PERTURBATION THEORY WITH NON-DIAGONAL PROPAGATORS AND ITS USE IN THE INTERMEDIATE-COUPLING REGIME

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An innovated method of construction of the Rayleigh-Schrödinger perturbation series in a seemingly nonperturbative regime is offered. Designed for the needs of condensed matter physics, nuclear physics and quantum chemistry, the flexibility of our new formalism is based on a nonstandard Lanczosean construction of unperturbed basis. With an asymmetric choice of the model space the recipe becomes recurrent not only order-by-order in a small parameter (as usual) but also projection-by-projection in the Hilbert space. Its idea and efficiency are illustrated on a few schematic examples.

1 Purpose

In the general perturbation theory a family of Hamiltonians $H = H(g)$ is usually being considered in a small-coupling regime, i.e., in a "sufficiently small" vicinity of an exactly solvable $H(g_0)$. One often has to extend this construction beyond the domain of its strict mathematical validity, i.e., to an intermediate-coupling regime which lies far from any exactly solvable approximant.

Here, we propose a novel perturbative start from a Hamiltonian which is *not* exactly solvable. We shall only assume that at a fixed parameter $g_0 \neq 0$ our operator $H(g_0)$ remains simplified by the Lanczosean tridiagonalization or block-tridiagonalization[1].

Our method is fairly universal. For paedagogical reasons, we shall not discuss its detailed manybody implementations and restrict our attention just to the clear and concise explanation of its Lanczosean plus recurrent perturbative essence.

2 Examples

In the usual harmonic-oscillator basis $\{|n\rangle\}_0^\infty$ the harmonic oscillator Hamiltonian itself is a diagonal matrix in each ($\ell-$th) partial wave,

$$H_{(HO)} = \sum_{n=0}^{\infty} |n\rangle \varepsilon_n \langle n|, \qquad \varepsilon_n = 4n + 2\ell + 3. \tag{1}$$

In the same basis the anharmonicities r^4, r^6, ... are banded matrices. The textbook (i.e., Rayleigh-Schrödinger, RS) perturbation theory is often recalled to specify the so called perturbed energies, i.e., functions $E(g)$ of a coupling g represented in the schematic power-series form

$$E(g) = E(g_0) + (g - g_0)\, E^{(1)} + (g - g_0)^2\, E^{(2)} + \ldots \tag{2}$$

near any g_0. The harmonic $g_0 = 0$ is exceptional. Its choice leads just to the divergent, asymptotic series (2). Unfortunately, all the "better" choices of $g_0 \neq 0$ leave $H(g_0)$ non-diagonal.

What we are going to show is that the expansion (2) may also fairly easily be constructed in a vicinity of some "better" $g_0 \neq 0$. The basic technical ingredient (and the source of feasibility of our generalized RS construction) will be found in the use of the well known finite-dimensional partial solvability of many Hamiltonians at some "exceptional" couplings. Usually, this means a break in the Lanczos numerical iterations. Within our perturbative scenario, such a termination is welcome and able to specify the eligible unperturbed system.

Thus, a mere *incomplete*, partial solvability of the Schrödinger equation at g_0 will be needed. For applicability of our method to perturbations $g \neq g_0$ the banded structure of Hamiltonians at these exceptional (though not necessarily vanishing) coupling(s) $g = g_0$ will prove sufficient. The non-hermitean zero-order Schrödinger operators will also be admitted,

$$H(g_0) - E(g_0) = \sum_{m,n=0}^{\infty} |\Xi_m\rangle \varepsilon_{m,n} \langle \xi_n|, \qquad |\psi(g_0)\rangle = \sum_{p=0}^{M(g_0)} |\Xi_p\rangle\, h_p \tag{3}$$

with termination $M(g_0) < \infty$, sparse $\varepsilon_{m,n} = 0$ for $|m-n| > t$ $[= t(m) > 0]$ and usual Lanczosean biorthogonality $\langle \xi_m | \Xi_n \rangle = 0$ for $m \neq n$.

Our most elementary *non-polynomial* illustration with a double well shape of the potential

$$V_{(DW)}(g,r) = r^2 + \frac{\sigma(g_0) + \lambda\, \sigma^{(1)}}{1+r^2}\,, \qquad \lambda = \lambda(g) = g - g_0 \tag{4}$$

has $|\Xi_n\rangle = (1+r^2)\,|n\rangle$ and $|\xi_n\rangle = (1+r^2)^{-1}\,|n\rangle$ after its Lanczos tridiagonalization ($t = 1$). Its triple well descendant

$$V_{(TW)}(g,r) = r^2 + \frac{[\mu(g_0) + \lambda\mu^{(1)}]\, r^2 + \nu(g_0) + \lambda\, \nu^{(1)}}{1 - r^2 + r^4} \tag{5}$$

with $|\Xi_n\rangle = (1-r^2+r^4)\,|n\rangle$ and $|\xi_n\rangle = (1-r^2+r^4)^{-1}\,|n\rangle$ will be pentadiagonal. The general Padé oscillators will be characterized by $2t+1$ diagonals and asymmetry, $H(g) \neq H^+(g)$.

3 Zero order

The usual complete solvability at g_0 is an unnecessarily strong constraint imposed upon $H^{(0)}$. In the numerical context, it is sufficient to work with arbitrary truncated matrices[2]. In the non-numerical treatment of polynomial potentials one may rely upon the analytic Taylor-series Ansatz[3]. In our *non-polynomial* double-well example (4) symbolic manipulations may still generate the necessary Lanczos-terminating couplings non-numerically. We get $\sigma(g_0) = (4\,\ell+6)e+4$ at $q = 0$. A longer expression and two roots result at $q = 1$. After a straightforward algebra, the three real roots may be shown to exist for $q = 2$, four real roots may be generated at $q = 3$, etc. A methodical challenge as well as phenomenological appeal of the related spectra lies in their quasi-degeneracy (see Table 1).

In the triple wells (5) we get, similarly,

$$\nu(g_0) = (4\ell+6)(f-2e)+8, \qquad \mu(g_0) = (8\ell+20)e^2+4f-8e\ , \quad q=0\ . \quad (6)$$

At $q = 1$, a single real Cardano root of $\nu^3 + 48\,\nu - 360 = 0$ exists and gives $\nu(g_0) \approx 4.959$ and $\mu(g_0) \approx 14.94$. The norm $h_1(g_0) = 1$ and the first nontrivial overlap $h_0(g_0) \approx -3.48$ characterize the wavefunction. Two real roots emerge for $q = 2$ (sextic) and $q = 3$ (decadic) case, etc. In the quartic-over-sextic example $V(g_0, r) = r^2 + [u(g_0) + v(g_0)\,r^2 + w(g_0)\,r^4]/[1 + r^6]$ with $w(g_0) = 2\,(\sqrt{2}\,a + 27)$, $v(g_0) = -\sqrt{2}\,(\sqrt{2}\,a^2 + 11\,a - 6\,\sqrt{2})$ and $u(g_0) = \sqrt{2}\,(2\,a^3 + 10\,\sqrt{2}\,a^2 - 23\,a + 18\,\sqrt{2})/2$, the two real parameters $x = \sqrt{2}\,a$ are obtainable from the Lanczos termination constraint $x^4 + 9\,x^3 - 33\,x^2 + 27\,x - 12 = 0$. In all these cases, the exact energies $E(g_0) = 4t + 4q + 2\ell + 7$ depend on the integer nodal number $q \geq 0$.

4 Recurrences for corrections

In contrast to the usual RS recipe which splits $\langle 0|H(0) - E(0)| = 0$ and $Q|\psi(0)\rangle = 0$ and keeps the propagator diagonal, our formalism is asymmetric. The knowledge of the left eigenstate $\langle\psi(g_0)|$ becomes redundant. A

Table 1: A sample of the quasi-degenerate spectra in a few double wells (4).

$\sigma(g_0)$	the four lowest (numerical) energies			
81.88	18.999999996	19.	22.765764732	22.765764788
64.89	17.	17.000000131	20.733677525	20.733679219
52.05	15.301693677	15.301695784	18.999974785	19.

weak assumption $\langle \xi_0 | [H(g_0) - E(g_0)] \neq 0$ is accepted. The most natural normalization $\langle \xi_0 | \psi^{(k)} \rangle = 0$ projects $\langle \xi_0 |$ out, $|\psi^{(k)}\rangle \equiv Q|\psi^{(k)}\rangle$. This splits the perturbed Schrödinger equation $H(g)\,|\psi(g)\rangle = E(g)\,|\psi(g)\rangle$ in $k-$th order into two separate components,

$$\langle \xi_0 | H(g_0) - E(g_0) | \psi^{(k)} \rangle = \langle \xi_0 | \tau \rangle + E^{(k)} \langle \xi_0 | \psi(g_0) \rangle \tag{7}$$

$$Q | H(g_0) - E(g_0) | Q \psi^{(k)} \rangle = Q | \tau \rangle + E^{(k)} Q | \psi(g_0) \rangle \ . \tag{8}$$

The meaning of the abbreviation τ is obvious.

4.1 Propagators are, in effect, triangular

Pentadiagonal example with $t = 2$ and ground-state $q = 0$ may be recalled,

$$\left(\begin{array}{cc|ccccc} (0) & d_0^{[1]} & d_0^{[2]} & 0 & 0 & 0 & \ldots \\ (0) & a_1 & d_1^{[1]} & d_1^{[2]} & 0 & 0 & \ldots \\ (0) & b_2^{[1]} & a_2 & d_2^{[1]} & d_2^{[2]} & 0 & \ldots \\ 0 & b_3^{[2]} & b_3^{[1]} & a_3 & d_3^{[1]} & d_3^{[2]} & \ldots \\ 0 & 0 & b_4^{[2]} & b_4^{[1]} & a_4 & d_4^{[1]} & \ldots \\ \vdots & & & \ddots & \ddots & \ddots & \ddots \end{array} \right) \left(\begin{array}{c} 0 \\ h_1^{(k)} \\ \hline h_2^{(k)} \\ h_3^{(k)} \\ h_4^{(k)} \\ \vdots \end{array} \right) = \left(\begin{array}{c} \tau_0 \\ \tau_1 \\ \tau_2 \\ \tau_3 \\ \tau_4 \\ \vdots \end{array} \right) + E^{(k)} \left(\begin{array}{c} h_0^{\{0\}} \\ h_1^{\{0\}} \\ h_2^{\{0\}} \\ 0 \\ 0 \\ \vdots \end{array} \right) . \tag{9}$$

It characterizes well the general situation. Before its trivial recurrent solution one has only to shift the "upper" $h_1^{(k)}$ to the right and interpret *both* $h_1^{(k)}$ (or, in general, $h_j^{(k)}$ with $j = 1, 2, \ldots, t-1$) and $E^{(k)}$ as "free" parameters. They only have to be fixed via the t "model-space" or asymptotic boundary condition requirements

$$h_{N+j}^{(k)} \left(E^{(k)}, h_1^{(k)}, h_2^{(k)}, \ldots, h_{t-1}^{(k)} \right) = 0, \qquad j = 1, 2, \ldots, t, \qquad N \gg 1 \tag{10}$$

in the limit $N \to \infty$ if necessary. This indicates the correct way of generalization of several older and immanently tridiagonal recurrent perturbative formalisms[4].

4.2 The lowest orders offer good approximations

The Lanczos termination generates a "comparatively dense" set of couplings g_0. This is the reason why the first-order estimates may become fairly reliable. Their sample is given in Table 2. As long as the ground and excited

Table 2: The first two triple-well energies in perturbative picture ($\ell = 0$)

order		ground state	excited state
zero		11.0000	15.0000
one		10.9551	14.9015
∞	(numerical)	10.9434	14.6332

terminations differ by a mere inessential modification of the couplings, the simultaneous first-order re-constructions of the other state both achieve a fairly good precision.

We may summarize that our recipe is based on the ease of the Lanczos zero-order construction of a biorthogonalized unperturbed basis and on a wealth of the suitable quasi-exact couplings $g_0 \neq 0$. Its efficiency and transparency was achieved by an appropriate split of the unknowns into their "model-space" subset ($E^{(k)}$ and $h_j^{(k)}$ with $j < t$) and its recurrently defined complement ($j \geq t$).

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