Constrained Imaginary Time-Step Method

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1 Imaginary Time-Step Method

In order to minimize the eigenvalues of our system we use an imaginary time-step method to iteritively improve the wavefunction at each orbital k. We bigin with the TDSE

$$i\hbar\frac{\partial\psi_k}{\partial t} = \hat{H}(t)\psi_k. \tag{1}$$

Now, by introducing discretized time $t_n = n\Delta t$ we can develop the solution for the wavefunction at time t_{n+1}

$$\psi_k^{n+1} = e^{-i\Delta t\hat{H}^n/\hbar}\psi_k^n, \tag{2}$$

where $\hat{H}^n$ signifies the hamiltonian at the n^{th} iteration. The imaginary time-step method then gains its namesake from the transformation $\Delta t \to -i\Delta t$. We can extract a trivial phase from ψ_k^n to write

$$\chi_k^{n+1} = e^{-x_0(\hat{H}^n - \epsilon_k^n)}\chi_k^n \tag{3}$$

where $x_0 = \Delta t/\hbar$. The first order expansion of the exponential in x_0 then yields the iterative scheme:

$$\chi_k^{n+1} = \mathcal{O}[\chi_k^n - x_0(\hat{H}^n - \epsilon_k^n)\chi_k^n], \tag{4}$$

where $\mathcal{O}$ indicates Gram-Schmidt orthonormalization. The index n no longer represents time steps but can be seen as iterations of an improvement on the wavefunction orbitals which minimizes the yielded eigenvalues. Similarly, x_0 no longer represents a time-step, but rather can be thought of as a damping constant, which here is set to 0.005.

2 Implementing Constraints

Next, we can implement a constraint for the system that will be taken into account at each iteration of our imaginary time-step minimization of the eigenvalues. The goal is to maintain the expectation value of an arbitraty operator

$\hat{Q}$ from one iteration to the next

$$\sum_k \left\langle \chi_k^{n+1} \right| \hat{Q} \left| \chi_k^{n+1} \right\rangle = \sum_k \left\langle \chi_k^n \right| \hat{Q} \left| \chi_k^n \right\rangle . \tag{5}$$

This expectation value is to be a fixed number Q_0. Through a Lagrange multiplier method, this constraint can be implemented by means of an additional term to the effective potential

$$\chi_k^{n+1} = \mathcal{O}[\chi_k^n - x_0(\hat{H}^n + \lambda \hat{Q} - \epsilon_k^n)\chi_k^n]. \tag{6}$$

In order to maintain accuracy while avoiding costly calculations we improve the method by calculating an intermediate step

$$\chi_k^{n+1/2} = \mathcal{O}[\chi_k^n - x_0(\hat{H}^n + \lambda^n \hat{Q} - \epsilon_k^n)\chi_k^n]. \tag{7}$$

along with the difference

$$\delta Q^{n+1/2} = \sum_k \left\langle \chi_k^{n+1/2} \right| \hat{Q} \left| \chi_k^{n+1/2} \right\rangle - \sum_k \left\langle \chi_k^n \right| \hat{Q} \left| \chi_k^n \right\rangle . \tag{8}$$

The Lagrange parameter λ is altered at each iteration to reduce this difference

$$\lambda^{n+1} = \lambda^n + c_0 \frac{\delta Q^{n+1/2}}{2x_0 \sum_k \left\langle \chi_k^n \right| \hat{Q}^2 \left| \chi_k^n \right\rangle d_0}, \tag{9}$$

where c_0 and d_0 are emperical parameters which replace the exchange terms and are chosen to be 0.9 and 7×10^{-5} respectively. The $(n+1)^{\text{st}}$ step can then be represented as

$$\chi_k^{n+1} = \mathcal{O}[\chi_k^{n+1/2} - x_0(\lambda^{n+1} - \lambda^n + \delta\lambda^n)\hat{Q}\chi_k^{n+1/2}], \tag{10}$$

where

$$\delta\lambda^n = \frac{\sum_k \left\langle \chi_k^n \right| \hat{Q} \left| \chi_k^n \right\rangle - Q_0}{2x_0 \sum_k \left\langle \chi_k^n \right| \hat{Q}^2 \left| \chi_k^n \right\rangle d_0}. \tag{11}$$

3 Example

As an example of this method, we can constrain the wavefunction to yeild

$$\sum_k \left\langle \chi_k \right| r^2 \left| \chi_k \right\rangle = r_0^2 \tag{12}$$

while also minimizing the eigenvalues. We simply replace $\hat{Q}$ in the previously described method with r^2, as well as Q_0 with r_0^2, and set $\lambda^0 = 1.0$.