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PERTURBATION THEORY FOR QUANTUM MECHANICS IN ITS HESSENBERG-MATRIX REPRESENTATION

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For years, the partial integrability in quantum mechanics [e.g., the exceptional terminating Lanczos solutions or the so called quasi-exactly solvable "next-to-elementary" systems] represented a challenge in perturbation theory. The main difficulty lied in an incompleteness of the available zero-order wavefunctions and in the related impossibility of an easy construction of the necessary zero-order propagators. We describe a solution of this problem, based on an unusual choice of the model space. A few examples illustrate the underlying technicalities: Paying detailed attention to the Hessenberg-matrix Hamiltonians, our formalism compensates the incompleteness of integrability by a slightly less elementary (viz., non-diagonal but still triangular) matrix structure of its propagators.

1. The two possible Hessenberg-matrix represenations of Hamiltonians

Integrable systems in quantum mechanics may be characterized as possessing the one- or two-diagonal matrix representation of Hamiltonians. The situation is particularly simple in the case of a single particle moving in a centrally symmetric potential $V(r)$. Indeed, we may write its (say, bound-state) Schrödinger equation in an ordinary differential-equation form with a radial Hamiltonian

$$H|\psi\rangle = E|\psi\rangle, \quad H = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + V(r), \quad r \in (0,\infty) \tag{1}$$

with one-dimensional parity ($\ell = -1,\ 0$) or three-dimensional angular momentum ($\ell = 0, 1, \ldots$). The auxiliary, so called "Jost" or "regular" and, in general, non-normalizable solutions $\psi(r)$ may be then defined, by the current power-series method,[1] as compatible with just one of boundary conditions,

$$\psi^{(Jost)}(r_\infty) = 0, \quad r_\infty \to \infty, \qquad \psi^{(regular)}(r_0) = \mathcal{O}(r^{\ell+1}), \quad r_0 \to 0. \tag{2}$$

In the next step, the imposition of the missing, complementary boundary-condition constraint fixes the energy and defines the final normalizable wavefunction $\langle r|\psi\rangle$. In this language, the integrability means that the underlying recurrences have a two-term form, solvable, generically, in terms of gamma functions.

As an illustration of the above "exact" or "special-function" solution scheme, one may recall the various regular-function solutions based on the use of hypergeometric functions[2] or the Jost-type Bessel-function construction of the $s-$wave bound states in an exponential potential (see, by the way, also a "forgotten" matrix generalization of the latter analytic procedure.[3])

1.1. *The Lanczos-type constructions*

An immediate generalization of the Jost-type two-term recurrences and special-function solutions to an arbitrarily complicated Hamiltonian H_0 may be found, for our present purposes, in the so called Lanczos tridiagonalization technique.[4] Basically, it is able to convert many Hamiltonians into tridiagonal matrices. The underlying idea lies in a choice (or rather a construction) of a basis $\{|n\rangle\}_{n=0}^{n=\infty}$ which, whenever arranged in a row, may be understood as satisfying the following three-term recurrence relations,

$$H_0 \times (|0\rangle, |1\rangle, \ldots) = (|0\rangle, |1\rangle, \ldots) \times \left(\begin{array}{cccc} A_0 + E_0 & C_1 & 0 & \ldots \\ B_0 & A_1 + E_0 & C_2 & \ldots \\ 0 & B_1 & A_2 + E_0 & \ldots \\ 0 & 0 & B_2 & \ldots \\ & \ldots & & \ldots \end{array} \right)$$

(later on, we shall need the "redundant" symbol E_0 for the energy; one might ignore it now and put, say, $E_0 = 0$).

In accord with the monograph[4] (cf. also our older methodical study[5]), several "next-to-solvability" features of the latter formula admit a straightforward generalization to the general, unconstrained recurrences of the form

$$(H_0 - E_0 I) \times (|0\rangle, |1\rangle, \ldots) = (|0\rangle, |1\rangle, \ldots) \times \left(\begin{array}{ccccc} A_0 & C_1^{(1)} & C_2^{(2)} & C_3^{(3)} & \ldots \\ B_0 & A_1 & C_2^{(1)} & C_3^{(2)} & \ldots \\ 0 & B_1 & A_2 & C_3^{(1)} & \ldots \\ 0 & 0 & B_2 & A_3 & \ldots \\ & \ldots & & \ldots & \end{array} \right) \qquad (3)$$

i.e., to the so called upper Hessenberg matrix representation of the Hamiltonian.

1.2. *The second, anti-Lanczosean possibility*

A generalization of regular solutions beyond their special-function implementation with bi-diagonal Hamiltonians may be achieved via an introduction of a lower-Hesseberg counterpart of the latter relation (3). We may speak about an "anti-Lanczos" method in such a case. Its explicit realization and exemplification may be spotted, in acord with our recent review,[6] within the framework of the so called Hill-determinant (HD) approach.[7] For analytic potentials, the power-series HD Ansatz

$$|\psi\rangle = (|0\rangle, |1\rangle, \ldots) \times \left(\begin{array}{c} c_0 \\ c_1 \\ \ldots \end{array} \right), \qquad \langle r|n\rangle = r^{2n+\ell+1} \mathrm{e}^{-f(r)} \qquad (4)$$

with a suitable n-independent auxiliary polynomial $f(r) > 0$ leads directly to the alternative action of the Hamiltonian,

$$(H_0 - E_0 I) \times (|0\rangle, |1\rangle, \ldots) = (|0\rangle, |1\rangle, \ldots) \times \begin{pmatrix} A_0 & B_0 & 0 & \ldots & \\ C_1^{(1)} & A_1 & B_1 & 0 & \ldots \\ C_2^{(2)} & C_2^{(1)} & A_2 & B_2 & \ldots \\ C_3^{(3)} & C_3^{(2)} & C_3^{(1)} & A_3 & \ldots \\ \ldots & & & & \ldots \end{pmatrix} \quad (5)$$

which is the transposition of the more usual Lanczos formula (3).

Summarizing, many different Hamiltonians may be encountered as represented by an asymmetric, infinite-dimensional matrix with the sparse (viz., upper or lower) Hessenberg-matrix structure in the applied quantum mechanics.

1.3. *Explicit solvability of the Hessenberg Schrödinger equations*

The Hessenberg-matrix structure of Hamiltonians introduces an immediate and important simplification of the Schrödinger eigenvalue problem. Indeed, the rigorous infinite-dimensional and, say, lower-Hessenberg (i.e., regular-type or Hill-determinant) algebraic equation which combines eqs. (4) and (5),

$$\begin{pmatrix} A_0 & B_0 & 0 & \ldots & \\ C_1^{(1)} & A_1 & B_1 & 0 & \ldots \\ C_2^{(2)} & C_2^{(1)} & A_2 & B_2 & \ldots \\ C_3^{(3)} & C_3^{(2)} & C_3^{(1)} & A_3 & \ldots \\ \ldots & & & & \ldots \end{pmatrix} \times \begin{pmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ \ldots \end{pmatrix} = 0$$

always possesses the complete and *closed* solution

$$c_{n+1} = \frac{c_0}{\Pi_{k=0}^{n}(-B_k)} \det\mathcal{H}^{\{n\}}, \quad n = 0, 1, \ldots \quad (6)$$

defined in terms of determinants of finite matrices,

$$\mathcal{H}^{\{n\}} = \begin{pmatrix} A_0 & C_1^{(1)} & \ldots & C_{n-1}^{(n-1)} & C_n^{(n)} \\ B_0 & A_1 & \ldots & C_{n-1}^{(n-2)} & C_n^{(n-1)} \\ 0 & B_1 & \ldots & C_{n-1}^{(n-3)} & C_n^{(n-2)} \\ & & \ldots & & \\ 0 & \ldots & 0 & B_{n-1} & A_n \end{pmatrix}.$$

In the special two-diagonal case, the determinants degenerate back to products of diagonal matrix elements. Formula (6) leads then immediately to the well known gamma-function factors in the corresponding (e.g., hypergeometric) analytic special-function solutions.

In accord with the long-lasting research[8] one may achieve an exact termination of certain exeptional solution(s), $c_{M+1}^{[0]} = c_{M+2}^{[0]} = \ldots = 0$. The Lanczos-type example of these zero-order states was found[9] at an exceptional set of energies $E_0 = \varepsilon_{M+1} =$

$4M+2\ell+7$ and couplings $g=g(M)$ in the potential $V(r)=r^2\left(1-\frac{4g+6g^2}{1+gr^2}\right)$. In an anti-Lanczos setting, the similar sextic example with $V(r)=a\,r^2+b\,r^4+c\,r^6$ may be recalled.[10] Similar states, used as the zero-order approximants, will form a starting point of our present perturbative considerations.

2. The new, Lanczos-type perturbation theory

In accord with the current textbooks,[1] an analytic $\lambda-$dependence of Hamiltonians, enables us to replace, via the pair of Ansätze

$$E=E(\lambda)=E_0+\lambda E_1+\lambda^2E_2+\ldots,$$

$$|\psi\rangle=|\psi(\lambda)\rangle=|\psi_0\rangle+\lambda\;|\psi_1\rangle+\lambda^2|\psi_2\rangle+\ldots,$$

the standard Schrödinger equation (1) by an infinite hierarchy of its independent $O(\lambda^k)$ components. In this way, the zero-order problem becomes complemented by the equations

$$(H_0-E_0)\;|\psi_k\rangle+(H_1-E_1)\;|\psi_{k-1}\rangle+\ldots+(H_k-E_k)\;|\psi_0\rangle=0,\quad k=1,2,\ldots. \tag{7}$$

which remain ambiguous and admit different adaptations.

In a nonstandard, "non-unperturbed" basis $\{|n\rangle\}_{n=0}^{\infty}$ which breaks the traditional coincidence of the eigenstates of H_0 with the basis elements themselves, an assumption of tridiagonality of H_0 may still lead to a non-numerical propagators defined in terms of continued fractions.[11] With a non-RS projector $P^{(0)}=|0\rangle\langle 0|=1-Q^{(0)}$, the normalization $|\psi_0\rangle\equiv P^{(0)}|\psi\rangle$ makes the standard out-of-the-model-space projectors over-complicated, and non-diagonal zero-order propagators must be used. Due to their non-diagonality people even return to the immediate numerical (i.e., coordinate) representation of wavefunctions.[12] Implicitly, such a challenge has encouraged and inspired our forthcoming proposal which, basically, introduces the general projectors $P^{(K)}=|K\rangle\langle K|$. Our new prescription realizes the idea of normalizing via $P^{(K_1)}$ and "projecting" via $P^{(K_2)}$ at any suitable K_1 and K_2.

For the sake of brevity, we shall pay the detailed attention, say, to the Lanczos-type upper Hessenberg case (the subsequent Lanczos $\to$ anti-Lanczos transition is under current research.[13]) At a fixed perturbation order $k\geq 1$, we take the general definition (7) of corrections $|\psi_k\rangle$ and E_k, namely, equation

$$(H_0-E_0)\;|\psi_k\rangle=|\tau_{k-1}\rangle+E_k|\psi_0\rangle. \tag{8}$$

The sum of the "old" or "known" terms

$$(H_j-E_j)\;|\psi_m\rangle=(|0\rangle,|1\rangle,\ldots)\times\left(\begin{array}{ccccc} A_0^{\{j\}} & C_1^{(1)\{j\}} & C_2^{(2)\{j\}} & \ldots\\ B_0^{\{j\}} & A_1^{\{j\}} & C_2^{(1)\{j\}} & \ldots\\ 0 & B_1^{\{j\}} & A_2^{\{j\}} & \ldots\\ 0 & 0 & B_2^{\{j\}} & \ldots\\ & \ldots & & \ldots \end{array}\right)\times\left(\begin{array}{c} c_0^{[m]}\\ c_1^{[m]}\\ c_2^{[m]}\\ \ldots\end{array}\right)$$

with $j = 1, 2, \ldots, k-1$ and $m \equiv k - j$ is collected here in the abbreviation

$$|\tau_{k-1}\rangle = (|0\rangle, |1\rangle, |2\rangle, \ldots) \times \left(\begin{array}{c} c_0^{(\tau)[k-1]} \\ c_1^{(\tau)[k-1]} \\ \ldots \end{array} \right) .$$

Our first and highly important technical step is an $(N+1)-$dimensional truncation of our linear problem (8) (with $N \to \infty$ at the end). This enables us to replace the standard RS normalization by its most natural Lanczos-inspired modification, $|\psi_0\rangle \equiv P^{(N)}|\psi\rangle$. In the other words, we employ the renormalization freedom and postulate

$$c_N^{[0]} \neq 0, \quad c_N^{[1]} = c_N^{[2]} = \ldots = c_N^{[N-1]} = 0 .$$

Now, the standard procedure may follow: In a way which reflects the matrix structure of $H_0 - E_0 I$, we pick up the model space projector $P^{(0)} = 1 - Q^{(0)}$. Let us notice its non-coincidence with the normalization: It enables us to define a new, $N-$dimensional square matrix $R_0^{(0N)} = \left[Q^{(0)}(E_0 - H_0)Q^{(N)}\right]^{-1}$ with an off-diagonal position of energies but with the *simplified, triangular* overall structure, $(R_0^{(0N)})_{mn} = 0$ for all $m > n$. This is our main achievement.

Our unusual "unperturbed" propagator $R_0^{(0N)}$ enables us to *decompose* eq. (8),

$$(H_0 - E_0)\ Q^{(N)}|\psi_k\rangle = |\tau_{k-1}\rangle + E_k|\psi_0\rangle \ . \tag{9}$$

with respect to the *not yet specified parameter* E_k,

$$|\psi_k\rangle = E_k\,|\psi_k^{(P)}\rangle + |\psi_k^{(Q)}\rangle, \qquad |\psi_k^{(P,Q)}\rangle = (|0\rangle, |1\rangle, \ldots, |N\rangle) \times \left(\begin{array}{c} c_0^{(P,Q)[k]} \\ c_1^{(P,Q)[k]} \\ \ldots \\ c_{N-1}^{(P,Q)[k]} \\ 0 \end{array} \right) . \tag{10}$$

The $Q^{(0)}-$projected eq. (9) becomes the pair of triangular inversions,

$$\left(\begin{array}{ccccc} B_0^{\{0\}} & A_1^{\{0\}} & C_2^{(1)\{0\}} & \ldots & C_{N-1}^{(N-2)\{0\}} \\ 0 & B_1^{\{0\}} & A_2^{\{0\}} & \ldots & C_{N-1}^{(N-3)\{0\}} \\ 0 & 0 & B_2^{\{0\}} & \ldots & C_{N-1}^{(N-4)\{0\}} \\ & \ldots & & \ldots & \\ 0 & 0 & 0 & \ldots & B_{N-1} \end{array} \right) \times \left(\begin{array}{c} c_0^{(P)[k]} \\ c_1^{(P)[k]} \\ \ldots \\ c_{N-1}^{(P)[k]} \end{array} \right) = \left(\begin{array}{c} c_1^{[0]} \\ c_2^{[0]} \\ \ldots \\ c_N^{[0]} \end{array} \right) \tag{11}$$

$$\left(\begin{array}{ccccc} B_0^{\{0\}} & A_1^{\{0\}} & C_2^{(1)\{0\}} & \ldots & C_{N-1}^{(N-2)\{0\}} \\ 0 & B_1^{\{0\}} & A_2^{\{0\}} & \ldots & C_{N-1}^{(N-3)\{0\}} \\ 0 & 0 & B_2^{\{0\}} & \ldots & C_{N-1}^{(N-4)\{0\}} \\ & \ldots & & \ldots & \\ 0 & 0 & 0 & \ldots & B_{N-1} \end{array} \right) \times \left(\begin{array}{c} c_0^{(Q)[k]} \\ c_1^{(Q)[k]} \\ \ldots \\ c_{N-1}^{(Q)[k]} \end{array} \right) = \left(\begin{array}{c} c_1^{(\tau)[k-1]} \\ c_2^{(\tau)[k-1]} \\ \ldots \\ c_N^{(\tau)[k-1]} \end{array} \right) . \tag{12}$$

In an upward direction, they define, step-by-step, all the "new" left-hand-side coefficients $c_n^{(P,Q)[k]}$ and components (10) of the wavefunction corrections $|\psi_k\rangle$.

The remaining linear relation (viz., a $P^{(0)}-$projection of eq. (9) defines now the energy. In terms of the known (just constructed and, notice, E_k-independent) $P-$ and $Q-$superscripted wavefunction components, we have

$$E_k = \frac{\langle 0|(H_0 - E_0)\, Q^{(N)}|\psi_k^{(Q)}\rangle - \langle 0|\tau_{k-1}\rangle}{\langle 0|\psi_0\rangle - \langle 0|(H_0 - E_0)\, Q^{(N)}|\psi_k^{(P)}\rangle}.$$

This is our final result, the new Lanczos-RS explicit formula for the energy corrections.

In practice, one must get rid of the auxiliary truncation-dependence. This is to be done numerically, via the "last-step" infinite-dimensional limiting transition, $N \to \infty$. For the sake of comfort, the energy formula may also be further modified. Thus, via an (= arbitrary) introduction of the "norm", say, $B_{-1} = 1$, we may also define the auxiliary "minus-first" components via an "upwards" extension of eqs. (11) and (12). Then, the obvious "boundary condition"

$$c_{-1}^{[k]} = E_k\, c_{-1}^{(P)} + c_{-1}^{(Q)[k]} = 0$$

offers a final, intuitively appealing interpretation and simplified definition of energies,

$$E_k = \frac{c_{-1}^{(Q)[k]}}{c_{-1}^{(P)}}, \qquad\qquad N \to \infty.$$

Its numerical tests are under preparation.

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