Application of a modified Lanczos method for reducing unnecessary information in the computation of observables' dynamics

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Abstract

Typically the simulation of a quantum mechanical system is focused on the dynamics of a small set of interesting quantities. Despite this, it is not always easy to carry out the necessary calculations, because one has usually to rely on the solution of the full quantum state dynamics. In this paper we show a method, valid in the context of finite dimension Hilbert spaces, for producing dynamics equations focused on the observables of interest, cutting unnecessary information, possibly saving memory and computation time.

1 Introduction

Numerical simulations in a quantum mechanical context are usually difficult. The problem is that the computation time increases exponentially with the number of coordinates, making the simulation of even small systems a possibly impractical task. However the number of quantities of interest is often very small if compared with the whole degrees of freedom of a certain system, thus it may be possible to reduce the descriptive information of a quantum state, saving memory and maybe computation time.

For some systems, it is well known that set of operators exist whose mean expectation values are linked together: sometimes a closed set of evolution equations can be found and from them the dynamics of such quantities can be easily calculated. An example relevant for this paper is in the context of finite fermionic quadratic systems: closed equations for a two-point correlation matrix can be found, allowing a fast calculation of any fermionic quadratic quantity [1, 2]. A more general example are the eigen-operators of the Liouville equation for isolated systems: they have very simple separated evolution laws, but they also are usually impractical to calculate because requiring a complete spectral analysis of the system's Hamiltonian.

In this paper we study a possible way to extend this principle to a generic observable of interest in finite dimensions Hilbert space systems, approximating its dynamics without a complete analysis the Hamiltonian structure and focusing only on the aspects relevant to the observable. To obtain this we adapt a method [3] originally used in solid state calculations to overcome the well known numerical instability of the Lanczos tridiagonalization algorithm [4]. Exploiting the same reasoning we can find approximated evolution equations for the observable's mean value and other complementary quantities, allowing the calculation of their dynamics.

2 The procedure

We consider an isolated system having state $\hat{\rho}$ and evolving through the Liouville equation

$$\frac{d}{dt}\hat{\rho}(t) = \frac{1}{i\hbar}\left[\hat{H},\, \hat{\rho}(t)\right] \tag{1}$$

where $\hat{H}$ is the Hamiltonian of the system. In the following we take units such that $\hbar = 1$. We are interested in the expectation value of a certain observable $\hat{O}_0$ as a function of time

$$\langle\, \hat{O}_0 \,\rangle(t) \equiv \mathrm{Tr}\left\{\hat{\rho}(t)\hat{O}\right\} : \tag{2}$$

we could calculate this quantity if we knew the full state of the system $\hat{\rho}$ as a function of time. This can be computed, in principle, through the equation (1). However for some systems it is possible to find set of observables that appear to be linked by linear relationships of the kind

$$\frac{d}{dt}O_j(t) = \sum_{k=0}^{N-1} S_{jk}O_k(t), \tag{3}$$

thus allowing a faster and more precise calculation of these quantities as a function of time. In this paper we show a way to find a set of complementary observables $\left\{\hat{O}_1 ... \hat{O}_{N-1}\right\}$ for any $\hat{O}_0$ of interest, leading to a relationship of the kind (3), at least in an approximate sense for generic systems on finite Hilbert spaces.

2.1 A set of recursive equations

Let L be the super-operator acting as

$$L\hat{\rho} = \frac{1}{\hbar}\left[\hat{H},\, \hat{\rho}\right] : \tag{4}$$

the time derivatives of the mean values of an operator $\hat{O}$ can be rewritten as

$$\frac{d}{dt}O(t) = i\mathrm{Tr}\left\{\hat{\rho}(t)L\hat{O}\right\}. \tag{5}$$

We define a scalar product between operators

$$\langle \hat{A},\, \hat{B}\rangle \equiv \mathrm{Tr}\left\{\hat{A}^\dagger\hat{B}\right\}, \tag{6}$$

valid for finite dimension Hilbert spaces. The super-operator L is Hermitian in respect to it

$$\langle L\hat{a},\, \hat{b}\rangle = \langle \hat{a},\, L\hat{b}\rangle. \tag{7}$$

We consider the sequence of normalized operators a_k, calculated recursively as follows. We define

$$\hat{a}_0 := \hat{O}_0 / \left|\left|\hat{O}_0\right|\right|, \tag{8}$$

$$\hat{B}_k := (1 - \hat{a}_k\langle \hat{a}_k,\, \cdot\rangle)\, L^2\hat{a}_k \tag{9}$$

and

$$\hat{b}_k := \hat{B}_k / \left|\left|\hat{B}_k\right|\right|. \tag{10}$$

Let

$$r_k := \langle \hat{a}_k,\, L^2\hat{a}_k\rangle, \tag{11}$$

the operator $\hat{a}_{k+1}$ is generated as a linear combination of $\hat{a}_k$, $\hat{b}_k$

$$\hat{a}_{k+1} = \alpha_k\hat{a}_k + \beta_k\hat{b}_k \tag{12}$$

where $\mathbf{v_k} := (\alpha_k, \beta_k)$ is a real normal vector taken in such a way to minimize r_{k+1}.

Let

$$s_k := \left|\left|\hat{B}_k\right|\right|, \tag{13}$$

and

$$t_k := \langle \hat{b}_k,\, L^2\hat{b}_k\rangle. \tag{14}$$

Theorem 1. *The sequence $\hat{a}_k$ approximates eigen-operators of L^2, that is $\left|\left|L^2\hat{a}_k - r_k\hat{a}_k\right|\right| \to 0$*

Proof. Being the lowest eigenvalue of L^2 null we have

$$r_k \geq r_{k+1} \geq 0, \tag{15}$$

and then

$$\lim_{k\to\infty} r_k = r_\infty := \inf\{r_j\}. \tag{16}$$

Adopting a Lagrange multiplicators approach we conclude that to satisfy the minimization requirements we have to find the lowest eigen-vector of the matrices

$$F_k := \begin{pmatrix} r_k & s_k \\ s_k & t_k \end{pmatrix}, \tag{17}$$

by means of which we can write

$$r_{k+1} = \mathbf{v_k}\cdot F_k\mathbf{v_k}. \tag{18}$$

Let $\mathbf{v}_k$ be the normal eigenvector with the lowest eigenvalue of F_k:

$$F_k\mathbf{v}_k = \lambda_k^-\mathbf{v}_k \tag{19}$$

where $\lambda_k^- = r_{k+1}$. We can write

$$s_k^2 = \left(r_k - \lambda_k^-\right)\left(t_k - \lambda_k^-\right), \tag{20}$$

thus, because t_k has an upper-bound (the maximum eigenvalue of L^2) and

$$r_k - r_{k+1} \to 0, \tag{21}$$

we have

$$s_k = \left|\left|L^2\hat{a}_k - r_k\hat{a}_k\right|\right| \to 0. \tag{22}$$

□

From the sequence $\hat{a}_k$ we can calculate a set of differential equations for its expectation values: recalling (12) and (9) we get

$$\langle\, \hat{a}_{k+1}\,\rangle = \alpha_k\langle\, \hat{a}_k\,\rangle + \beta_k\langle\, \hat{b}_k\,\rangle \tag{23}$$

and

$$s_k\langle\, \hat{b}_k\,\rangle(t) = -\frac{d^2}{dt^2}\langle\, \hat{a}_k\,\rangle(t) - r_k\langle\, \hat{a}_k\,\rangle(t). \tag{24}$$

2.2 Approximations of the dynamics

Chosen an arbitrary small positive ϵ we continue the sequence until the first index $k = N$ such that

$$s_N < \epsilon \tag{25}$$

and we approximate the N-th differential with

$$\frac{d^2}{dt^2}\langle\, \hat{a}_N\,\rangle \simeq -r_N\langle\, \hat{a}_N\,\rangle. \tag{26}$$

Let us consider the indexes with $k < N$. If $r_{k+1} = r_k$ then we could see that the Lagrange multiplier problem would have a solution only for $s_k = 0$, meaning that k could not be less than N: it must be $r_k > r_{k+1}$. Being $r_{k+1} \neq r_k$, we can see from the equation (12) that $\beta_k \neq 0$, thus we can cast the dynamics equations (23) and (24) in the equivalent form

$$\frac{d^2}{dt^2}\langle\, \hat{a}_k\,\rangle(t) = p_k\langle\, \hat{a}_k\,\rangle(t) + q_k\langle\, \hat{a}_{k+1}\,\rangle(t) \tag{27}$$

where

$$p_k := \left(\frac{\alpha_k s_k}{\beta_k} - r_k\right) \leq 0 \tag{28}$$

and

$$q_k := -\frac{s_k}{\beta_k} \neq 0 \text{ (because } s_k > \epsilon). \tag{29}$$

The approximated dynamics equations can be then cast in the following matrix picture: let

$$\mathbf{a}(t) = \begin{pmatrix} \langle\, \hat{a}_0\,\rangle(t) \\ \vdots \\ \langle\, \hat{a}_N\,\rangle(t) \end{pmatrix} \tag{30}$$

and

$$M = \begin{pmatrix} p_1 & q_1 & & & \\ & p_2 & q_2 & & \\ & & \ddots & \ddots & \\ & & & p_{N-1} & q_{N-1} \\ & & & & r_N \end{pmatrix}, \tag{31}$$

we have

$$\ddot{\mathbf{a}}(t) \simeq M\mathbf{a}(t). \tag{32}$$

The coefficients p_k and q_k are independent from the state of the system and characterize the dynamics equations. The dynamics of the $\{\langle\, \hat{a}_k\,\rangle\}$ can then be calculated by stating the necessary initial conditions for the equation (32).

2.3 Necessary conditions for a periodic solution

Being the system evolving autonomously and being the Hilbert space of finite dimension, any related observable has a periodic behavior, thus, we have

$$\mathbf{a}(t) = \sum_{\omega \in W} \mathrm{cas}(\omega t)\mathbf{m}(\omega), \tag{33}$$

where

$$\mathrm{cas}(\omega t) := \cos(\omega t) + \sin(\omega t), \tag{34}$$

$\mathbf{m}(f)$ are real vectors and W is a set of frequencies characterizing the signal. Let

$$\mathbf{A}(t) = \begin{pmatrix} \mathbf{a}(t) \\ \dot{\mathbf{a}}(t) \end{pmatrix} : \tag{35}$$

we are interested in the cases where the dynamics can be identified by the specification of the initial condition $\mathbf{A}(0)$.

Looking at the matrix M we note some facts:

- considering the equation (32) as exact we get

$$-\omega^2 \mathbf{m}(\omega) = M\mathbf{m}(\omega) \tag{36}$$

- because the M matrix is triangular its eigenvalues are $\{p_1 ... p_N\}$ and then

$$W = \left\{-\sqrt{-p_1}, ..., -\sqrt{-p_N}, \sqrt{-p_1}, ..., \sqrt{-p_N}\right\} \tag{37}$$

- let the m eigenvectors of M be

$$\mathbf{e}_k(t) = \begin{pmatrix} e_k^1 \\ \vdots \\ e_k^N \end{pmatrix}, \tag{38}$$

the numbers e_k^j can be calculated through the recursive relation

$$e_k^0 = 1 \tag{39}$$

$$e_k^{j+1} = \begin{cases} -\frac{p_j - p_k}{q_j} e_k^j & 0 < j < k \\ 0 & j \geq k \end{cases} \tag{40}$$

Rearranging them in a matrix E we get that

$$E = (\mathbf{e_1}, ..., \mathbf{e_m}) \tag{41}$$

is triangular. We note that each eigenspace of M must have dimension 1.

Summarizing we can rewrite

$$\mathbf{a}(t) = \sum_{\omega \in W} \mathrm{cas}(\omega t) g(\omega)\mathbf{e}(|\omega|) \tag{42}$$

where $g(\omega)\mathbf{e}(|\omega|) \equiv \mathbf{m}(\omega)$. By the latter relation we have

$$\mathbf{a}(0) = \sum_{\omega \geq 0} \frac{g(\omega) + g(-\omega)}{2} \mathbf{e}(\omega) \tag{43}$$

and

$$\dot{\mathbf{a}}(0) = \sum_{\omega \geq 0} \omega \frac{g(\omega) - g(-\omega)}{2} \mathbf{e}(\omega) : \tag{44}$$

it is clear from these equations that to obtain the coefficients of the expansion (42) for each starting vector $\mathbf{A}(0)$ it is necessary to provide exactly N of $\mathbf{e_k}$ vectors, condition satisfied only when the p_k coefficients are all different.

2.4 Necessary input values

In this section we show the input values needed to carry out the whole computation up to a degree of depth N. The following theorems prove the requirements and describe the details of the calculation.

Theorem 2. *The characteristic coefficients of the equations can be obtained by the knowledge of the terms*

$$\left\{\langle \hat{a}_0,\, L^{2j}\hat{a}_0\rangle,\ \text{with } j \in [0, 2N]\right\}, \tag{45}$$

Proof. Let

$$R_{n,k} := \langle \hat{a}_k,\, L^{2(n+1)}\hat{a}_k\rangle, \tag{46}$$

we can rewrite

$$r_k = R_{0,k} \tag{47}$$

$$s_k = \sqrt{R_{1,k} - r_k^2} \tag{48}$$

$$t_k = \frac{1}{s_k^2}(R_{2,k} - 2r_k R_{1,k} + r_k^3), \tag{49}$$

that is, we can calculate them and α_k and β_k starting from

$$R_{0,k},\, R_{1,k},\, R_{2,k}.$$

Let

$$u_k := \alpha_k - \frac{r_k \beta_k}{s_k}, \tag{50}$$

$$v_k := \frac{\beta_k}{s_k}, \tag{51}$$

the $\{R_{n,k}\}$ numbers are related by the following recurrence relation:

$$R_{n,k+1} = u_k^2 R_{n,k} + 2u_k v_k R_{n+1,k} + v_k^2 R_{n+2,k}, \tag{52}$$

thus we can calculate $R_{n,k+1}$ by the knowledge

$$R_{0,k},\, R_{1,k},\, R_{2,k},\, R_{n,k},\, R_{n+1,k},\, R_{n+2,k}.$$

The only characteristic coefficient of the equation N coincides with $r_N \equiv R_{0,N}$, that to be calculated requires the numbers $R_{0,N-1}, R_{1,N-1}, R_{2,N-1}$ and so on: let

$$C_m = \{R_{n,m} \text{ with } n \in [0, j_m]\}, \tag{53}$$

the numbers for the stage N are contained in C_N with a $j_N = 0$. It is clear by (52) that if the numbers characterizing the stage m are in C_m then the stage $m-1$ requires the set C_{m-1} with $j_{m-1} = j_m + 2$. Let

$$C_N = \{R_{n,N} \text{ with } n \in [0, 0]\} \tag{54}$$

by induction we conclude that

$$C_0 = \{R_{n,0} \text{ with } n \in [0, 2N]\}. \tag{55}$$

□

Theorem 3. *To calculate the vector* $\mathbf{A}(0)$ *we need the values*

$$\left\{ \langle\, L^j \hat{a}_0 \,\rangle \text{ with } j \in [0, 2N+1] \right\}. \tag{56}$$

Proof. We start proving that it holds

$$\hat{a}_k = \sum_{j=0}^{k} Q(j,k) L^{2j} \hat{a}_0, \tag{57}$$

where $Q(j,k)$ are real numbers null for $j \notin [0,k]$. We set

$$Q(0,0) = 1 \tag{58}$$

and proceed by induction assuming that the hypothesis holds for the stage k: it then would be

$$\hat{a}_{k+1} = \sum_{j=0}^{k} Q(j,k) \left(u_k L^{2j} + v_k L^{2j+2} \right) \hat{a}_0. \tag{59}$$

By setting

$$Q(j,k+1) = Q(j,k) u_k + Q(j-1,k) v_k, \tag{60}$$

we obtain

$$\hat{a}_{k+1} = \sum_{j=0}^{k+1} Q(j,k+1) L^{2j} \hat{a}_0, \tag{61}$$

thus confirming the relation (59) for each k. Thus we have the equations

$$\langle\, \hat{a}_k \,\rangle = \sum_{j=0}^{k} Q(j,k) \langle\, L^{2j} \hat{a}_0 \,\rangle \tag{62}$$

and

$$\langle\, iL\hat{a}_k \,\rangle = \sum_{j=0}^{k} Q(j,k) i \langle\, L^{2(j+1)} \hat{a}_0 \,\rangle, \tag{63}$$

that can be calculated by knowing the values $\left\{ \langle\, L^j \hat{a}_0 \,\rangle \text{ with } j \in [0, 2k+1] \right\}$: because the set with $k = N$ contains all the previous ones we obtain the thesis. □

3 Conclusion

The scheme for finite dimension Hilbert spaces we have presented is a possible way to deduce closed evolution equations specific of generic observable of interest, thus cutting superfluous information about the dynamics of other observables. The recursive relationships of this method make it numerically unstable, making prohibitive the calculation of a great number of high quality characteristic coefficients. An other point of concern is represented by the condition necessary to enforce periodic dynamics, as they are expected for isolated systems in finite dimensions Hilbert spaces: nothing seems assuring the condition $p_k \neq p_j \Leftrightarrow k \neq j$. Provided this, the number of evolution equations is bound by the numerical error, that must not grow bigger than the minimum distance appearing between the p_k values. The most promising conditions for an application of this scheme are when the $R_{j,1}$ and $\langle\, L^j a_0 \,\rangle$ values can be easily obtained, as an example, by algebraic means. In such cases the method has the advantage of a contained memory usage and it allows a fast integration of the dynamics.

4 License

References

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