Master CompuPhys - Fortran Numerical Project Scope statements

Numerical methods to find the ground state of a quantum Hamiltonian

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1 Description of the project

The eigenstates of a quantum Hamiltonian play important roles in quantum mechanics, especially the ground state (the state with the lowest energy). At the equilibrium at low temperature, the ground state is the one which is essentially populated. It is then the starting state in the study of light-matter interaction; it describes the equilibrium properties of a material, it is the incoming state for a collision of particles. The goal of this project consists to study and code (in Fortran) algorithms to partially diagonalize Hamiltonians in order to compute ground states.

Their exists two families of algorithms to diagonalize matrices. The direct methods consist to compute the root of the characteristic polynomial. This needs a rapid method to evaluate this polynomial which exists for hermitian tridiagonal matrices by using a recurrence relation. In atomic and molecular physics, the quantum Hamiltonians become tridiagonal matrices in the numerical representation by the finite difference method (see the quantum mechanics course). The zeros of the characteristic polynomial could be then found for example by a dichotomy method. Once known an eigenvalue λ, the associated eigenvector ψ can be computed by solving the equation $(H-\lambda \mathrm{id})\psi = 0$ by using the fixed point method for example. The direct methods are efficient only on matrices with very particular structures (as tridiagonal) for which the evaluation of the characteristic polynomial is rapid. For the general case, the computation of the characteristic polynomial at a point x by a direct computation of $\det(H - x\mathrm{id})$ is very slow and finally inefficient. The second family of diagonalization methods are the iterative methods which are based on the matrix power method. The more important methods are called Lanczos and Davidson methods for hermitian matrices, and Arnoldi method for non-hermitian matrices (their exists also non-hermitian adaptated Lanczos and Davidson methods). Here we consider only hermitian matrices.

1.1 Diagonalization algorithms

1.1.1 The power method algorithm

Let H be an hermitian matrix with unkown **negative** spectrum $\mathrm{Sp}(H) = (\lambda_0, \lambda_1, ..., \lambda_N)$ sorted by increasing values. For the sake of simplicity, we suppose that the eigenvalues are not degenerate. Let ψ a normalized nonspecial state. By nonspecial state, we mean that ψ has components onto all unkown eigenvectors $(\phi_0, ..., \phi_N)$: $\psi = \sum_{i=0}^{N} c_i \phi_i$ with $c_i \in \mathbb{C}$ unkown complex numbers. ψ is kown in the work basis used to represent H but not in the eigenbasis. The power method algorithm is based on the following fact:

$$H^k \psi = \sum_{i=0}^{N} c_i \lambda_i^k \phi_i \simeq c_0 \lambda_0^k \phi_0 \quad \textit{if } k \textit{ is very large} \tag{1}$$

Since $|\lambda_0| > |\lambda_i|$ $(\forall i > 0)$, $\lim_{k\to+\infty} \frac{|\lambda_i|^k}{|\lambda_0|^k} = 0$ $(\forall i > 0)$. Finally

$$\lim_{k\to+\infty} \frac{H^k \psi}{\|H^k \psi\|} = \phi_0 \tag{2}$$

We can then find the ground state of H by studying the sequence $\left(\frac{H^k\psi}{\|H^k\psi\|}\right)_{k\in\mathbb{N}}$. The ground level is found as $\lambda_0 = \langle\phi_0|H|\phi_0\rangle$ with ϕ_0 the limit of the sequence.

If the spectrum of H is not negative, we simply use the method onto a shifted matrix $H' = H - \mu\mathrm{id}$ where $\mu > 0$ is sufficiently large such that the spectrum of H' be negative. H and H' have the same eigenvectors and $\mathrm{Sp}(H) = \mathrm{Sp}(H') + \mu$.

If λ_0 is degenerate, the algorithm converges to an arbitrary state (which depends on the choice of ψ) into the eigensubspace associated with λ_0.

To find the second eigenvector, we apply the same method but with a more special state ψ_0 which has no component onto ϕ_0 but has components onto all other eigenstates. In practice $\psi_0 = (1 - |\phi_0\rangle\langle\phi_0|)\psi$. We have then

$$\lim_{k\to+\infty} \frac{H^k\psi_0}{\|H^k\psi_0\|} = \phi_1 \tag{3}$$

and so on for the other eigenvectors.

The pseudo-code of the power method algorithm for the ground eigenvector is the following:

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take random vector ϕ_0
normalize ϕ_0
$H \leftarrow H - shift * \mathrm{id}$
while $\|H\phi_0 - \langle\phi_0|H|\phi_0\rangle\phi_0\| > \epsilon$ and $k \leq k_{max}$ do
    $\phi_0 \leftarrow H\phi_0$
    normalize ϕ_0
    $k \leftarrow k + 1$
end while
$H \leftarrow H + shift * \mathrm{id}$
$\lambda_0 \leftarrow \langle\phi_0|H|\phi_0\rangle$

The parameters of the algorithm are

- $shift$ (positive real number): the shifting value used to ensure a negative spectrum;
- ϵ : the desired precision concerning the verification of the eigenequation (typically $\epsilon = 10^{-8}$);
- k_{max} : the maximal number of iterations, if k reaches k_{max} before the eigenequation be satisfied with the precision ϵ then the algorithm has not converged.

For the first excited eigenstate the pseudo-code is the following:

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take random vector ϕ_1
$\phi_1 \leftarrow \phi_1 - \langle\phi_0|\phi_1\rangle\phi_0$
normalize ϕ_1
$H \leftarrow H - shift * \mathrm{id}$
while $\|H\phi_1 - \langle\phi_1|H|\phi_1\rangle\phi_1\| > \epsilon$ and $k < k_{max}$ do
    $\phi_1 \leftarrow H\phi_1$
    $\phi_1 \leftarrow \phi_1 - \langle\phi_0|\phi_1\rangle\phi_0$
    normalize ϕ_1
    $k \leftarrow k + 1$
end while
$H \leftarrow H + shift * \mathrm{id}$

$\lambda_1 \leftarrow \langle\phi_1|H|\phi_1\rangle$

Note that we project onto the orthogonal complement of ϕ_0 at each iteration (and not only at the begining) because non-zero components onto ϕ_0 appears into ϕ_1 due to the numerical errors.

1.1.2 The Lanczos algorithm

The Lanczos method consists to consider the projection of the Hamiltonian to the subspaces generated by the power method. These subspaces are called Krilov subspaces:

$$\mathcal{K}^n(H,\psi_0) = \mathrm{Lin}(\psi_0, H\psi_0, H^2\psi_0, ..., H^{n-1}\psi_0) \tag{4}$$

with ψ_0 a normalized "nonspecial" vector (anew for H with a **negative** spectrum). We need an orthonormal basis $\mathcal{B}^n = (\psi_0, \psi_1, ..., \psi_{n-1})$ of $\mathcal{K}^n(H,\psi_0)$. For that we use a modified Gram-Schmidt orthonormalization algorithm:

$$\psi_1 = \frac{\psi_1'}{\|\psi_1'\|} \quad \text{with } \psi_1' = H\psi_0 - \langle\psi_0|H|\psi_0\rangle\psi_0 \tag{5}$$

$$\psi_j = \frac{\psi_j'}{\|\psi_j'\|} \quad \text{with } \psi_j' = H\psi_{j-1} - \sum_{k=0}^{j-1}\langle\psi_k|H|\psi_{j-1}\rangle\psi_k \tag{6}$$

By construction we have

$$H\psi_j = \psi_{j+1}' + \sum_{k=0}^{j}\langle\psi_k|H|\psi_j\rangle\psi_k \tag{7}$$

$$\Rightarrow \langle\psi_{j+i}|H|\psi_j\rangle = \|\psi_{j+1}'\|\delta_{i1} + \langle\psi_j|H|\psi_j\rangle\delta_{i0} \tag{8}$$

It follows that $\langle\psi_{j+i}|H|\psi_j\rangle = 0$ for $i > 1$ (and then by hermiticity $\langle\psi_j|H|\psi_{j+i}\rangle = 0$ for $i > 1 \iff \langle\psi_{j-i}|H|\psi_j\rangle = 0$ for $i > 1$). Finally we can write

$$H\psi_j = \sum_k \langle\psi_k|H|\psi_j\rangle\psi_k \tag{9}$$

$$= \langle\psi_{j-1}|H|\psi_j\rangle\psi_{j-1} + \langle\psi_j|H|\psi_j\rangle\psi_j + \langle\psi_{j+1}|H|\psi_j\rangle\psi_{j+1} \tag{10}$$

The representation of the projection of H into the Krilov subspace in the basis $\mathcal{B}^n$ is then a tridiagonal matrix:

$$H_{\mathcal{B}^n} = \begin{pmatrix} \alpha_0 & \bar{\beta}_1 & & 0 \\ \beta_1 & \alpha_1 & \ddots & \\ & \ddots & \ddots & \bar{\beta}_{n-1} \\ 0 & & \beta_{n-1} & \alpha_{n-1} \end{pmatrix} \tag{11}$$

with $\alpha_j = \langle\psi_j|H|\psi_j\rangle$ and $\beta_j = \langle\psi_{j+1}|H|\psi_j\rangle$.
We can now diagonalize $H_{\mathcal{B}^n}$ by a direct diagonalization method. Finally the Lanczos method to find the ground state of H consists to iteratively build $H_{\mathcal{B}^n}$ with respect to n until the ground state $\phi_0^{(n)}$ of $H_{\mathcal{B}^n}$ be such that $\|H\phi_0^{(n)} - \lambda_0^{(n)}\phi_0^{(n)}\| < \epsilon$ (for the required precision ϵ).
In comparison with the power method, the Lanczos method faster converge since the ground state is not searched as $H^n\phi_0$ but as a linear superposition of $(\psi_0, H\psi_0, ..., H^n\psi_0)$.

For the direct diagonalization method applied to tridiagonal matrices, we can use the following result:

$$p_n(\lambda) = \begin{vmatrix} \alpha_0 - \lambda & \bar{\beta}_1 & & 0 \\ \beta_1 & \alpha_1 - \lambda & \ddots & \\ & \ddots & \ddots & \bar{\beta}_{n-1} \\ 0 & & \beta_{n-1} & \alpha_{n-1} - \lambda \end{vmatrix} \tag{12}$$

satisfies the following recurrence relation:

$$p_0(\lambda) = 1 \tag{13}$$
$$p_1(\lambda) = \alpha_0 - \lambda \tag{14}$$
$$p_k(\lambda) = (\alpha_{k-1} - \lambda)p_{k-1}(\lambda) - |\beta_{k-1}|^2 p_{k-2}(\lambda) \quad \forall k \in \{2, ..., n\} \tag{15}$$

Question: Prove by recurrence this relation.

Let $\omega(\lambda)$ be the number of sign changes in the sequence $(p_k(\lambda))_{k\in\{0,...,n\}}$. $\omega(b) - \omega(a)$ is the number of eigenvalues into $[a, b]$.

Question: Prove this property.

Finally to find the ground eigenvalue of $H_{\mathcal{B}^n}$ (we suppose that $\mathrm{Sp}(H_{\mathcal{B}^n}) \leq 0$) we use the following dichotomy algorithm:

$b \leftarrow 0$
while $\omega(b) - \omega(a) \neq 1$ do $b \leftarrow (a + b)/2$
while $(b - a) > \epsilon$ do
    if $\omega((b + a)/2) - \omega(a) = 1$ then
        $b \leftarrow (b + a)/2$
    else
        $a \leftarrow (b + a)/2$
    end if
end while
$\lambda_0^{(n)} \leftarrow (b + a)/2$

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with an initial value of a choosen such that $a < \lambda_0 < 0$.

Question: Explain the previous algorithm.

To find the ground state $\phi_0^{(n)}$, we study the convergence of the sequence $\left(\left(H_{\mathcal{B}^n} - (\lambda_0^{(n)} - 1)\mathrm{id}\right)^k \psi_0\right)_{k\in\mathbb{N}}$ which has $\phi_0^{(n)}$ as fixed point. Remark: the found ground state $\phi_0^{(n)}$ is expressed in the basis $\mathcal{B}^n$, a basis change is necessary at the end of the computation to come back to the initial basis.

1.2 Studied systems

For the sake of simplicity, we choose the atomic units system where $\hbar = 1$.

1.2.1 2 or 3 level atom interacting with laser fields

To test the codes, we can first consider small Hamiltonians as a 2 or 3-level atom in interaction with laser fields in the RWA approximation:

$$H = \frac{1}{2}\begin{pmatrix} 0 & \Omega e^{\imath\varphi} \\ \Omega e^{-\imath\varphi} & 2\Delta \end{pmatrix}$$

$$H = \frac{1}{2}\begin{pmatrix} 0 & \Omega_P e^{\imath\varphi_P} & 0 \\ \Omega_P e^{-\imath\varphi_P} & 2\Delta_P & \Omega_S e^{\imath\varphi_S} \\ 0 & \Omega_S e^{-\imath\varphi_S} & 2(\Delta_P - \Delta_S) \end{pmatrix}$$

where Ω is the laser amplitude multiplied by the atomic dipolar moment amplitude, φ is the laser phase and Δ is the detuning (the level energy gap minus the energy of one photon).

1.2.2 Molecular systems in DVR representation

We consider the Hilbert space $\mathcal{H} = L^2(\mathbb{R}, dx)$ with a molecular Hamiltonian $H = H_K + \hat{V}$. In the following DVR basis:

$$u_j(x) = \frac{1}{\sqrt{(N+1)L}} \sum_{n=0}^{N} e^{\imath k_n (x - x_j)}$$

for an equipartition $0 = x_0 < x_1 < ... < x_N = L$ of $[0, L] \subset \mathbb{R}$; we have for the kinetic Hamiltonian:

$$[H_{K,DVR}]_{ij} = \frac{1}{2m} \begin{cases} \frac{\pi^2((N+1)^2+2)}{3L^2} & \text{if } i = j \\ \frac{(-1)^{j-i} 2\pi^2}{L^2 \sin^2((j-i)\pi/(N+1))} & \text{if } i \neq j \end{cases}$$

(where m is the mass); and for the potential:

$$\hat{V}_{DVR} = \begin{pmatrix} V(x_0) & & 0 \\ & \ddots & \\ 0 & & V(x_N) \end{pmatrix}$$

$x \mapsto V(x)$ being the potential function. We can consider different cases:

- Particle in a box
$$V(x) = \begin{cases} +\infty & \text{if } x = 0 \\ 0 & \text{if } x \in]0, L[\\ +\infty & \text{if } x = L \end{cases}$$
- Harmonic oscillator
$$V(x) = \frac{1}{2} k (x - \frac{L}{2})^2$$
- Vibration of the H_2^+ molecule (in the bound electronic state $^2\Sigma_g^+$):
$$V(x) = V_0 (e^{-2a(x-x_0)} - 2e^{-a(x-x_0)})$$

1.2.3 Heisenberg spin system

We consider M spins representing a magnetic medium in the Heisenberg-XXX model: $H_0 + H_{int}$

$$H_0 = \frac{1}{2}\sum_{i=1}^{M} \omega_i \sigma_{z,i}$$

$$H_{int} = -\frac{1}{4}\sum_{i=1}^{M-1}\sum_{j=i+1}^{M} J_{ij}(\sigma_{1,i}\otimes\sigma_{1,j} + \sigma_{2,i}\otimes\sigma_{2,j} + \sigma_{3,i}\otimes\sigma_{3,j})$$

where ω_i are the Larmor frequencies and J_{ij} the exchange integrals. Note that

$$A_i \equiv \mathrm{id}\otimes ... \otimes \mathrm{id} \otimes \underset{\text{position } i}{A} \otimes \mathrm{id} \otimes ... \otimes \mathrm{id}$$

$$A_i \otimes B_j \equiv \mathrm{id}\otimes ... \otimes \mathrm{id} \otimes \underset{\text{position } i}{A} \otimes \mathrm{id} \otimes ... \otimes \mathrm{id} \otimes \underset{\text{position } j}{B} \otimes \mathrm{id} \otimes ... \otimes \mathrm{id}$$

(the identity matrices being of order 2).
The simplest case is the open spin chain where only the elements $J_{i,i+1}$ are non-zero with the same value. For a closed spin chain, $J_{1,M}$ is also non-zero. The more interesting case is the spin glass where (J_{ij}) are randomly choosen in $[-J_{max}, J_{max}]$. When $\forall i,j,\ J_{ij} \geq 0$, the material is ferromagnetic; and when $J_{ij} \leq 0$ it is antiferromagnetic.

To be reasonable in the numerical computation, we can consider a number of spins equal to $M = 6$ to 12 (the matrix size being 2^M).

2 Expected deliverables

2.1 Pre-Alpha version

Code developments:

- Code Fortran functions to create the 2 and 3-level Hamiltonian matrices depending from the parameters $(\Omega, \varphi, \Delta)$ (or $(\Omega_P, \varphi_P, \Delta_P, \Omega_S, \varphi_S, \Delta_S)$.
- Code a Fortran subroutine computing by the power matrix method the ground state of an Hamiltonian, with inputs $dimH$ (matrix dimension), H (Hamiltonian), μ (shift value), ϵ (precision), k_{max} (maximum iteration order) and ouputs ϕ_0 (ground state), ϵ_0 (ground eigenvalue), $conv$ (boolean variable with value True if the algorithm has converged, False otherwise).
- Code a Fortran main program to compute the ground state of a 2 or 3 level atoms. Try to find a method to fix correctly the shift value.

Physical study:
Study the eigenvalues and the eigenvectors of the atom for different values of the parameters (you can draw with an external software graphs as $\Omega \mapsto \lambda_0(\Omega)$ for example). Compare with analytic results.

2.2 Alpha version

Code developments:

- Modify the subroutine computing the ground state by the power matrix method to compute also the first excited state and its associated eigenvalue.

- Code Fortran functions to create the Hamiltonian of a molecular system.
- Modify the main program to compute also the first excited state of an atom; and code a new main program to compute the ground state and the first excited state of a molecule.

Physical study:
Study the eigenvalues and the eigenvectors of the atomic or molecular systems for different values of the parameters. Draw the eigenvectors of molecular systems as wavefunctions of x.

2.3 Beta version

Code developments:

- Code a Fortran function or subroutine to compute the representation of an Hamiltonian in the Krilov subspace representation.
- Code a Fortran function computing the characteristic polynomial of a tridiagonal matrix.
- Code a Fortran function computing the smallest eigenvalue of an Hamiltonian by the dichotomy method.
- Code a Fortran subroutine computing the ground state of an Hamiltonian with the Lanczos method.
- Modify the main programs to replace the subroutine computing the ground state by the one using the Lanczos method.

Physical study:
Compare the results obtained with the two diagonalization methods. Study the convergence speed of the two algorithms.

2.4 Gold version

Code developments:

- Code a recursive Fortran function permetting to compute the tensor product of several matrices.
- Code Fortran functions creating the Hamiltonians of spin chains and of spin glasses.
- Modify the main programs to compute the ground state of spin systems.

Physical study:
Study the ground state of the spin systems for different values of the parameters. Try to graphically represent the ground states (for example by a lattice of arrows indicating the spin state direction onto the Bloch sphere for all spins). Compare the case of a ferromagnetic spin chain with an antiferromagnetic spin chain. Try to study the quantum entanglement between the spins in the ground state.