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Residue decompositions of the propagator for time-independent Hamiltonian operators

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The formal equivalence and algorithmic differences between the Leverrier-Bateman resolvent method and the recursive residue generation method for constructing the evolution operator of time-independent Hamiltonian operators are discussed.

The author has promoted the usage of the Leverrier-Bateman resolvent method (LBRM) for evaluating the evolution operator $U(t)$ of a multilevel system interacting with a constant-intensity[1(a),1(b)] or a time-varying-intensity[1(a),1(c)] laser field. For fixed-amplitude fields, Nauts and Wyatt and co-workers[2] have advanced the application of the recursive residue generation method (RRGM) in calculating $U(t)$. Both methods address the problem of exponentiating a time-independent Hamiltonian operator H to yield $U(t)=\exp(-iHt)$. While one can often accomplish this through a complete spectral decomposition of H in a finite basis, a strategy that is clearly costly in computational and storage resources, both the LBRM and the RRGM require only the eigenvalues of H and obviate the need for the corresponding eigenvectors. This common feature of the LBRM and RRGM suggests that the two schemes are somehow related, and it is the exposure of this linkage that is the object of this Rapid Communication. In brief, I show that the methods are formally equivalent but differ in their algorithmic generation of the residues of the Laplace-weighted resolvent of H at its poles in the complex plane.

Consider a quantized system whose time-independent Hamiltonian operator H has the discrete spectral resolution

$$H=\sum_k \omega_k |\psi_k\rangle\langle\psi_k| \ , \tag{1a}$$

in terms of its complete set of orthonormal energy (ω_k, assumed nondegenerate) eigenstates $|\omega_k\rangle$ which satisfy the closure relation

$$\sum_k |\psi_k\rangle\langle\psi_k| = I \ , \tag{1b}$$

I being the identity operator. The propagator $U(t)=\exp(-iHt)$ is the inverse Laplace transform of the resolvent of H, i.e.,

$$U(t)=\frac{1}{2\pi i}\int_{i\gamma+\infty}^{i\gamma-\infty} ds \exp(-ist)(sI-H)^{-1} \ , \tag{2a}$$

where γ is an arbitrary real number to be chosen so that all singularities of the integrand lie below $s=\gamma$ and the integration is to be performed along the straight line $\mathrm{Im}(s)=\gamma$ parallel to the real axis. Evaluating Eq. (2a) by use of the residue theorem[3] gives

$$U(t)=\sum_k \exp(-i\omega_k t)N_k \ , \tag{2b}$$

where the time-independent operator N_k, when weighted by the phase factor $\exp(-i\omega_k t)$, is the residue of the integrand in Eq. (2a) at the pole $s=\omega_k$. However, taking the Maclaurin expansion of $U(t)$ and using Eq. (1) as necessary gives as an alternative to Eq. (2b),

$$U(t)=\sum_k \exp(-i\omega_k t)|\psi_k\rangle\langle\psi_k| \ . \tag{2c}$$

Consequently, from Eqs. (2b) and (2c), the N_k operators are given by

$$N_k=|\psi_k\rangle\langle\psi_k| \ , \tag{3a}$$

and have the projection

$$N_k N_l = 0 \text{ if } k\neq l \ , \tag{3b}$$

and idempotent

$$N_k^l = N_k \text{ for } l=1,2,\ldots \tag{3c}$$

properties, by virtue of Eq. (1), and obey the sum rule

$$\sum_k \omega_k^l N_k = H^l \text{ for } |l|=0,1,\ldots, \tag{3d}$$

as follows from Eq. (2b).

In the field-free finite (N, say) complete orthonormal basis $|\phi\rangle$, the transition amplitude between the states $|\phi_r\rangle$ and $|\phi_s\rangle$ is given by

$$U_{rs}(t)=\sum_k \exp(-i\omega_k t)N_{k,rs} \ , \tag{4a}$$

where

$$N_{k,rs}=\langle\phi_r|\psi_k\rangle\langle\psi_k|\phi_s\rangle \tag{4b}$$

and $U_{rs}(t)$ are general entries in $\mathbf{U}(t)$ and $\mathbf{N}_k$, respectively, the matrix representations of the operators in the $|\phi\rangle$ basis. Equation (4a) is the point of formal equivalence of the LBRM and the RRGM. At this stage no progress has been made as a result of the $\mathbf{N}_k$'s dependence of the unknown $|\psi_k\rangle$ through Eq. (4b), save for the realization that no matter how they are obtained they continue to satisfy the relations given in Eqs. (3b)–(3d) in the $|\phi\rangle$ basis. Both the LBRM and the RRGM schemes circumvent direct use of $|\psi_k\rangle$ through different algorithmic constructions of the $\mathbf{N}_k$'s.

The $\mathbf{N}_k$'s are computed in the LBRM approach[1(a),1(b)] by first determining the eigenvalues ω_k using the EISPAK library,[4] or an equivalent package, followed by the recursive generation of the $N\times N$ auxiliary matrices $\mathbf{Z}_k$ via

Faddeev's and Sominskii's[5-7] modified Leverrier algorithm[8] $\mathbf{Z}_k = -i\mathbf{H}\mathbf{Z}_{k-1} + \theta_{k-1}\mathbf{I}$ for $k = 2, \ldots, N$ starting with $\mathbf{Z}_1 = \mathbf{I}$, where $\theta_k = i\,\mathrm{Tr}(\mathbf{H}\mathbf{Z}_k)/k$ for $k = 1,2,\ldots,N$ and $\mathbf{H}$ and $\mathbf{I}$ are matrix representations in the $|\phi\rangle$ basis of the corresponding operators. The $\mathbf{N}_k$'s can be evaluated concurrently by parallel array processors as

$$\prod_{l\neq k}(\omega_k - \omega_l)\mathbf{N}_k = \sum_l \omega_k^{N-l}\mathbf{Z}_l \ .$$

However, when N is large the storage requirements of the LBRM become a matter of concern, since even if $\mathbf{H}$ is sparse, the $\mathbf{Z}_k$'s and $\mathbf{N}_k$'s are generally dense. Following Nauts and Wyatt and co-workers[2] in their implementation of the RRGM, one can conserve core resources by first tridiagonalizing $\mathbf{H}$ via the Lanczos recursion method,[9] after which its eigenvalues are calculated and transferred to disk until required. One then proceeds to serially construct each of a total of N^2 N-vectors of $Z_{k,rs}$'s from the core-resident $\mathbf{H}$ and the N-vector of $Z_{k-1,rs}$'s, while capitalizing on the Jocobi structure of $\mathbf{H}$ to minimize the number of floating-point operators to evaluate the $Z_{k,rs}$'s and θ_k, following which the N-vector of $Z_{k-1,rs}$'s is transferred to disk. This strategy demands core and disk capacities of $5N$ and $O(N^3)$, respectively. With both $\mathbf{H}$ and its N-vector of eigenvalues core resident, an N-vector of $N_{k,rs}$'s can be computed from each N-vector of $Z_{l,rs}$'s in core, the entire calculation requiring a core capacity of $5N$ and involving N^2 transfers of N-vectors of $N_{k,rs}$'s to disk and N retrievals of N-vectors of $Z_{l,rs}$'s from disk. If, for fixed r and s, $|N_{k,rs}| < \varepsilon$ for some k, where ε is arbitrarily small, then these components make negligible contributions to $U_{rs}(t)$ through Eq. (4a) and their omission assures continued fulfillment of the relations in Eqs. (3b)–(3d) to within acceptable tolerance(s). Physically one may interpret this numerical artifice as implying that not all of the dressed states $|\psi_k\rangle$ play significant roles in mediating the $r \rightarrow s$ transition. If $\mathbf{H}$ has degenerate eigenvalues, the summation in Eq. (4a) is over the n distinct eigenvalues with corresponding multiplicities n_k so that $\sum_k n_k = N$, and, for $\mathbf{U}(t)$ to be always bounded, the Bateman matrices $\mathbf{N}_k$ are generalized[1(b)] to

$$(n_k - 1)!\mathbf{N}_k = \sum_l \mathbf{Z}_l \frac{d^{n_k-1}}{ds^{n_k-1}}\left[s^{N-l}/\prod_{l\neq k}(s-\omega_l)^{n_l}\right]_{s=\omega_k} .$$

Implementation of the LBRM on any of the emerging multiprocessor machines will depend on the specifics of the parallel architecture, in particular on whether core memory is shared or distributed, the interprecessor connectivity and communication links, and the disk storage available per processor, with the degree of parallelism being such as to minimize the synchronization and communication overheads.

In the RRGM approach,[2(b)] the $N_{k,rs}$'s are computed as contributions from two or four residues of diagonal Green's functions according as $|\phi_r\rangle$, $|\phi_s\rangle$, and $\mathbf{H}$ are real or general complex, respectively. These residues are products of $N-1$ quotients of eigenvalue differences requiring determination of the ω_k's in addition to the eigenvalues of from two to four $(N-1)\times(N-1)$ reduced Hamiltonian matrices in an orthonormal transition vector basis comprised of symmetric and antisymmetric linear combinations of $|\phi_r\rangle$ and $|\phi_s\rangle$. The diagonalizations via EISPACK are preceded by use of Paige's reformulated[9(a),9(b)] Lanczos recursion method[9(c)] to transform $\mathbf{H}$ and the reduced Hamiltonian matrices from the $|\phi\rangle$ basis to tridiagonal form in a so-called recursion basis. By exploiting the structural sparsity of the tridiagonalized form of a generic laser-molecule Hamiltonian operator, Castillo and Wyatt[2(g)] succeeded in reducing storage requirements to the extent that calculations on systems with $N \geq 10^4$ were feasible; furthermore, by representing a multidimensional potential in a direct product of one-dimensional potentials, significant reductions in computation time were achieved[2(h)] in an implementation of the RRGM on a vector processor. The LBRM should also benefit from use of these features of the Hamiltonian operator describing the interaction of a polyatomic molecule with a classical laser field of fixed or time-varying intensity. Nauts[2(c)] and Nauts and Chapuisat[2(d)] have discussed the extension of the RRGM to the case where $\mathbf{H}$ has a degenerate spectrum by noting that through the restriction of the Hamiltonian operator to the subspace of the total space of state vectors spanned by the recursion basis, its nondegenerate eigenvalues are the only ones needed for the computation of the residues.

Development[1] of the LBRM was prompted by investigations[10] of the evolution of radionuclide inventories in open systems—hence the Bateman[11] appellation for the $\mathbf{N}_k$'s—and in a related context the method has been applied[12] to the point nuclide kinetics of ^{2}H, ^{3}H, and ^{3}He in the thermal-neutron flux prevailing within the heavy-water moderator of a CANDU (Canada Deuterium Uranium) commercial power reactor. The LBRM is currently being used to gauge the photon economics during the initial stages of multiphoton excitation of polyatomic molecules by continuous-wave[1(b)] and pulsed[1(c)] high-intensity lasers for isotope-separation applications. Development of the RRGM was inspired by use[13] of similar techniques in calculations of the local density of electronic states about a site in a disordered solid and, in addition to its use[2] in the laser-molecule context, it has been applied[14] to the evaluation of thermal and temporal propagators arising in approximations to quantum statistical averages.

Finally, it is interesting to note that even if N is sufficiently small as to render a complete spectral decomposition of $\mathbf{H}$ competitive with the LBRM and RRGM approaches to the calculation of $\mathbf{U}(t)$, there is no assurance[15] that a similarity transformation for diagonalizing $\mathbf{H}$ can be determined if $\mathbf{H}$ is not Hermitian, such as when its eigenvalues have finite radiative widths.

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