Definitions: The AIMS wavefunction is,

$$|\Psi(x,t)\rangle \equiv \sum_I c_I(t)|\chi_I(x,t)\rangle|I\rangle$$

where $c_I(t)$ is the TBF amplitude, $|\chi_I(x,t)\rangle$ is a frozen Gaussian nuclear basis function, and $|I\rangle$ is the adiabatic electronic state.

Approximation 1: We wish to compute an arbitrary time-dependent observable depending on the nuclear coordinates,

$$\bar{O}(t) \equiv \langle\Psi(x,t)|O(x)|\Psi(x,t)\rangle$$

Plugging in, this is,

$$\bar{O}(t) = \sum_{IJ} c_I^* c_J \delta_{IJ}^{\mathrm{e}} \langle\chi_I(x,t)|O(x)|\chi_J(x,t)\rangle$$

I think an OK approximation is,

$$\bar{O}(t) \approx \sum_{IJ} c_I^*(t) S_{IJ}(t) c_J(t) O(\bar{x}_{IJ}(t))$$

Here,

$$\bar{x}_{IJ}(t) \equiv \frac{\langle\chi_I(x,t)|x|\chi_J(x,t)\rangle}{\langle\chi_I(x,t)|\chi_J(x,t)\rangle} = \frac{\alpha_I x_I(t) + \alpha_J x_J(t)}{\alpha_I + \alpha_J} = \frac{1}{2}\left[\bar{x}_I(t) + \bar{x}_J(t)\right]$$

Here the last equality holds only for $\alpha_I = \alpha_J$ (common in AIMS).

The approximation invoked above is,

$$\langle\chi_I(x,t)|O(x)|\chi_J(x,t)\rangle \approx \langle\chi_I(x,t)|O(\bar{x}_{IJ})|\chi_J(x,t)\rangle = S_{IJ} O(\bar{x}_{IJ})$$

This will be accurate if $O(x)$ varies slowly from $O(\bar{x}_{IJ})$ relative to the integration weight $\chi_I^*(x,t)\chi_J(x,t)$. In AIMS, the TBFs are quite narrow, so this is probably a fine approximation.

Approximation 2: Another possible approximation is,

$$\bar{O}(t) \approx \sum_{IJ} c_I^*(t) S_{IJ}(t) c_J(t) \frac{1}{2}\left[O(\bar{x}_I(t)) + O(\bar{x}_J(t))\right]$$

$$= \sum_I O(\bar{x}_I(t)) \sum_J \frac{1}{2}\left[c_I^*(t) S_{IJ}(t) c_J(t) + c_J^*(t) S_{JI}(t) c_I(t)\right]$$

$$\equiv \sum_I O(\bar{x}_I(t)) q_I(t)$$

This is the Mulliken-charge-based estimate, or as Todd prefers, the "bra-ket averaged Taylor approximation"