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Superconvergent perturbation theory for an anharmonic oscillator

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A computationally facile superconvergent perturbation theory for the energies and wavefunctions of the bound states of one-dimensional anharmonic oscillators is suggested. The proposed approach uses a Kolmogorov repartitioning of the Hamiltonian with perturbative order. The unperturbed and perturbed parts of the Hamiltonian are defined in terms of projections in Hilbert space, which allows for zero-order wavefunctions that are linear combinations of basis functions. The method is demonstrated on quartic anharmonic oscillators using a basis of generalized coherent states and, in contrast to usual perturbation theories, converges absolutely. Moreover, the method is shown to converge for excited states, and it is shown that the rate of convergence does not deteriorate appreciably with excitation.

KEY WORDS: perturbation theory, time-independent Schrödinger equation, quantum mechanical oscillators, superconvergence

1. Introduction

The energies and wavefunctions of bound states of quartic anharmonic oscillators, i.e., systems with Hamiltonians

$$H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + gx^4, \tag{1}$$

continue to be actively studied as a result of their occurrence in important but disparate areas such as quantum field theory and the study of molecular vibrations (see, e.g., [1,2]). Specifically, the known divergence of Rayleigh–Schrödinger (RS) perturbation theory for the quartic anharmonic oscillator [3,4] is assumed to be a good model of divergences in quantum field theory [5]. Attention has focused on resummation techniques of the series [2,6 and references therein]. However, Patnaik [7] has demonstrated that with an alternative choice of basis an initially stronger convergent RS perturbation theory can be obtained, and Znojil [8] proposed a modified RS treatment that obtains convergent series

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for sufficiently small perturbations. In this paper, we propose a superconvergent perturbation theory and demonstrate numerically its convergence behavior for the quantum quartic anharmonic oscillator.

Following the pioneering work of Kolmogorov [9], superconvergent perturbation methods have become widely used in the study of classical dynamics (see, e.g., [10]). Superconvergent perturbation theories are based on the notion of absorbing all solvable parts into the unperturbed Hamiltonian in each order of the perturbation theory,

$$H = H_0^{(n)} + V^{(n)}. \tag{2}$$

Whereas an elegant statement of the idea of Kolmogorov can be made in terms of Lie methods, through the Deprit power series expansions (see, e.g., [10]), Berry [11] demonstrated that superconvergent perturbation theories can be expressed equivalently in the intuitively appealing framework of local quadratic approximations and function minimizations. The presentation herein uses the Berry framework.

Despite the widespread use of superconvergent perturbation theories in classical dynamics, such approaches are apparently unreported for bound state quantum problems. Consequently, in the following section, we present a superconvergent perturbation theory for the energies and wavefunctions of the time-independent Schrödinger equation. Our proposed superconvergent perturbation theory could, in principle, be used in conjunction with any reasonable basis set. For example, the discrete variable representation (DVR), which has been shown to give substantial numerical improvements over continuous basis representations in variational calculations of molecular vibrations [12 and references therein], may be expected to be useful in the present approach as well. In this paper, in order to focus attention on the perturbation theory, only one specific continuous basis representation (i.e., the generalized coherent state basis) is used. In section 3, after briefly reviewing the generalized coherent state basis set for quartic oscillators, introduced by Hsue and Chern [13] and used in Patnaik's RS treatment [7], we provide numerical results of application of our proposed superconvergent perturbation theory for the quantum mechanical quartic anharmonic oscillator. It is shown that, while the generalized coherent state basis functions prove to be adequate zero-order functions for ground and low-lying states, they are unreliable for more highly excited states. We introduce a straightforward method for generating zero-order functions for such more highly excited states. The conclusions are given in a final section.

2. Superconvergent perturbation theory

2.1. Basic equations

As mentioned in the introduction, the basic idea of all superconvergent perturbation theories is to redefine the partitioning of the Hamiltonian with order, so as to effect as small of a perturbation as possible. Although there are similarities between Kolmogorov-type superconvergent methods and methods of averaging, the latter can lead to convergence to erroneous results and are not pursued further in the present work [10,14]. Un-

fortunately, each step in Kolmogorov's technique is much more complicated than the corresponding steps in ordinary perturbation theory, which has hindered practical application. This observation is particularly relevant vis-à-vis computational perturbation theory. However, Berry observed that a repeated application of a Newton minimizer [11] (also see Moser [15]) produces a series analogous to Kolmogorov's; specifically, the order of convergence is the same. Hence, we develop our perturbation theory in the framework of Berry's function minimization.

The action of the nth order perturbation operator on the nth order approximation to the wavefunction is

$$V^{(n)}\big|\psi_k^{(n)}\big\rangle = H\big|\psi_k^{(n)}\big\rangle - E_k^{(n)}\big|\psi_k^{(n)}\big\rangle, \tag{3}$$

where $E_k^{(n)}$ is the nth order estimate of the energy, and in accord with Kolmogorov,

$$H_0^{(n)}\big|\psi_k^{(n)}\big\rangle = E_k^{(n)}\big|\psi_k^{(n)}\big\rangle. \tag{4}$$

In all of the equations presented subsequently, a subscript designating the particular state of interest is understood and suppressed. We demonstrate numerically in section 3 that the proposed method is capable of describing excited as well as ground states.

Rather than expanding the wavefunction and energy in the conventional order-by-order manner of perturbation theory, consider the first-order variation of the residual vector:

$$r_j^{(n)} \equiv \big\langle\phi_j^{(n)}\big|V^{(n)}\big|\psi^{(n)}\big\rangle, \tag{5}$$

where $|\phi_j^{(n)}\rangle$ is a function in an orthonormal basis set. Since the exact wavefunction must be a vector of the relevant Hilbert space, and, under the mild restriction that all approximations thereof are as well, the residual vectors are Fréchet differentiable so that a Taylor series exists (see, e.g., [16]), i.e.,

$$r_j^{(n+1)} = r_j^{(n)} + \sum_k G_{jk}^{(n)} s_k^{(n)} + \cdots, \tag{6}$$

where the elements of the Jacobian matrix are

$$G_{jk}^{(n)} \equiv \frac{\partial r_j^{(n)}}{\partial c_k^{(n)}} = \big\langle\phi_j^{(n)}\big|H\big|\phi_k^{(n)}\big\rangle - c_j^{(n)}\frac{\partial E^{(n)}}{\partial c_k^{(n)}} - E^{(n)}\delta_{jk}, \tag{7}$$

$\boldsymbol{s}^{(n)}$ is a search direction (alternatively referred to as a descent direction or step direction),

$$\big|\xi^{(n)}\big\rangle = \sum_i s_i^{(n)}\big|\phi_i^{(n)}\big\rangle, \tag{8}$$

and $\boldsymbol{c}^{(n)}$ is the representation of the current wavefunction in the current basis. The energy gradient is given by

$$\frac{\partial E^{(n)}}{\partial c_k^{(n)}} = \frac{2}{\langle\psi^{(n)}|\psi^{(n)}\rangle}\sum_i c_i^{(n)}\Big[\big\langle\phi_i^{(n)}\big|H\big|\phi_k^{(n)}\big\rangle - E^{(n)}\delta_{ik}\Big], \tag{9}$$

and δ_{ij} is used to designate the Kronecker delta function ($\delta_{ij} = 1$, $i = j$; 0, otherwise). Then, in the spirit of Berry, we suggest that a superconvergent perturbation theory for eigenvalues and eigenvectors be developed by requiring that $r_j^{(n+1)}$, from the truncated form of equation (6), be minimized. Specifically, the nth order correction to the wavefunction (cf. equation (8)) is determined from the solution of the set of simultaneous linear equations,

$$\mathbf{G}^{(n)}\boldsymbol{s}^{(n)} = -\boldsymbol{r}^{(n)}. \tag{10}$$

Equations (10) are, in general, infinite dimensional and not solvable in closed form. Moreover, as an eigenvector is determined only up to normalization, the issue of necessary and sufficient number of equations must be considered. In order to obtain a perturbative approximation, we examine the partitioning of the Hamiltonian in closer detail than needed above. Block-diagonal unperturbed Hamiltonians have been shown previously to be effective in developing Hilbert space perturbation theories [17,18], and we adopt this approach. Here, let

$$H_0^{(n)} = P^{(n)} H P^{(n)} + Q_1^{(n)} H Q_1^{(n)} + Q_2^{(n)} H Q_2^{(n)}, \tag{11a}$$

and so,

$$V^{(n)} = P^{(n)} H Q_1^{(n)} + Q_1^{(n)} H P^{(n)} + Q_1^{(n)} H Q_2^{(n)} + Q_2^{(n)} H Q_1^{(n)}, \tag{11b}$$

where $P^{(n)}$ is the projector of the nth order wavefunction, i.e., $P^{(n)} = |\psi^{(n)}\rangle\langle\psi^{(n)}|$, $Q_1^{(n)}$ is the projector of the space connected to $|\psi^{(n)}\rangle$ by the Hamiltonian, but excluding $|\psi^{(n)}\rangle$ itself, and $Q_2^{(n)}$ is the (infinite dimensional) remainder. Clearly, $Q_2^{(n)} H P^{(n)}$ and $P^{(n)} H Q_2^{(n)}$ vanish and so these terms do not appear in either equation (11a) or (11b). With this partitioning, the given equations are valid as written, except that the Hamiltonian contribution to the Jacobian (cf. equation (7)) is replaced

$$\langle \phi_j^{(n)} | H | \phi_k^{(n)} \rangle \quad \Longrightarrow \quad \langle \phi_j^{(n)} | Q_1^{(n)} H Q_1^{(n)} + Q_2^{(n)} H Q_2^{(n)} | \phi_k^{(n)} \rangle. \tag{12}$$

Consequently, equations (10) decouple into $Q_1^{(n)}$ and $Q_2^{(n)}$, and the summations in equations (6) and (8) become restricted to functions in $Q_1^{(n)}$.

2.2. Update

One essential detail remains in specifying the suggested superconvergent perturbation theory. Recognizing the similarity between the suggested method, for solution of an eigenvalue/eigenvector problem, and the Gauss–Newton method for the nonlinear least squares problem (see, e.g., [19]), we should expect it necessary to distinguish small-residual and large-residual problems. As Gauss–Newton is superlinearly convergent in the small residual case (and superquadratically convergent for zero residual) [19], we should expect that an update of the form

$$\boldsymbol{c}^{(n+1)} = \frac{\boldsymbol{c}^{(n)} + \boldsymbol{s}^{(n)}}{1 + [\boldsymbol{s}^{(n)}]^{\mathrm{T}}[\boldsymbol{s}^{(n)}]} \tag{13}$$

will prove satisfactory for small-residual cases. We shall present numerical evidence in the following section to this effect. On the other hand, Gauss–Newton is not necessarily locally convergent for sufficiently large residuals (or highly nonlinear problems). One alternative, which is locally convergent on almost all problems, is to use a line search in connection with a Gauss–Newton search direction; i.e., the so-called damped Gauss–Newton method [19]. In the context of our suggested superconvergent perturbation theory, the update becomes the solution of the one-dimensional subproblem,

$$\min_{\alpha\in[0,1]} \big\| R(\alpha) \big\| = \frac{\| H|\psi(\alpha)\rangle - E(\alpha)|\psi(\alpha)\rangle \|}{\langle\psi(\alpha)|\psi(\alpha)\rangle^{1/2}}, \tag{14}$$

where

$$\big|\psi(\alpha)\big\rangle = \big|\psi^{(n)}\big\rangle + \alpha\big|\xi^{(n)}\big\rangle, \tag{15a}$$

$$\big|\psi(\alpha)\big\rangle = \sum_i c_i^{(n)}\big|\phi_i^{(n)}\big\rangle + \alpha\sum_i s_i^{(n)}\big|\phi_i^{(n)}\big\rangle. \tag{15b}$$

Equivalently, we can solve the subproblem,

$$\min_{\alpha\in[0,1]} \big\| R(\alpha) \big\|^2 = \frac{\| H|\psi(\alpha)\rangle - E(\alpha)|\psi(\alpha)\rangle \|^2}{\langle\psi(\alpha)|\psi(\alpha)\rangle}. \tag{16}$$

Explicitly,

$$\big\| R(\alpha) \big\|^2 = \frac{(\langle\psi(\alpha)|H - \langle\psi(\alpha)|E(\alpha))(H|\psi(\alpha)\rangle - E(\alpha)|\psi(\alpha)\rangle)}{\langle\psi(\alpha)|\psi(\alpha)\rangle}, \tag{17a}$$

which simplifies to

$$\big\| R(\alpha) \big\|^2 = \frac{\langle\psi(\alpha)|H^2|\psi(\alpha)\rangle}{\langle\psi(\alpha)|\psi(\alpha)\rangle} - \big(E(\alpha)\big)^2, \tag{17b}$$

and

$$\begin{aligned}\big\| R(\alpha) \big\|^2 = {} & \frac{\sum_i (\sigma_i^{(n)} + \alpha\kappa_i^{(n)})^2}{1 + \sum_i (s_i^{(n)})^2} \\ & - \left[\frac{E^{(n)} + \alpha\sum_i (c_i^{(n)}\kappa_i^{(n)} + s_i^{(n)}\sigma_i^{(n)}) + \alpha^2\sum_i s_i^{(n)}\kappa_i^{(n)}}{1 + \sum_i (s_i^{(n)})^2}\right]^2.\end{aligned} \tag{17c}$$

In equations (17), the following definitions were introduced:

$$\sigma_i^{(n)} = \big\langle\phi_i^{(n)}\big|H\big|\psi^{(n)}\big\rangle = \sum_j c_j^{(n)}\big\langle\phi_i^{(n)}\big|H\big|\phi_j^{(n)}\big\rangle \tag{18}$$

and

$$\kappa_i^{(n)} = \big\langle\phi_i^{(n)}\big|H\big|\xi^{(n)}\big\rangle = \sum_j s_j^{(n)}\big\langle\phi_i^{(n)}\big|H\big|\phi_j^{(n)}\big\rangle. \tag{19}$$

In order to understand the essence of the residual minimization more fully, it is productive to consider the dimensionality of the nth order vectors, or, more precisely, their inner products. The energy term, i.e., the second term in equation (17c), involves only summations over $Q_1^{(n)}$. Specifically, $\boldsymbol{c}^{(n)}$ is completely within $Q_1^{(n)} \oplus P^{(n)}$ and $\boldsymbol{s}^{(n)}$ is completely within $Q_1^{(n)}$. However, as $\boldsymbol{\kappa}^{(n)}$ is *not* within $Q_1^{(n)}$, the first term in equation (17c) must be performed in $Q_1^{(n)}$ and a small part of $Q_2^{(n)}$. Heuristically, the minimization of residual we propose as a final step of our suggested superconvergent perturbation theory provides a best fit for the current order balanced against the introduction of large error in the subsequent order.

With regard to the observation of the last paragraph, we address two details. First, as $\boldsymbol{s}^{(n)} \in Q_1^{(n)}$ and determination of the step direction did not explicitly consider $P^{(n)}$, it can be seen that the minimization of residual not only considers the effect of $Q_2^{(n)}$ but also introduces explicit consideration of $P^{(n)}$ into the calculation. As the small residual case results in small changes in P from iteration to iteration, it should not be surprising that update (13) suffices in this case. Secondly, as the step $\alpha|\xi^{(n)}\rangle$ is based on the topology near the unperturbed vector, we search for the *first* minimum between 0 and 1, ascending, during the line search, and, if such minimum does not exist, accept $\alpha = 1$. Although a conservative line search may slow convergence, it also enhances the integrity of the approximation of the eigenvector from order to order. In particular, we should expect at least some resistance to the so-called root-flipping problem.

3. Results

3.1. Quartic anharmonic oscillator

In terms of the standard creation and annihilation operators, $a^+ = (x - \mathrm{i}p)/\sqrt{2}$ and $a = (x + \mathrm{i}p)/\sqrt{2}$, the quartic anharmonic oscillator Hamiltonian (i.e., equation (1)), can be written (e.g., [13])

$$H = \frac{1}{2} + a^+a + \frac{g}{4}\left(a^+ + a\right)^4. \tag{20}$$

As shown by Hsue and Chern [13], a Bogoliubov transformation

$$b = \frac{a - ta^+}{\sqrt{1-t^2}}, \tag{21a}$$

$$b^+ = \frac{a^+ - ta}{\sqrt{1-t^2}} \tag{21b}$$

leads to

$$\begin{aligned} H = E_0 &+ \left[\frac{4\omega(1-\omega)}{(1+\omega)^3} + \frac{3g}{2\omega^2}\right]\left(b^2 + \left(b^+\right)^2\right) \\ &+ \left[\frac{1+\omega^2}{2\omega} + \frac{3g}{\omega^2}\right]b^+b + \frac{g}{4\omega^2} : \left(b + \left(b^+\right)^4\right) :, \end{aligned} \tag{22}$$

and the ground state energy is

$$E_0 = \frac{1}{2} + \frac{(1-\omega)^2}{4\omega} + \frac{3g}{4\omega^2}. \tag{23}$$

Following Hsue and Chern, the transformed variable $\omega = (1-t)/(1+t)$ is used; : : represents normal ordering. Although equations (22) and (23) are valid for arbitrary ω (and, thus, t), the variational ground state energy is obtained by minimizing E_0. As might be expected, such choice makes the quadratic term of the Hamiltonian (i.e., the second term on the first line) vanish and the b and b^+ correspond to normal modes. A so-called generalized coherent state basis is generated by applying the raising operator to the Bogoliubov transformed, energy minimized, ground state:

$$|n\rangle = \frac{(b^+)^n}{\sqrt{n!}}\big|\tilde{0}\big\rangle. \tag{24}$$

The only unique nonzero matrix elements of the Hamiltonian in this basis are:

$$\langle n|H|n\rangle = E_0 + n\omega + \frac{3g}{2\omega^2}n(n-1), \tag{25a}$$

$$\langle n-2|H|n\rangle = \frac{g}{\omega^2}\big[n(n-1)\big]^{1/2}(n-2), \tag{25b}$$

$$\langle n-4|H|n\rangle = \frac{g}{4\omega^2}\big[n(n-1)(n-2)(n-3)\big]^{1/2}. \tag{25c}$$

Patnaik [7] demonstrated that a RS perturbation expansion of the quartic anharmonic oscillator wavefunction, based on Hsue and Chern's generalized coherent states, gives rapid initial convergence for low-lying states. Unfortunately, such a procedure does not circumvent the eventual divergent, or at best asymptotic, behavior. In table 1, we show the results of a RSPT series to high order with the generalized coherent state basis for a coupling strength (g) of 0.1. Examination of this table shows the expected divergence, although the lowest two roots might be considered to be converged to useful accuracy for the given coupling strength before the onset of increasing oscillatory behavior. Moreover, the oscillations are such that series resummations, e.g., by Euler transformation, produces a limit that is stable with order, even for excited states (also see [2,6 and references therein]). Nonetheless, it is clear that the basic RSPT series becomes increasingly dubious for higher excited states and, though not shown in this paper, for greater coupling strength.

Table 2 shows the results of our suggested superconvergent perturbation theory for the same coupling strength, basis functions and initial guesses as in table 1. Several comments can be made. First, all roots converge absolutely, i.e., $|E^{(n+1)}| < |E^{(n)}|$. Second, the convergence is rapid. Calculations were performed in double precision arithmetic, with values below 1×10^{-14} reported as 0. Iterations were continued at least 5 orders beyond that reported to monitor the re-emergence of nonzero values. In figure 1, the logarithm of the energy error, $\big|\sum_{i=0}^{n} E^{(i)} - E^*\big|$, where E^* is the converged value, is

Table 1
Energy corrections from RSPT for quartic anharmonic oscillator ($g = 0.1$) (in units of $\hbar\omega_0$, where ω_0 is the angular frequency of the unperturbed oscillator).

Order	E_0	E_1	E_2	E_5
0	0.560307371139	1.781504057320	3.203864631308	8.677929680119
1	0.0	0.0	0.0	0.0
2	−0.001107147000	−0.013747017005	−0.075726727366	−0.883101440006
3	0.0	0.002583575981	0.016349445468	0.234921848863
4	−0.000058125565	−0.001127018557	−0.008422419924	−0.194081357346
5	0.000009818729	0.000453794775	0.004132826855	0.124267785681
6	−0.000007347317	−0.000245193023	−0.002504594893	−0.105188876394
7	0.000002931929	0.000130452644	0.001563855633	0.086255764990
8	−0.000001773204	−0.000079916801	−0.001066538381	−0.077485405532
9	0.000000982756	0.000049954645	0.000752851673	0.070494187294
10	−0.000000623697	−0.000033636695	−0.000558632796	−0.066725485716
11	0.000000403061	0.000023373132	0.000427239050	0.064301052534
12	−0.000000277673	−0.000017004995	−0.000337941799	−0.063387074093
13	0.000000197665	0.000012761911	0.000274236138	0.063478118383
14	−0.000000146671	−0.000009900725	−0.000228269946	−0.064576000655
15	0.000000112243	0.000007893968	0.000194170806	0.066547763147
16	−0.000000088640	−0.000006462411	−0.000168605931	−0.069413168439
17	0.000000071893	0.000005416322	0.000149151482	0.073177292404
18	−0.000000059816	−0.000004640933	−0.000134266478	−0.077907999574
19	0.000000050917	0.000004057925	0.000122835405	0.083690082394
20	−0.000000044279	−0.000003616012	−0.000114098541	−0.090650034619
21	0.000000039270	0.000003279475	0.000107503971	0.098945408180
22	−0.000000035472	−0.000003023754	−0.000102662676	−0.108776844622
23	0.000000032592	0.000002831407	0.000099293658	0.120390123236
24	−0.000000030427	−0.000002690123	−0.000097199866	−0.134087032663
25	0.000000028834	0.000002591114	0.000096245592	0.150234590634
26	−0.000000027710	−0.000002528204	−0.000096344468	−0.169279377516
27	0.000000026985	0.000002497134	0.000097449819	0.191763811400
28	−0.000000026607	−0.000002495140	−0.000099549344	−0.218347387607
29	0.000000026546	0.000002520651	0.000102661600	0.249832482037
30	−0.000000026782	−0.000002573102	−0.000106834697	−0.287196798966
31	0.000000027307	0.000002652816	0.000112146396	0.331633508251
32	−0.000000028124	−0.000002760954	−0.000118705730	−0.384601382119

plotted against perturbation order for roots 0, 2, and 5. Also plotted are linear regression curves. Taking into account that the definition of linear convergence [19] is

$$\left|\sum_{i=0}^{n} E^{(i)} - E^*\right| = c\left|\sum_{i=0}^{n-1} E^{(i)} - E^*\right|, \tag{26a}$$

so that

$$\ln\left|\sum_{i=0}^{n} E^{(i)} - E^*\right| = n\ln c + k. \tag{26b}$$

Table 2
Energy corrections from superconvergent perturbation theory for quartic anharmonic oscillator ($g = 0.1$).

Order	E_0	E_1	E_2	E_5
0	0.560307371139	1.781504057320	3.203864631308	8.677929680119
1	0.0	0.0	0.0	0.0
2	−1.117956E−03	−1.151009E−02	−6.336603E−02	−7.810828E−01
3	−4.237021E−05	−4.879391E−04	−1.869152E−03	3.440153E−03
4	−7.156280E−07	−3.378017E−06	−4.852122E−06	−5.096795E−04
5	−1.598591E−09	−9.588685E−09	−2.835430E−07	−9.756857E−06
6	−8.960316E−11	−1.343786E−09	−5.922517E−09	−3.116278E−07
7	−1.735781E−12	−3.687939E−12	−4.058620E−11	−1.298756E−08
8	−1.264809E−14	−7.600587E−13	−4.919620E−12	−2.336575E−10
9	0	0	−1.554312E−14	−1.742517E−11
10			0	−3.650413E−13
11				−2.398082E−14
12				0

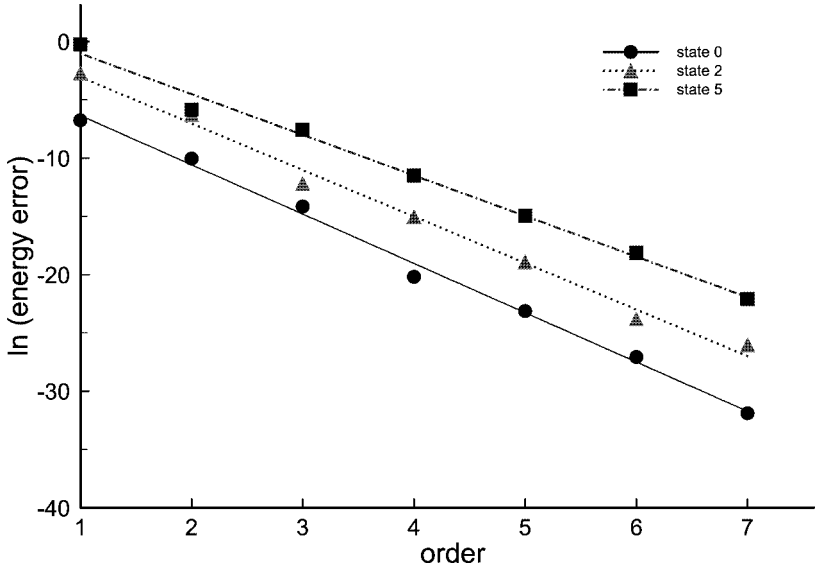

Figure 1. Energy errors from superconvergent perturbation theory for states 0 (■), 2 (▲) and 5 (●) of quartic anharmonic oscillator ($g = 0.1$).

Figure 1 demonstrates that the suggested superconvergent perturbation theory is linear for ground and low-lying excited states.

3.2. More highly excited states

More highly excited states can be calculated within the framework of the suggested superconvergent perturbation theory, although naïve application can produce undesirable results. Table 3 shows the wavefunctions of several states of the system of interest,

Table 3
Wavefunctions of lowest roots of even symmetry of quartic anharmonic oscillator ($g = 0.1$) in Hsue and Chern basis from large variational calculations.

Amplitude	ψ_0	ψ_2	ψ_4	ψ_6	ψ_8	ψ_{10}	ψ_{12}	ψ_{14}
c_0	0.99990	−0.00396	0.01363	0.00248	−0.00093	−0.00032	0.00012	−0.00005
c_2	0.00226	0.99190	0.11057	0.05870	−0.01956	−0.00804	0.00336	−0.00148
c_4	−0.01414	−0.12446	0.93916	0.27496	−0.14520	−0.06558	0.03152	−0.01534
c_6	0.00186	−0.02166	−0.32312	0.78950	−0.41402	−0.26184	0.14771	−0.08302
c_8	0.00033	0.01258	0.02431	−0.52517	−0.52368	−0.45593	0.36463	−0.25151
c_{10}	−0.00019	−0.00190	0.02154	0.14617	0.64736	−0.18190	0.35736	−0.39155
c_{12}	0.00003	−0.00046	−0.01037	0.00068	−0.32679	0.61604	−0.13816	−0.13697
c_{14}	0.00001	0.00034	0.00173	−0.01947	0.08091	−0.50050	−0.41176	0.32027
c_{16}		−0.00008	0.00048	0.00914	0.00820	0.22980	0.57407	0.10051
c_{18}		−0.00001	−0.00042	−0.00174	−0.01782	−0.05326	−0.40450	−0.47887
c_{20}			0.00013	−0.00044	0.00866	−0.01025	0.18037	0.51914
c_{22}			< 0.00001	0.00049	−0.00195	0.01676	−0.04144	−0.34635
c_{24}			−0.00002	−0.00019	−0.00034	−0.00871	−0.01011	0.15566
c_{26}			0.00001	0.00003	0.00054	0.00234	0.01614	−0.03768
c_{28}				0.00002	−0.00026	0.00017	−0.00914	−0.00873
c_{30}				−0.00001	0.00006	−0.00056	0.00294	0.01574
c_{32}					0.00001	0.00033	−0.00010	−0.00987
c_{34}					−0.00002	−0.00011	−0.00056	0.00375
c_{36}					0.00001	< 0.00001	0.00041	−0.00051
c_{38}						0.00002	−0.00017	−0.00049
c_{40}						−0.00001	0.00003	0.00048
c_{42}							0.00001	−0.00025
c_{44}							−0.00002	0.00007
c_{46}							0.00001	< 0.00001
c_{48}								−0.00002
c_{50}								0.00001
c_{52}								−0.00001

from a large variational calculation which may be considered to be essentially exact. In particular, it may be noted that the first 4 even parity roots are dominated by the expected Hsue and Chern basis function, but, in roots 5 and higher, the expected basis function is not the dominant component. Consequently, an initial wavefunction comprising this nondominant component may lead to unexpected results. In fact, an initial guess of the 8th basis function, i.e., ${}^{(8)}c_8^{(0)} = 1.0$, does converge quickly to the 8th state (cf. table 4), although an initial guess of the 10th basis function converges to the 14th state. It is interesting to note that ψ_{14} has the largest contribution from the 10th basis function, c_{10}, of nearby states. (NB: table 3 does not include ψ_{16} and above, but the preceding statement applies.) So, the suggested superconvergent perturbation theory apparently maintains integrity to initial guess.

The structure of the suggested superconvergent perturbation theory does not require an initial guess that consists of only 1 basis function. Indeed, equation (11a), which is valid in any iteration, is specifically valid for the initial guess. Although many

Table 4
Energies from superconvergent perturbation theory for quartic anharmonic oscillator ($g = 0.1$).

Order	E_8	E_{10}[a]
0	15.962469719197	21.824649184287
1	15.962469719197	21.824649184287
2	12.841547050777	27.602084718042
3	13.371764919364	29.950381846269
4	13.382643382719	27.111301854539
5	13.382486728449	25.950140769719
6	13.382475187546	25.919942560541
7	13.382474827945	25.915738480272
8	13.382474808359	25.915674721312
9	13.382474807480	25.915660718837
10	13.382474807449	25.915659848379
11	13.382474807446	25.915659822746
12	13.382474807446	25.915659815104
13		25.915659815079
14		25.915659815049
15		25.915659815048
16		25.915659815048

[a] Generated with an initial guess of ${}^{(10)}c_{10}^{(0)} = 1.0$. (See text for details concerning the nature of this excited state.)

zero-order wavefunctions are possible, a straightforward possibility uses the Bogoliubov transformed raising operator actively; e.g.,

$$\left|\psi_k^{(0)}\right\rangle \approx \left(b^+\right)^2 \left|\psi_{k-2}^*\right\rangle, \tag{27a}$$

$$\left|\psi_k^{(0)}\right\rangle \approx \sum_j {}^{(k-2)}c_j^* \sqrt{(j+1)(j+2)}\,|j+2\rangle, \tag{27b}$$

where the superscript * refers to converged values, and the state subscripting (and left-superscripting for coefficient) that has been suppressed in the majority of the paper is included here for clarity. In order to form an initial wavefunction that is reasonably compact, the result of equation (27b) is, after normalization, truncated such that coefficients below a threshold (e.g., 0.1) are eliminated and the wavefunction renormalized. Table 5 shows the produced zero-order wavefunctions and table 6 gives the energy corrections produced by application of the suggested superconvergent perturbation series on these zero-order wavefunctions. In consideration of the observation from the preceding paragraph, that the Hsue and Chern basis functions are not the dominant components of more highly excited states, the results of table 5 are not remarkable. Perhaps surprising is the extent to which these zero-order wavefunctions, which are constructed from adjacent states, differ from single basis function wavefunctions. In particular, $\psi_{10}^{(0)}$ and $\psi_{12}^{(0)}$ have largest components one (same symmetry) function removed from the simple choices of ${}^{(10)}c_{10}^{(0)} = 1.0$ and ${}^{(12)}c_{12}^{(0)} = 1.0$, but with substantial major contributions from

Table 5
Initial wavefunctions of several excited states of even symmetry of quartic anharmonic oscillator ($g = 0.1$) in Hsue and Chern basis using equation (27).

Amplitude	ψ_{10}	ψ_{12}	ψ_{14}	ψ_{16}
c_8	−0.29460	−0.14929	0.0	0.0
c_{10}	−0.47238	−0.32955	0.21832	−0.12862
c_{12}	0.70720	−0.15923	0.25913	−0.24249
c_{14}	−0.41920	0.63320	−0.11764	0.0
c_{16}	0.11919	−0.59076	−0.40260	0.26745
c_{18}		0.30628	0.63381	0.0
c_{20}			−0.49766	−0.50318
c_{22}			0.24469	0.60148
c_{24}				−0.43863
c_{26}				0.21392

Table 6
Energy corrections from superconvergent perturbation theory for quartic anharmonic oscillator ($g = 0.1$).

Order	E_{10}	E_{12}	E_{14}	E_{16}
0	16.690923775648	21.180814375770	25.193165605811	30.208996260805
1	0.0	0.0	0.0	0.0
2	6.736495E−01	3.583068E−01	6.932784E−01	2.686601E−01
3	−1.219400E−02	5.963419E−04	2.997823E−02	−1.307253E−03
4	−4.566698E−04	−2.809040E−03	−6.917797E−04	−4.741584E−03
5	−1.371290E−05	−2.336257E−05	−5.585804E−05	−2.138870E−04
6	−1.226452E−06	−1.057451E−05	−1.392378E−05	−1.544837E−05
7	−2.190026E−08	−1.972272E−07	−8.693082E−07	−2.982517E−06
8	−4.660112E−09	−2.498825E−08	−2.563340E−08	−1.505178E−08
9	−2.361844E−11	−1.639361E−09	−7.641713E−09	−1.838156E−08
10	−1.632472E−11	−3.913314E−11	−2.491163E−11	−2.317861E−10
11	−3.552714E−14	−1.167422E−11	−2.991740E−11	−5.067236E−11
12	0	−2.131628E−14	−4.902745E−13	−4.799716E−12
13		0	0	0

several basis functions. On the other hand, $\psi_{14}^{(0)}$ and $\psi_{16}^{(0)}$ have largest components that are two and three removed from the simple choices. Calculation of the overlaps of these initial wavefunctions with the converged function gives 0.89310, 0.87396, 0.84574, and 0.87736 for $\psi_{10}^{(0)}$ through $\psi_{16}^{(0)}$, respectively. A comparison of table 6 with table 2 shows that the rate of convergence of more highly excited states is not significantly worse than that of low-lying excited states provided that a reasonable initial wavefunction is used.

3.3. Approximate steplength

In the preceding two subsections, it has been demonstrated that the suggested superconvergent perturbation theory converges linearly for ground and excited states of

the quartic anharmonic oscillator, which is asymptotically convergent, at best, with a Rayleigh–Schrödinger perturbation theory (RSPT) series. As part of the suggested method, a one-dimensional line search is performed (cf. equations (14)–(17) and accompanying text). And, although this line search is not particularly difficult computationally, the requirement of generating the Hamiltonian projection of the step vector, i.e., $\boldsymbol{\kappa}^{(n)}$ (cf. equation (19)), requires that a larger part of the full Hilbert space be considered for this final step than for the generation of the step vector itself. For problems in which this projection is of small incremental dimensionality, such as the quartic anharmonic oscillator under current consideration (i.e., the increment is exactly 2), this issue is computationally unimportant, although it is sure to be significanct for other problems. Based on this consideration, and the known enhanced convergence of the Gauss–Newton method for small residual simultaneous equation problems (see, e.g., [19]), we investigated whether an approximate updating scheme suffices.

At the simplest approximation, one could accept the step without any line search; in other words, use equation (13). Table 7 presents energy corrections for several states using this scheme. Comparison of table 7 with table 2, for states 0, 1, 2, and 5, and, less directly, with table 4, for states 8 and 10, shows that the simple scheme does not compromise convergence. It is worth noting that series starting from Hsue and Chern basis function 10 converge to different final states using the line-search and non-line-search methods: the line search method converges to the final state with greatest overlap (i.e., state 14), but the non-line-search method converges to an inexplicable final state (i.e., state 12). As was the case for the line search variant, initial wavefunctions produced by application of raising operator on the next lower state of same parity, as described in the preceding subsection, produced rapidly convergent series to the correct final states. Since the convergence for the non-line-search variant is generally similar to those given in table 6, this data is not reproduced here. So, at least for the quartic anharmonic oscillator, one should conclude that the line search for step length may be skipped.

4. Conclusion

A superconvergent perturbation theory for the bound states Hamiltonian eigenvalues and eigenvectors of a one-dimensional quantum system was suggested. The approach is based on redefining the partitioning with iteration and thus follows Kolmogorov. Implementation is in the framework of Berry's insight that the approach of Kolmogorov can be realized in terms of local quadratic approximations. The proposed theory has similarity to the Gauss–Newton method for the solution of simultaneous nonlinear equations. In particular through the work presented here, a computationally facile superconvergent perturbation theory has been realized.

We demonstrated the effectiveness of the suggested superconvergent perturbation theory on the quantum quartic anharmonic oscillator. It is well known, and easily shown numerically, that a Rayleigh–Schrödinger perturbation theory is divergent, but summable, even for relatively small coupling strength. Our results using the suggested theory converge absolutely for ground and excited states.

Table 7
Energy corrections from superconvergent perturbation theory, without line search, for quartic anharmonic oscillator ($g = 0.1$).

Order	E_0	E_1	E_2	E_5	E_8	E_{10}[a]
0	0.56030737113	1.78150405732	3.20386463130	8.67792968011	15.9624697191	21.8246491842
1	0.0	0.0	0.0	0.0	0.0	0.0
2	−1.121970E−03	−1.157941E−02	−6.353813E−02	−7.332945E−01	−8.858731E−01	5.629351E−01
3	−3.839431E−05	−4.186576E−04	−1.697047E−03	−4.431907E−02	−1.305783E+00	−3.861492E−01
4	−6.774734E−07	−3.330220E−06	−4.911495E−06	−5.390118E−04	−3.840052E−01	−4.557893E−01
5	−1.614738E−09	−9.347720E−09	−2.243689E−07	−9.602908E−06	−4.322011E−03	−5.808791E−03
6	−7.349163E−11	−1.246931E−09	−5.669469E−09	−2.640838E−07	−1.135148E−05	−2.933001E−03
7	−1.700620E−12	−3.893552E−12	−3.847811E−11	−1.250897E−08	−3.033483E−07	−1.985903E−05
8	−1.201578E−14	−5.542233E−13	−4.658052E−12	−2.134302E−10	−1.916969E−08	−9.726047E−06
9	0	0	−1.554312E−14	−1.688250E−11	−7.200693E−10	−1.716962E−07
10			0	−3.232969E−13	−3.135980E−11	−2.438217E−08
11				−2.664535E−14	−2.255973E−12	−1.274930E−09
12				0	−4.618528E−14	−4.263967E−11
13					0	−7.513989E−12
14						−3.907985E−14
15						−3.552714E−14
16						0

[a] Generated with an initial guess of ${}^{(10)}c_{10}^{(0)} = 1.0$. (See text for details concerning the nature of this excited state.)

It was shown that, in accord with Patnaik's work using RSPT, the Hsue and Chern generalized coherent state basis functions are excellent initial wavefunctions for ground and low-lying excited states. For more highly excited states, it was shown by numerical example that the line search variant of the suggested superconvergent perturbation theory converges to an excited state with largest overlap with the zero-order function, but that the approximate non-line-search variant does not. Consequently, we conclude that the generalized coherent state basis will not be the most desirable initial zero-order functions for studies of highly excited states. However, we showed that initial states generated from lower states, by straightforward application of raising operators, are reliable initial wavefunctions for all states examined. Furthermore, for such zero-order wavefunctions, the line search and non-line-search variants had very similar convergence characteristics. With reasonable initial wavefunctions, the rate of convergence was shown to be linear for ground and excited states.

We expect to consider other quantum mechanical bound state systems using the suggested superconvergent perturbation theory.

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