Dependence of the computer time on the number of coefficients

For computing of the exact 1/*D*-series, we use the inhomoheneous equation

$$(H_0 - E_0)\psi = W\psi\,, \quad W = \delta E - \delta V\,.$$

It leads to the equation for the wavefunction at any order $n = 1,2,\ldots$:

$$(H_0 - E_0)\psi^{(n)} = \sum_{m=0}^{n} W^{(n-m)}\psi^{(m)}$$

that is solved in a matrix form.

For the problem with two independent degrees of freedom, the number of components of the vector $\psi^{(n)}$ rises as n^2, and the number of components of the matrix $W^{(n)}$ rises as $n^2 \cdot n^2$. So, the calculation of every component of $\psi^{(n)}$ needs $\sim n \cdot n^2$ summations, and the calculation of all $\sim n^2$ components of $\psi^{(n)}$ needs $\sim n^5$ summations. Thus, the calculation of all $\psi^{(n)}$, $n = 1,2,\ldots$ needs $\sim n^6$ summations. For the particular case of diamagnetic hydrogen atom, we should take into account that every component of the matrix $W^{(n)}$ represents a sum of $\sim n$ elements (since $V^{(n)}(q_1, q_2)$ represents a sum of three homogeneous polynomials of degree $n+2$, $n+1$, and n). As a result, the total number of operations rises more strongly, as n^7.

For the problem with only one independent degree of freedom, the similar estimate gives $\sim n^4$ operations (without considering the structure of every component of the matrix $W^{(n)}$). In the case of the SCF equations, every component of the matrix $W^{(n)}$ represents a sum of $\sim n$ elements (since $V^{(n)}(q_1)$ represents a sum of $\sim n$ terms of a polynomial of degree $n+2$). As a result, the total number of operations rises as n^5. Note that for one-particle spherically-symmetric problem, $V^{(n)}(q_1)$ represents a sum of only three terms, so the total number of operations rises more slowly as n^4.

Numerical evidence confirms our estimates. On the attached figure, we plot the computing time vs the number of perturbation coefficients in a double logarithmic scale. According to this numerical estimate, the time rises as $n^{6.8}$ for the exact series, and as $n^{5.2}$ for SCF series.