Analytic derivatives for UCC

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$$
\begin{aligned}
|\psi\rangle &= e^{T-T^\dagger}|0\rangle && (1)\\
E &= \langle\psi|H|\psi\rangle && (2)\\
\frac{\partial E}{\partial t_{ij}^{ab}} &= \frac{\partial\langle\psi|}{\partial t_{ij}^{ab}}H|\psi\rangle + \langle\psi|\frac{\partial H}{\partial t_{ij}^{ab}}|\psi\rangle + \langle\psi|H\frac{\partial|\psi\rangle}{\partial t_{ij}^{ab}} && (3)\\
\frac{\partial E}{\partial p} &\equiv \frac{\partial\langle\psi|}{\partial p}H|\psi\rangle + \langle\psi|\frac{\partial H}{\partial p}|\psi\rangle + \langle\psi|H\frac{\partial|\psi\rangle}{\partial p} && (4)\\
&= \frac{\partial\langle\psi|}{\partial p}H|\psi\rangle + \langle\psi|H\frac{\partial|\psi\rangle}{\partial p}. && (5)
\end{aligned}
$$

Let's focus on just one of these terms:

$$
\begin{aligned}
\frac{\partial|\psi\rangle}{\partial t_{ij}^{ab}} &= \frac{\partial}{\partial t_{ij}^{ab}}e^{T-T^\dagger}|0\rangle && (6)\\
&= \frac{\partial\left(T-T^\dagger\right)}{\partial t_{ij}^{ab}}e^{T-T^\dagger}|0\rangle && (7)\\
\frac{\partial\left(T-T^\dagger\right)}{\partial t_{ij}^{ab}} &= \frac{\partial}{\partial t_{ij}^{ab}}\left(\frac{1}{4}\sum_{ijab}t_{ij}^{ab}a^\dagger b^\dagger ji\right) && (8)\\
&= \frac{1}{4}a^\dagger b^\dagger ji && (9)\\
\frac{\partial|\psi\rangle}{\partial t_{ij}^{ab}} &= \frac{1}{4}a^\dagger b^\dagger jie^{T-T^\dagger}|0\rangle && (10)
\end{aligned}
$$

The quantum computer will give us $|\psi\rangle$ and $E|\psi\rangle = H|\psi\rangle$. Substituting $E|\psi\rangle$ into $\frac{\partial\langle\psi|}{\partial p}H|\psi\rangle$ gives: $E\frac{\partial\langle\psi|}{\partial p}|\psi\rangle$, so all we have to do is evaluate $\frac{\partial\langle\psi|}{\partial p}|\psi\rangle$ (and $\langle\psi|\frac{\partial|\psi\rangle}{\partial p}$ for the second term).

$$
\begin{aligned}
\langle\psi|\frac{\partial|\psi\rangle}{\partial t_{ij}^{ab}} &= \langle 0|e^{T^\dagger-T}a^\dagger b^\dagger jie^{T-T^\dagger}|0\rangle && (11)\\
&= \frac{1}{4}\langle 0|e^{T^\dagger-T}a^\dagger b^\dagger jie^{T-T^\dagger}|0\rangle && (12)
\end{aligned}
$$

Since this does not envolve diagonalizing H, a classical computer should surely have enough RAM to approximate $\frac{1}{4}\langle 0|e^{T^\dagger-T}a^\dagger b^\dagger jie^{T-T^\dagger}|0\rangle$, even including the first terms of the Taylor series should give a decent approximation to the derivatives. **This does not involve calculating the energy several times for various values of t_{ij}^{ab} in order to get "finite difference" derivatives.**

Alternatively, we may think about calculating $\frac{\partial|\psi\rangle}{\partial t_{ij}^{ab}}$ using linear respose theory (as we do for calculating $\frac{\partial|\psi\rangle}{\partial c_{ij}^{ab}}$ for a CI coefficient c_{ij}^{ab}).