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Concurrent multiple-state analytic perturbation theory via supersymmetry

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Conventional nondegenerate perturbation theory for some *n*th state starts with the corresponding unperturbed state. The present formulation yields recursively perturbation expansions for any bound state using the sole information of the unperturbed ground state. Logarithmic perturbation theory is exploited along with supersymmetric quantum mechanics to achieve this end. As the method involves ground-state perturbations of a series of supersymmetric Hamiltonians, concern about nodal shifts of targeted excited states arises only at the ultimate step, thus, minimizing considerably the labor of clumsy computations involved in dealing with excited states. © *2011 American Institute of Physics*. [doi:10.1063/1.3570817]

Given a solvable eigenvalue problem

$$h_0\phi_n = \varepsilon_n\phi_n, \tag{1}$$

perturbation theory sets out to find approximate solutions of E_n and ψ_n in

$$(h_0 + \lambda\upsilon)\psi_n = E_n\psi_n \tag{2}$$

in the form of Taylor expansions in λ. This is typically the strategy through which the Rayleigh–Schrödinger perturbation theory in quantum mechanics[1–4] is developed. However, the theory tackles each given stationary state ψ_n and the corresponding energy E_n at a time. This feature continues to be true for other versions of perturbation theories[5,6] as well. Also, there is no way to connect results for two different states; hence, the knowledge of correction terms for one state cannot be used in anyway to estimate the same for another one. On the other hand, we know that the outcomes of perturbation theory, summed to infinite orders, are equivalent to those of linear variations with basis functions $\{\phi_j\}$ that are eigenfunctions of h_0. We also know that the variational route yields results for all the states at a time, unlike perturbation theory. Therefore, it would be nice to seek if there exists at all an avenue that allows perturbative corrections to be had for any number of states simultaneously. Fortunately, we have found one such that starts with the ground state and requires no other extra information.

To proceed, we choose a useful variant of the Rayleigh–Schrödinger formulation, called the logarithmic perturbation theory (LPT) .[7–15] In LPT, one first transforms the Schrödinger eigenvalue equation to a nonlinear Riccati form and then develops a perturbative treatment.[7,8] Interest on LPT really grew around the 1980s when, for varying problems reducible to one dimension, it was found to be very convenient.[9,10] Here, one bypasses the "sum-over-states" representations and integral evaluations in the energy- and wave function-correction terms. Although the method was initially developed for the ground state, approaches soon followed to deal with excited states.[11–13] Nevertheless, the prevalent schemes required an integration step to evaluate energy corrections or corrections to nodal point shifts. Later, we formulated a simpler route[14] that avoided such an exercise, clarified some earlier discrepancies,[13] offered perturbation series for properties directly and simplified excited-state calculations. Further applications followed soon.[15]

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The basic idea of supersymmetry (SUSY) (Ref. 16) has been found useful in several areas of nonrelativistic quantum mechanics.[17,18] Its connection with the Riccati form is also apparent. Therefore, it seemed to us that LPT could somehow be linked up with SUSY theory to achieve our end in a natural way, as outlined below.

We consider the Schrödinger energy-eigenvalue equation in one dimension (x), with $h = 2\pi$, $m = \frac{1}{2}$, and real potentials. The unperturbed problem, $h_0\phi_n = \varepsilon_n\phi_n$, is then

$$-\phi_n'' + (\upsilon_0 - \varepsilon_n)\phi_n = 0, \tag{3}$$

that may be rewritten as

$$\theta_n^2 + \theta_n' + \varepsilon_n - \upsilon_0 = 0, \tag{4}$$

where $\theta_n = \phi_n'/\phi_n$. The perturbed problem likewise simplifies to

$$-\psi_n'' + (\upsilon_0 + \lambda\upsilon - E_n)\psi_n = 0. \tag{5}$$

Both E_n and ψ_n are expandable in powers of λ, and the interest is to find the expansion coefficients. For convenience, however, we designate the perturbed problem as

$$H_0\psi_{0n} = E_{0n}\psi_{0n}. \tag{6}$$

The total potential in H_0 is symbolized by V_0, where $V_0 = \upsilon_0 + \lambda\upsilon$. We now rewrite (6) in the Riccati form

$$\chi_{0n}^2 + \chi_{0n}' + E_{0n} - V_0 = 0 \tag{7}$$

by defining the ratio $\psi_{0n}'/\psi_{0n} = \chi_{0n}$, where the prime refers to differentiation with respect to x. We now expand the quantities of interest in terms of the perturbation parameter λ:

$$\begin{aligned} E_{0n} &= E_{0n0} + \lambda E_{0n1} + \lambda^2 E_{0n2} + ..., \\ V_0 &= \upsilon_0 + \lambda\upsilon, \\ \chi_{0n} &= \chi_{0n0} + \lambda\chi_{0n1} + \lambda^2\chi_{0n2} + ... \end{aligned} \tag{8}$$

Putting the above expansions in (7), and equating terms of a fixed power of λ, we obtain the LPT equations of various orders.[8] The most convenient way to solve these equations is to suppose polynomial forms for $\chi_{0nj}(j \neq 0)$ at the onset, whose coefficients are determined by satisfying each of the above equations. This route yields simultaneously the energy corrections, without quadratures.[14] However, such a scheme is best suited for the ground state. In case of excited states, we have found it expedient[14] to write

$$\psi_{0n} = f_{0n}\exp[g_{0n}], \tag{9}$$

where the prefactor f_{0n} is a polynomial that takes account of the nodes, while the exponential part determines the overall behavior. Obviously, in LPT we need to use expansions of both f_{0n} and g_{0n}' in place of χ_{0n} in (8), An order-by-order relationship of the latter with f_{0n} and g_{0n}' is known.[14]

In the present approach, we proceed to define a series of eigenvalue problems, in addition to (6), given by

$$H_j\psi_{jn} = E_{jn}\psi_{jn}, \quad j = 1, 2, ..., \tag{10}$$

where the potential parts V_j in Hamiltonians H_j are estimated recursively as

$$\begin{aligned} V_1 &= V_0 - 2\chi_{00}', \\ V_2 &= V_1 - 2\chi_{10}', ..., \end{aligned} \tag{11}$$

and

$$\chi_{jn} = \psi_{jn}'/\psi_{jn}.$$

Note that (10) can be cast in the Riccati form too:

$$\chi_{jn}^2 + \chi_{jn}' + E_{jn} - V_j = 0. \tag{12}$$

Since V_j and V_{j-1} are the two SUSY partner potentials, SUSY theory guarantees that

$$E_{j0} = E_{0j}, \tag{13}$$

$$-(d/dx + \chi_{j0})\,\psi_{(j+1)n} \sim \psi_{j(n+1)}, \tag{14}$$

where normalization is relegated for convenience. Now, we are in a position to outline the basic steps of our endeavor.

Start a perturbation theory for the ground state ($n = 0$) of the parent Hamiltonian with (7) using expansions (8) and the knowledge of (4). This yields χ_{00} to some desired order, say λ^k. Employ the same to get V_1 in (11) to $\boldsymbol{O}(\lambda^k)$. Put expansions similar to (8) in (12) to obtain χ_{10} correct up to $\boldsymbol{O}(\lambda^k)$. This gives V_2 to $\boldsymbol{O}(\lambda^k)$. Employ (12) for $j = 2$ and $n = 0$ now. The process thus continues. We get a set of ground states in the form of $\{\chi_{j0}\}$ for the SUSY partner Hamiltonians H_j. At the last step, we revert to excited states of H_0 by employing (14) and then rearrange them in keeping with (9).

A few important points are now in order. First, only the information of unperturbed ground state is required in the overall process. Second, each perturbation expansion is aimed at getting some ground state and hence LPT need not bother about nodes. Third, the association (13) at each λ implies that the correction terms would obey

$$E_{j0k} = E_{0jk}. \tag{15}$$

Fourth, the route to get back χ_{0n} from χ_{n0} is accomplished through (14), rewritten more conveniently as

$$\chi_{j(n+1)} = \chi_{(j+1)n} + \frac{(\chi'_{(j+1)n} + \chi'_{j0})}{\chi_{(j+1)n} + \chi_{j0}}. \tag{16}$$

Finally, after getting a specific χ_{0n}, we extract[14] separately the perturbation series for both f_{0n} and g'_{0n}.

Example 1: We demonstrate the workability by first choosing the quartic anharmonic oscillator problem[19,20] for which $\theta_0 = -x$, $\upsilon_0 = x^2$, $\varepsilon_0 = 1$, and $\upsilon = x^4$. For brevity, we display the results up to the fifth order in λ, first for the ground states of H_j, $j = 0, 1, 2,$ and 3. This allows us to proceed up to the third excited state of H_0 and demonstrates the smoothness of the strategy. Of course, one can go beyond.

The perturbation $\upsilon = x^4$ yields $\chi_{000} = -x$ and

$$\chi_{001} = -\frac{3x}{4} - \frac{x^3}{2},$$

$$\chi_{002} = \frac{21x}{16} + \frac{11x^3}{16} + \frac{x^5}{8},$$

$$\chi_{003} = -\frac{333x}{64} - \frac{45x^3}{16} - \frac{21x^5}{32} - \frac{x^7}{16},$$

$$\chi_{004} = \frac{30\,885x}{1024} + \frac{8669x^3}{512} + \frac{1159x^5}{256} + \frac{163x^7}{256} + \frac{5x^9}{128}, \text{ and}$$

$$\chi_{005} = -\frac{916\,731x}{4096} - \frac{33\,171x^3}{256} - \frac{19\,359x^5}{512} - \frac{823x^7}{128} - \frac{319x^9}{512} - \frac{7x^{11}}{256}.$$

The energy series comes out as

$$E_{00} = 1 + \frac{3}{4}\lambda - \frac{21}{16}\lambda^2 + \frac{333}{64}\lambda^3 - \frac{30\,885}{1024}\lambda^4 + \frac{916\,731}{4096}\lambda^5 - \dots\ .$$

Using the above results, we can quickly solve for $\{\chi_{10j}\}$. We get $\chi_{100} = -x$ and

$$\chi_{101} = -\frac{9x}{4} - \frac{x^3}{2},$$

$$\chi_{102} = \frac{123x}{16} + \frac{33x^3}{16} + \frac{x^5}{8},$$

$$\chi_{103} = -\frac{3249x}{64} - \frac{267x^3}{16} - \frac{63x^5}{32} - \frac{x^7}{16},$$

$$\chi_{104} = \frac{458\,715x}{1024} + \frac{86\,493x^3}{512} + \frac{6913x^5}{256} + \frac{489x^7}{256} + \frac{5x^9}{128}, \text{ and}$$

$$\chi_{105} = \frac{-19\,471\,023x}{4096} - \frac{63\,291x^3}{32} - \frac{194\,913x^5}{512} - \frac{4921x^7}{128} - \frac{957x^9}{512} - \frac{7x^{11}}{256}.$$

The energy series is obtained as

$$E_{10} = 3 + \frac{15}{4}\lambda - \frac{165}{16}\lambda^2 + \frac{3915}{64}\lambda^3 - \frac{520\,485}{1024}\lambda^4 + \frac{21\,304\,485}{4096}\lambda^5 - \ldots\ .$$

Utilizing χ_{00} and χ_{10}, we get the expansion for the ground state of H_2, with $\chi_{200} = -x$. Results are

$$\chi_{201} = -\frac{15x}{4} - \frac{x^3}{2},$$

$$\chi_{202} = \frac{327x}{16} + \frac{55x^3}{16} + \frac{x^5}{8},$$

$$\chi_{203} = -\frac{12\,915x}{64} - \frac{711x^3}{16} - \frac{105x^5}{32} - \frac{x^7}{16},$$

$$\chi_{204} = \frac{25\,97\,055x}{1024} + \frac{345\,775x^3}{512} + \frac{18\,421x^5}{256} + \frac{815x^7}{256} + \frac{5x^9}{128}, \text{ and}$$

$$\chi_{205} = -\frac{1\,51\,223\,085x}{4096} - \frac{2\,894\,937x^3}{256} - \frac{780\,975x^5}{512} - \frac{13\,117x^7}{128} - \frac{1595x^9}{512} - \frac{7x^{11}}{256},$$

and

$$E_{20} = 5 + \frac{39}{4}\lambda - \frac{615}{16}\lambda^2 + \frac{20\,079}{64}\lambda^3 - \frac{35\,76\,255}{1024}\lambda^4 + \frac{191\,998\,593}{4096}\lambda^5 - \ldots\ .$$

Likewise, the above results are used to solve for $\{\chi_{30j}\}$ and we get $\chi_{300} = -x$,

$$\chi_{301} = -\frac{21x}{4} - \frac{x^3}{2},$$

$$\chi_{302} = \frac{633x}{16} + \frac{77x^3}{16} + \frac{x^5}{8},$$

$$\chi_{303} = -\frac{33\,831x}{64} - \frac{1377x^3}{16} - \frac{147x^5}{32} - \frac{x^7}{16},$$

$$\chi_{304} = \frac{90\,11\,265x}{1024} + \frac{907\,485x^3}{512} + \frac{35\,683x^5}{256} + \frac{1141x^7}{256} + \frac{5x^9}{128}, \text{ and}$$

$$\chi_{305} = -\frac{681\,755\,697x}{4096} - \frac{2\,520\,897x^3}{64} - \frac{20\,51\,217x^5}{512} - \frac{25\,411x^7}{128} - \frac{2233x^9}{512} - \frac{7x^{11}}{256},$$

and

$$E_{30} = 7 + \frac{75}{4}\lambda - \frac{1575}{16}\lambda^2 + \frac{66\,825}{64}\lambda^3 - \frac{15\,184\,575}{1024}\lambda^4 + \frac{10\,24\,977\,375}{4096}\lambda^5 - \ldots\ .$$

Excited states of the parent H_0 are next obtained via (16). The simplest is to get χ_{01} from χ_{10} and χ_{00}. Then, in accordance with (9), we separate the nodal and exponential parts. Here, by symmetry, no nodal shift occurs. We find $f_{01} = x$ and

$$g'_{010} = -x,$$

$$g'_{011} = -\frac{5x}{4} - \frac{x^3}{2},$$

$$g'_{012} = \frac{55x}{16} + \frac{17x^3}{16} + \frac{x^5}{8},$$

$$g'_{013} = -\frac{1305x}{64} - \frac{103x^3}{16} - \frac{31x^5}{32} - \frac{x^7}{16},$$

$$g'_{014} = \frac{173\,495x}{1024} + \frac{28\,269x^3}{512} + \frac{2437x^5}{256} + \frac{233x^7}{256} + \frac{5x^9}{128}, \text{ and}$$

$$g'_{015} = -\frac{7\,101\,495x}{4096} - \frac{187\,391x^3}{256} - \frac{56\,061x^5}{512} - \frac{1629x^7}{128} - \frac{445x^9}{512} - \frac{7x^{11}}{256}.$$

For the second excited state, we need to use χ_{20}, χ_{10}, and χ_{00}. Thus, one obtains $\chi_{02}$from which follows

$$f_{02} = (2x^2 - 1) + 2\lambda - \frac{191}{16}\lambda^2 + \frac{6697}{64}\lambda^3 - \frac{1\,183\,907}{1024}\lambda^4 + \frac{61\,616\,025}{4096}\lambda^5 - \ldots$$

$$g'_{020} = -x,$$

$$g'_{021} = -\frac{7x}{4} - \frac{x^3}{2},$$

$$g'_{022} = \frac{107x}{16} + \frac{23x^3}{16} + \frac{x^5}{8},$$

$$g'_{023} = -\frac{3467x}{64} - \frac{187x^3}{16} - \frac{41x^5}{32} - \frac{x^7}{16},$$

$$g'_{024} = \frac{617\,539x}{1024} + \frac{67\,967x^3}{512} + \frac{4225x^5}{256} + \frac{303x^7}{256} + \frac{5x^9}{128}, \text{ and}$$

$$g'_{025} = -\frac{33\,389\,117x}{4096} - \frac{252\,491x^3}{128} - \frac{125\,883x^5}{256} - \frac{2729x^7}{128} - \frac{571x^9}{512} - \frac{7x^{11}}{256}.$$

Results for the third excited state (χ_{03}), found through χ_{30}, χ_{20}, χ_{10}, and χ_{00}, are finally rearranged to yield

$$f_{03} = (2x^3 - 3x) + 9x\lambda - \frac{1215x}{16}\lambda^2 + \frac{57\,591x}{64}\lambda^3 - \frac{13\,308\,003x}{1024}\lambda^4 + \frac{882\,448\,749x}{4096}\lambda^5 - \ldots\ .$$

$$g'_{030} = -x,$$

$$g'_{031} = -\frac{9x}{4} - \frac{x^3}{2},$$

$$g'_{032} = \frac{177x}{16} + \frac{29x^3}{16} + \frac{x^5}{8},$$

$$g'_{033} = -\frac{7335x}{64} - \frac{297x^3}{16} - \frac{51x^5}{32} - \frac{x^7}{16},$$

$$g'_{034} = \frac{1\,656\,345x}{1024} + \frac{135\,359x^3}{512} + \frac{6523x^5}{256} + \frac{373x^7}{256} + \frac{5x^9}{128}, \text{ and}$$

$$g'_{035} = -\frac{112\,222\,881x}{4096} - \frac{298\,851x^3}{64} - \frac{240\,153x^5}{512} - \frac{4123x^7}{128} - \frac{697x^9}{512} - \frac{7x^{11}}{256}.$$

All the above results for energy corrections, in view of (15), agree with earlier works.[19,20] However, only a few data for LPT corrections g'_{0nk} could be checked against the available[11–15] ones. The primary reason for meager existing records is the complexity in dealing with terms f_{0nk} from the beginning. This is avoided nicely in our recipe.

Example 2: We next choose the spiked oscillator problem,[21,22] with $\upsilon = 1/x^2$, defined in the domain $[0, \infty)$. Here, a remarkable feature is that the corrections are summable for the ground state.[14] So, one gets closed-form results for the quantities sought. More surprising is that the exact summability of the perturbation series for each of the SUSY partners continues to hold. This makes the eigenstates of H_0 obtainable in closed forms too. Specifically, starting from $\theta_0 = -x + 1/x$, $\upsilon_0 = x^2$, and $\varepsilon_0 = 3$, we find first that

$$\chi_{00} = -x + \beta/x,\ \ E_{00} = 1 + 2\beta, \tag{17}$$

with

$$\beta = \frac{1 + \sqrt{1 + 4\lambda}}{2}. \tag{18}$$

Using (17), one can proceed stepwise as above, and obtain the summable SUSY partner states in the form

$$\begin{aligned} \chi_{10} &= -x + (\beta + 1)/x,\ \ E_{10} = 5 + 2\beta; \\ \chi_{20} &= -x + (\beta + 2)/x,\ \ E_{20} = 9 + 2\beta; \end{aligned} \tag{19}$$

etc. The inherent symmetry of the problem is quite apparent now. By employing (19) in (14), it is easy to evaluate the actual wave functions for the first two excited states as

$$\begin{aligned} \psi_{01} &= [2x^2 - (2\beta + 1)]x^{\beta} \exp[-x^2/2]; \\ \psi_{02} &= [4x^4 - 4x^2(2\beta + 3) + (2\beta + 3)(2\beta + 1)]x^{\beta} \exp[-x^2/2]. \end{aligned} \tag{20}$$

For any state, the true perturbation corrections can be found by expanding β in (18) in powers of λ. Convergence, however, is ensured as long as $|\lambda| < 1/4$. One may further note that the pre-exponential parts in (20) reduce to the desired odd Hermite polynomials as $\lambda \to 0$ whence $\beta = 1$. The process may continue for still higher states easily. However, the labor involved in getting (20) from the corresponding unperturbed state via conventional LPT is quite cumbersome. Results (20) are not previously known either.

In summary, we have first found that the present formulation capably furnishes perturbation series for any excited state of H_0 starting from the ground state of h_0. Since Schrödinger's introduction of perturbation theory in 1926, there exists no way of getting perturbation corrections for some nth eigenstate starting from the sole information of the ground unperturbed state. We have shown here that such a wonderful route is available. To obtain results up to some nth excited state, we need n auxiliary SUSY partner Hamiltonians H_j and their perturbation series for ground states. All calculations are simple, analytic, and involve terms up to a fixed order in λ. Second, excited-state calculations via LPT are plagued with various difficulties, particularly, in respect of changes of nodal structures. References 11–13 reveal the painstaking efforts (e.g., idea of ghost states, etc.) made in this issue. Although we have considerably simplified it later,[14] the need of two separate expansions, one for the exponential part and the other for the nodal structure, could not be eliminated. The present work shows how simply one can tackle these cases. Only at the final step, the nodal changes show up and one need not bother about two separate expansions at each step. This is a definite advantage in LPT that has not been explored before. Third, our work rests mainly on the principles of SUSY, as applied to nonrelativistic quantum mechanics. While a lot of work has been done on SUSY, here we have probably exploited its full strength to notice that, by deliberately avoiding linear-space properties, one may sometimes gain a lot more, as has sometime been emphasized.[23] Strengths of both the SUSY theory and LPT are quite apparent in this context. Finally, bound-state variation method has been enriched considerably by invoking SUSY in course of studies in excited-state energies,[24] wave functions,[25] and excitation energies via the Monte Carlo technique.[26] The present work shows instead the advantages in a perturbative context.

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