have achieved.

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VARIATIONALLY INSPIRED PERTURBATION THEORY

Consider a system under the Hamiltonian

$$H = H_0 + V_1 + V_2 \ , \tag{1}$$

where the part $H_0 + V_1$ is soluble and V_2 is normally treated as a perturbation but the strength of V_2 is so large that the normal perturbation approach is inapplicable. The VIPT handles the problem by using $Hp(s) = H_0 + (1-s)V_1$ as the unperturbed Hamiltonian, with s chosen variationally, treating

$$H' = \sigma V_1 + V_2 \tag{2}$$

as the new perturbation. This judicious choice of s gives a better first approximation to energy so that the new perturbation approach will improve in convergence property. The VIPT is done as follows: first, we evaluate the expectation value of the total Hamiltonian using eigenfunctions of $Hp(s)$,

$$Hp(\sigma)\phi_n(\sigma) = E_n^0(\sigma)\phi_n(\sigma) \ , \tag{3}$$

as trial functions to get the optimal value of s. Note here that the unperturbed eigenvalues and eigenfunctions actively depend on s. The meaning of the optimal parent Hamiltonian means that we are choosing the optimal value of the potential $(1-s)V_1$ to best approximate the true potential $V_1 + V_2$ for the particular eigenstate. Thus the optimal parent Hamiltonian can be used as the unperturbed Hamiltonian and the regular Schrodinger perturbation theory can be applied with the perturbation given by Eq. (2). The variational calculation actually gives the energy up to first order. Higher-order perturbative calculations for energy are calculated by regular perturbation techniques.

For the potential we will investigate, we choose a double well potential

$$V(x) = \frac{1}{2}m\omega^2\Omega x^2 + \lambda\frac{m^2\omega^3 x^4}{h} \ , \tag{4}$$

with the parameter W < 0 and l = 1. This form of the potential is a double-well potential whose depth is controlled by the value of W, i.e., the more negative W

is, the deeper the double well. In particular, we investigate the potential for three values of the parameter W, W = –1, –4, –10. The potential in Eq. (4) is chosen because the matrix elements of the potential is particularly simple. The results of perturbation calculations, done to first and third orders, are given in Tables 1 and 2 as follows:

Table 1. First-order VIPT results for ground state.

Ω	σ_0	$E_{0,calc}$	$E_{0,exact}$	Error
-1	-3.6712	0.5364	0.5148	0.0216
-4	-5.2876	-0.0151	-0.1304	0.1253
-10	-10.3370	-1.9359	-4.1358	2.1990

Table 2. Third-order VIPT results for ground state.

Ω	σ_0	$E_{0,calc}$	$E_{0,exact}$	Error
-1	-3.6712	0.5364	0.5148	0.0226
-4	-5.2876	0.3820	-0.1304	0.5124
-10	-10.3370	34.3614	-4.1358	37.50

We notice that when the wells deepen, i.e., as W becomes more negative, convergence becomes bad. In fact the case W = –10 is an extremely divergent case.

VARIATIONAL PERTURBATION THEORY

If perturbation theory converges, the results can be obtained in a quick fashion by calculating the expectation value of the Hamiltonian H with respect to the normalized perturbative series for wave function

$$\psi = (\phi_n + K\phi_n)/\left(1 + \langle \phi_n | KK | \phi_n \rangle\right)^{1/2} \ , \tag{5}$$

where the perturbation operator K can be obtained in series form from the equation (Speisman, 1957)

$$K = \frac{Q}{E_n^0 - H_0}(Q - K)H'(P + K) \ . \tag{6}$$

It was shown that using K to order n gives an energy to order $2n+1$. Thus, using

$$K^{(1)} = \frac{Q}{E_n^0 - H_0}H'P' \tag{7}$$

will give energy up to the third order. Since we are dealing with the expectation value of *H*, we can optimize the results by regarding the parameters s and l as variational parameters. This modification can be very advantageous if the results of applying VIPT turns out to be divergent, the optimization process in VPT could still give convergent results.

The first-order VPT is the same as the first-order VIPT since in both cases it is s that is used as the variational parameter. For third-order VPT, we use two variational parameters S and L for the term *H'* in Eq. (5) so that now the trial wave functions depend on three parameters:

$$\psi(\sigma) = \frac{\left(1 + K^{(1)}\right)\phi_0(\sigma)}{\left[1 + \left\langle \phi_0(\sigma) \left| K^{(1)} K^{(1)} \right| \phi_0 \right\rangle \right]^{1/2}} \qquad (8)$$

$$= \frac{\left(1 + \dfrac{Q}{E_0^0 - H_p} H' \phi_0(\sigma)\right)}{\left[1 + \left\langle \phi_0(\sigma) \left| H' \dfrac{Q}{\left[E_0^0 - H_p\right]^2} H' \phi_0(\sigma) \right\rangle \right]^{1/2}} \qquad (9)$$

with

$$H' = \frac{1}{2} \Sigma m\omega^2 x^2 + \Lambda \frac{m^2\omega^3}{h} x^4. \qquad (10)$$

Substituting, we get

$$\langle H \rangle = \frac{\left\langle \phi_0 \left| \left(1 + K^{(1)}\right)\left(H_p + H'\right)\left(1 + K^{(1)}\right) \right| \phi_0 \right\rangle}{1 + \left\langle \phi_0 \left| H' \dfrac{Q}{\left(E_0^0 - H_p\right)^2} H' \right| \phi_0 \right\rangle}$$

The results of third-order VPT is given in Table 3 as follows:

Table 3. Third-order VPT results for ground state.

Ω	σ_0	Σ	Λ	$E_{0,calc}$	$E_{0,exact}$	Error
-1	-5.254	-5.657	1.0075	0.5151	0.5148	0.0003
-4	-6.569	-7.577	1.0321	-0.1263	-0.1304	0.0041
-10	-14.000	44.522	-29.7200	-4.0475	-4.1358	0.0883

We noticed that instead of diverging, this third-order result represents a tremendous improvement over the first-order results. We shall also investigate the situation for the first excited state in the next section.

HIGHER EXCITED STATES

In this section, we give the corresponding results for the first excited state. For first-order VIPT and VPT results we have:

Table 4. First-order VIPT and VPT results for first excited state.

Ω	σ_0	$E_{0,calc}$	$E_{0,exact}$	Error
-1	-5.0000	2.0625	2.0206	0.0419
-4	-6.4235	0.7878	0.6614	0.1264
-10	-10.8490	-3.0317	-4.1191	1.0874

The third-order VIPT results are given in Table 5 as follows:

Table 5. Third-order VIPT results for first excited state.

Ω	σ_0	$E_{0,calc}$	$E_{0,exact}$	Error
-1	-5.0000	2.0334	2.0206	0.0419
-4	-6.4235	0.9110	0.6614	0.2494
-10	-10.8490	10.8930	-4.1191	15.0840

Notice again that the result is very highly divergent for W = –10. On the other hand, when the third-order VPT is performed the results are as given in Table 6:

Table 6. Third-order VPT results for first excited state.

Ω	σ_1	Σ	Δ	$E_{1,calc}$	$E_{1,exact}$	Error
-1	-6.1425	-6.5036	1.0622	2.0154	2.0206	0.0052
-4	-7.9329	-7.4540	1.0321	0.6660	0.6614	0.0046
-10	-12.733	-7.1704	0.0000	-3.9138	-4.1191	0.2053

Again, the convergence is much improved over first order results.

DISCUSSIONS AND CONCLUSIONS

We have observed in one particular example, in which the ordinary perturbation or the improved VIPT results were not convergent, that the use of VPT in which the perturbed wavefunctions were used as variational trial functions with variational parameters inserted for each term in the perturbation series has been able to render convergence to the results. The reason for the good convergence property of the VPT lies in the fact that it is a variational method. In a variational method, as one increases the number of parameters, one is sampling over greater numbers of trial functions, with the consequence of always increasing the accuracy, and therefore, in general, the higher the order of perturbation, the more perturbation parameters would be used, and the more accurate the result becomes.

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