Fast Time-Evolution Method for Dynamical Systems

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A fast time-evolution method is developed for systems for which the dynamical behavior can be reduced to the eigenvector/eigenvalue problem. The method does not use the eigenvectors/eigenvalues themselves and is based on a polynominal expansion of the formal operator solution in the eigenfrequency domain. It is complementary to the standard time-integration approaches and allows one to calculate or simulate the state of a system at arbitrary times. The time evolution of, e.g., classical harmonic atomic systems and quantum systems described by linear Hamiltonians can be treated by this method.

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Suppose that the time-evolution problem for a dynamical system can be reduced to the eigenfunction-eigenvalue problem. If the eigenfunctions and corresponding eigenvalues are known, then all dynamical variables describing the system with certain initial and boundary conditions can be found at any other moment of time. Let us suppose that the eigenfunctions and eigenvalues of the system exist but cannot be found either analytically or numerically (e.g., because of the very large number of variables involved). The question is can we predict (calculate or simulate) the dynamical state of the system at any moment of time knowing only the equations of motion, initial conditions, and the fact that the eigenfunctions and eigenvalues exist? The answer is positive (obvious in the case of an available analytical solution) and the standard but inefficient way uses numerical time-integration schemes, according to which normally many integration time steps have to be used in order to reach a desired moment of time (see, e.g., [1]). Such schemes are applicable to general dynamical systems which are not necessarily described by eigenfunctions and eigenvalues and therefore the advantage related to the existence of eigenfunctions and eigenvalues is not used at all.

In this Letter, we suggest a general, numerically efficient approach for the solution of the dynamical evolution problem for systems which can be described by eigenfunctions and eigenvalues. Our approach is quite opposite to the time-integration schemes treating the problem in the time domain. Instead, we solve the time-evolution problem in the frequency (eigenvalue) domain directly using the fact of the existence (only) of eigenfunctions and eigenvalues. This gives us an opportunity to find all dynamical variables at any moment of time using, in fact, only one time-evolution step of any required length. Such an approach is applicable to a broad class of dynamical systems which includes, e.g., some quantum mechanical systems characterized by time-independent Hamiltonians and classical harmonic atomic systems described by a dynamical matrix. Among the physical problems to which this fast evolution method (FEM) can be applied include stochastic transport theory [2], quantum (and classical) diffusion and electron-localization problems [3,4], wave propagation in disordered atomic structures [5,6], etc.

The basic idea of the FEM suggested here is to expand the formal (operator) solution of the problem in a series of suitable (Chebyshev) polynomials defined on the set of Hermitian operators. The coefficients in such expansions depend on time (and external field parameters) and on the form of the time-evolution operator only (not on the number of variables and their type, i.e., the dimensionality of the linear vector space), while the polynomials defined on Hermitian operators can be easily treated numerically in their matrix representation. The idea for the FEM came from the kernel polynomial method [7] for the calculation of the spectral functions for large systems and from the unstable oscillator method [8], exploiting the idea of a large time-integration step.

The FEM is easily adapted for computations. It can treat numerically a large number of dynamical variables ($\lesssim 10^7$) [9] and the computation time scales linearly with the number of variables and evolution time in the case of systems characterized by sparse matrices.

Let us consider a system, a dynamical state of which can be described by a vector, $\mathbf{u}(t)$ in an N-dimensional linear vector space spanned by the basis set $\{\mathbf{s}_1, \ldots, \mathbf{s}_N\}$ evolving with time t according to the following equation of motion: $\{\hat{\mathbf{T}}(t) + \hat{\mathbf{A}}\}\mathbf{u} = 0$, with $\hat{\mathbf{T}}(t)$ being a time-evolution operator and $\hat{\mathbf{A}}$ being the time-independent linear Hermitian operator responsible for interactions. Two applications of such an equation are straightforward. For classical motion of N_a coupled harmonic oscillators in D-dimensional real space, $\hat{\mathbf{T}} = \partial^2/\partial t^2$, $\{\mathbf{s}_i\}$ $(i = 1, \ldots, DN_a)$ could be a site basis and $\mathbf{A}$ then is a dynamical matrix in the site representation [10]. In the quantum case, $\hat{\mathbf{T}} = -i\partial/\partial t$ ($\hbar = 1$), $\{\mathbf{s}_i\}$ is a finite basis (e.g., the site basis for the tight-binding and the Anderson Hamiltonians [3]) suitable for a particular problem and $\mathbf{H} = \mathbf{A}$ is the Hamiltonian matrix in the same representation, $H_{ij} = \langle \mathbf{s}_i | \hat{\mathbf{H}} | \mathbf{s}_j \rangle$. In the general case, the operator $\hat{\mathbf{T}}$ can be any integrodifferential operator, for which an analytical or numerical solution, $\mathbf{u}(t, \lambda)$, of the auxiliary equation, $\{\hat{\mathbf{T}}(t) + \lambda\}\mathbf{u} = 0$ (with λ being a scalar, e.g., an eigenvalue of the matrix $\mathbf{A}$), is available.

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In that case, the FEM described below is directly applicable. In what follows, for definiteness, we consider mainly the classical motion problem, bearing in mind that, e.g., the quantum case can be treated similarly.

The formal operator solution (in the matrix representation) of the classical harmonic motion problem [with the initial conditions in the form $\mathbf{u}(t=0)=\mathbf{u}_0$ and $\dot{\mathbf{u}}(0)=\mathbf{v}_0$] for the displacement vector $\mathbf{u}$ of N_a coupled particles can be written as

$$\mathbf{u}(t)=\cos(\sqrt{\mathbf{A}}\,t)\mathbf{u}_0+(\mathbf{A}^{-1/2}\sin\sqrt{\mathbf{A}}\,t)\mathbf{v}_0\,, \qquad (1)$$

which is obvious for a matrix $\mathbf{A}$ in its eigenvector (diagonal) representation and can be easily obtained by linear transformation to another basis (e.g., site basis) in which the matrix $\mathbf{A}$ is not necessarily diagonal. We assume that the dynamical matrix $\mathbf{A}$ in the site basis and initial vectors $\mathbf{u}_0$ and $\mathbf{v}_0$ are known, while the eigenvectors/eigenvalues of $\mathbf{A}$ exist but are not available (because of, e.g., a large number of variables) and our aim is to find $\mathbf{u}(t)$ at an arbitrary time t. The formal solution is of no direct use for this aim because the dynamical matrix $\mathbf{A}$ in the site basis is not diagonal in general (because of couplings between oscillators) so that the symbolic scripts, e.g., $(\cos\sqrt{\mathbf{A}}\,t)\mathbf{u}_0$, in Eq. (1), should be understood as the power series (for example, Taylor) for this function around, e.g., $t_0=0$. The expansion in time is the basis for the numerical time-integration schemes (e.g., Verlet [1]), according to which a desired time t can be reached by making a necessary number of small time steps for which the Taylor expansion is appropriate.

An alternative way to the integration schemes based on time expansions relates to the expansion of the formal solution Eq. (1) in the eigenvalue domain of the dynamical matrix. Let us consider the time t as a parameter and $\mathbf{A}$ as a matrix variable for the functions $\cos\sqrt{\mathbf{A}}\,t$ and $\mathrm{sinc}\sqrt{\mathbf{A}}\,t\equiv\sin\sqrt{\mathbf{A}}\,t/\sqrt{\mathbf{A}}\,t$. These functions can then be expanded in a series of the appropriate complete set of functions $\phi_p(\mathbf{A})$ with time-dependent coefficients. The choice of the basis set for the expansion is dictated by the following requirements. The functions $\phi_p(\mathbf{A})$ preferably should be polynomials because the variable $\mathbf{A}$ is a matrix and it is easy to treat them computationally for polynomials. The functions $\phi_p(\mathbf{A})$ have to be defined on a finite interval because the spectrum of $\mathbf{A}$ is bounded. The coefficients in the expansion should be easily and rapidly computed. All these requirements are met by the Chebyshev polynomials $T_p(\mathbf{A}')=\cos(p\cos^{-1}\mathbf{A}')$ [7] which are the complete set for the matrix $\mathbf{A}'=2\mathbf{A}/\lambda_{\max}-\mathbf{I}$ (with $\lambda_{\max}$ being the maximum eigenvalue) having the spectrum in the interval $[-1,1]$. The formal solution can then be rewritten as follows:

$$\mathbf{u}(t)=\left[\sum_{p=0}^{\infty}a_p(t)T_p(\mathbf{A}')\right]\mathbf{u}_0+\left[t\sum_{p=0}^{\infty}b_p(t)T_p(\mathbf{A}')\right]\mathbf{v}_0\,. \qquad (2)$$

In practice, the infinite upper limit in the series above can be replaced by $P-1$, with P being the appropriate (cutoff) number of polynomials which give the most significant contributions in the series (see Fig. 1 and below). The expansion coefficients $c_p(t)$ [$a_p(t)$ and $b_p(t)$ in Eq. (2)] can be easily calculated using the orthogonality conditions for T_p,

$$c_p(t)=\frac{2}{(1+\delta_{p,0})P}\sum_{q=0}^{P-1}\cos\left(\frac{\pi pq}{P}\right)F\left[\sqrt{\frac{\lambda_{\max}}{2}\left(1+\cos\frac{\pi q}{P}\right)}\,t\right], \qquad (3)$$

with $\delta_{p,0}$ being the Kronecker symbol. The form of the function $F(x)$ is defined by the concrete form of the time-evolution operator and, in the particular case of harmonic vibrations of coupled oscillators, is $F(x)=\cos(x)$ and $F(x)=\mathrm{sinc}(x)$ for the coefficients $c_p(t)=a_p(t)$ and $c_p(t)=b_p(t)$, respectively. These coefficients can be rapidly computed using the fast Fourier transformation because of the cosinelike functional form of the Chebyshev polynomials. We should also stress that expression (3) is quite general and depends on the particular form or properties of operator $\hat{\mathbf{A}}$ only via the maximum eigenvalue $\lambda_{\max}$ entering the argument of the function F.

The Chebyshev polynomials in Eq. (2) are defined by the recursion relations: $T_0(\mathbf{A}')\mathbf{u}=\mathbf{u}$, $T_1(\mathbf{A}')\mathbf{u}=\mathbf{A}'\mathbf{u}$, and $T_{p+1}(\mathbf{A}')\mathbf{u}=2\mathbf{A}'T_p(\mathbf{A}')\mathbf{u}-T_{p-1}(\mathbf{A}')\mathbf{u}$. These polynomials actually enter the solution (2) as products with the initial vectors $\mathbf{u}_0$ and $\mathbf{v}_0$. This fact significantly improves the computational performance, so that for a sparse matrix $\mathbf{A}$ this method scales linearly with the number of variables and evolution time.

It appears that at fixed t the coefficients a_p and b_p first oscillate with increasing p and then decay exponentially with further increase of p (see Fig. 1 for the particular case of the time evolution of a δ-functional initial perturbation in a linear harmonic atomic chain). Such behavior of the coefficients a_p and b_p with p allows us to truncate the series in Eq. (2) at a certain order P of the polynomials. The number of polynomials used in the expansion, not surprisingly, grows with time t, and the maximum order of the polynomials (number of roots of the polynomial) can be estimated as the number of oscillations with a typical frequency, $\omega_*=\sqrt{\lambda_*}$ in time t, i.e., $P\simeq\omega_* t/\pi$. The typical frequency is normally of the same order as the maximum frequency, $\omega_*=\chi\omega_{\max}$, with $\chi\sim 1$ [in the case of a linear chain, the value of χ is roughly $\chi\simeq 1.6$ (see Fig. 1)]. The rest of the series for the expansion coefficients with $p\geq P$ does not give a significant contribution because of the very rapid (exponential) decrease of a_p and b_p with increasing p.

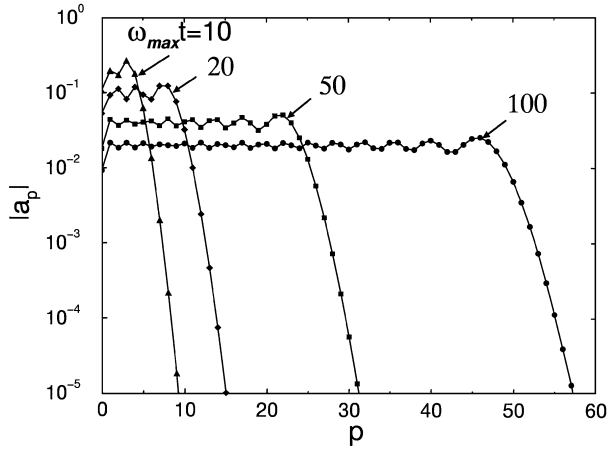

FIG. 1. The magnitude of the expansion coefficients, $|a_p|$, in Eq. (2) as a function of the order p of the Chebyshev polynomials for different evolution times t as indicated (with $\omega_{\max} = 2$ relevant for a 1D ideal atomic linear chain model).

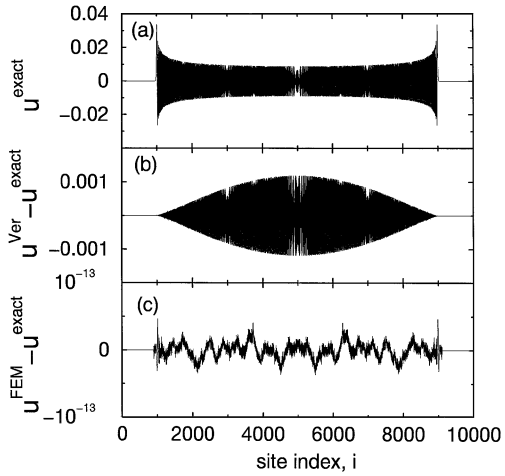

FIG. 2. Displacement pattern (the displacement u_i of atom i vs its equilibrium coordinate $R_i \equiv i$) for a δ-functional initial displacement perturbation at $i = 5000$ in an ideal linear harmonic chain of 10^4 atoms at $\omega_{\max} t = 4000$: (a) the exact solution, u_i^{exact}; (b) the difference between the approximate solution obtained by the Verlet method (with the integration time step, $\tau = 0.01$, and the number of steps, $N_\tau = 4 \times 10^5$) and the exact solution, $u_i^{\text{Ver}} - u_i^{\text{exact}}$; (c) the difference between the approximate solution obtained by the FEM (with the integration time step, $\tau = 4 \times 10^3$, the number of steps, $N_\tau = 1$, and the maximum order of the polynomials, $P = 4105$) and the exact solution, $u_i^{\text{FEM}} - u_i^{\text{exact}}$.

The FEM developed here can also be used as an elementary single-step calculation procedure in the integration algorithm, but the time step can be arbitrary. This means that an efficient integration method based on the Chebyshev polynomial expansion can be used to solve the equation of motion for the system in question. It appears to be much faster and more accurate than other known schemes, e.g., the Verlet algorithm. In order to compare its performance with the popular Verlet scheme, we have computed the Green function for the simplest harmonic model, an ideal linear chain of atoms coupled to the nearest neighbors only (see, e.g., [10,11], and references therein) with periodic boundary conditions. The potential energy of such a model is $V = (1/2)\sum_n (u_n - u_{n+1})^2$, assuming that all masses, $m_n = 1$, interatomic distances, $a_{n,n+1} = 1$, and spring constants, $\kappa_n = 1$, with a resulting $\omega_{\max} = 2$. Such a choice of model has been dictated by two reasons: (i) a displacement pattern with initial conditions, $u_n(0) = \delta_{nn_0}$ and $\dot{u}_n(0) = 0$, contains all the eigenmodes of the system, and (ii) the solution is known analytically [10], $u_n^{\text{exact}}(t) = J_{2n}(2t)$ [with $J_m(x)$ being the Bessel function], allowing us to judge the quality of the approximate numerical solutions obtained by the FEM, $\mathbf{u}^{\text{FEM}}(t)$, and by the Verlet method, $\mathbf{u}^{\text{Ver}}(t)$ (see Fig. 2). Approximate solutions have been found numerically for $N = 10^4$ atoms and $t = 4000$ ($\omega_{\max} t = 8000$). The results presented in Table I and in Fig. 2 show that the FEM is much faster and much more precise (cf. Figs. 2b and 2c). Indeed, the Verlet method can be either relatively fast but not precise (the third column in the Table) or relatively precise but slow (the first column in the Table) in comparison with the always precise, very fast single step (the sixth column) and relatively fast, multiple step (fourth column) FEM. The dramatic increase in speed for the FEM is related to the relatively small number of matrix-vector operations needed as compared to the Verlet scheme. As follows from the Table (cf. the fourth, fifth, and sixth columns), the strategy in accessing the best performance for the FEM is to choose the smallest number of integration steps, preferably just a single evolution step (sixth column) to the desired time t.

The FEM can be easily generalized for a classical system subject to an external force field, $\mathbf{F}^{\text{ext}}(\mathbf{R}_i^{(0)}, t)$ (with $\mathbf{R}_i^{(0)}$

TABLE I. Comparison of the performance of the simple Verlet (leapfrog) method and FEM for the time evolution of a δ-functional displacement perturbation in an ideal linear harmonic chain, with $\epsilon = |\mathbf{u}^{\text{exact}} - \mathbf{u}|$ and $\epsilon_{\text{gain}} = (|\mathbf{u}|/|\mathbf{u}^{\text{exact}}|) - 1$ (for $\mathbf{u} = \mathbf{u}^{\text{FEM}}$ or $\mathbf{u} = \mathbf{u}^{\text{Ver}}$).

Quantity	Verlet	Verlet	Verlet	FEM	FEM	FEM
Time step τ	0.01	0.1	1	1	10	4000
Number of steps N_τ	4×10^5	4×10^4	4×10^3	4×10^3	400	1
Order P for FEM	...	...	...	9	25	4105
CPU/R10 000 time (sec)	760	77.0	54.4	217	49.7	18.7
ϵ	5.5×10^{-2}	0.82	0.98	9.5×10^{-13}	8.4×10^{-13}	1×10^{-12}
ϵ_{gain}	-5×10^{-4}	-4×10^{-4}	2×10^{-3}	-5×10^{-13}	5×10^{-14}	-1×10^{-15}

being the equilibrium positional vector of atom i), and described by an equation of motion in the form, $\ddot{\mathbf{u}} + \hat{\mathbf{A}}\mathbf{u} = \hat{\mathbf{C}}\mathbf{F}^{\mathrm{ext}}(\mathbf{R}_i^{(0)}, t)$, with $\mathbf{C}$ being the matrix representation of the coupling operator $\hat{\mathbf{C}}$ of the external field with the system. In the case of an electromagnetic field, for example, this matrix contains atomic charges (around the diagonal for local interactions and in a distributed fashion for nonlocal interactions). Considering an external field in the form $\mathbf{F}^{\mathrm{ext}}(\mathbf{R}_i^{(0)}, t) = \sum_j \mathbf{f}_j^{\mathrm{ext}}(\mathbf{R}_i^{(0)}) \exp\{i\omega_j t\}$, with the time-independent force field $\mathbf{f}_j^{\mathrm{ext}}(\mathbf{R}_i^{(0)})$, depending on the equilibrium atomic positions $\mathbf{R}_i^{(0)}$ and arbitrary initial conditions, we can easily find the nonsingular formal solution of the problem and expand it in Chebyshev polynomials (to be published elsewhere).

We have also tested the method for more complicated atomic dynamical problems, such as the wave-propagation problem in disordered structures (see, e.g., [5,6,11]), and found excellent performance there (the results for the Ioffe-Regel crossover analysis by means of wave-packet propagation will be published elsewhere).

In conclusion, we have developed a new fast evolution method for dynamical systems characterized by linear Hermitian interaction operators and quite general time-evolution operators (e.g., quantum mechanical systems defined in a finite linear vector space and classical coupled harmonic oscillators). The advantage of the method lies in its computational efficiency (fast and precise, scaling linearly with the number of variables and evolution time) and the ability to treat large dynamical systems containing up to 10^7 variables.

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[1] D. Frenkel and B. Smit, *Understanding Molecular Simulations* (Academic Press, San Diego, 1996).
[2] T. Odagaki and M. Lax, Phys. Rev. B **24**, 5284 (1981).
[3] B. Kramer and A. MacKinnon, Rep. Prog. Phys. **56**, 1469 (1993).
[4] T. Brandes, B. Huckestein, and L. Schweitzer, Ann. Phys. (Leipzig) **5**, 633 (1996).
[5] *Scattering and Localization of Classical Waves in Random Media*, edited by P. Sheng (World Scientific, Singapore, 1990).
[6] S. N. Taraskin and S. R. Elliott, J. Phys. Condens. Matter **11**, A219 (1999).
[7] R. N. Silver and H. Röder, Phys. Rev. E **56**, 4822 (1997).
[8] Y. Okamoto and H. J. Maris, Comput. Phys. Commun. **76**, 191 (1993).
[9] Rough estimates of random access memory and CPU time requirements for a vibrational problem in a 3D cubic lattice of 10^7 atoms are 10 gigabytes and 10 h/R10 000 for $\omega_{\max} t = 10^2$.
[10] A. A. Maradudin, E. W. Montroll, G. H. Weiss, and I. P. Ipatova, *Theory of Lattice Dynamics in the Harmonic Approximation* (Academic Press, New York, 1971).
[11] P. B. Allen and J. Kelner, Am. J. Phys. **66**, 497 (1998).