1 GFN2-xTB E^{Γ}

$$E^{\Gamma} = \frac{1}{3}\sum_{A}\sum_{\mu\in A}(q_{A,\mu})^3\Gamma_{A,\mu} \tag{1}$$

where $q_{A,\nu} = \sum_B \sum_{\nu\in B} P_{\mu\nu}S_{\mu\nu}$ is the partial charge of shell μ associated with atom A. P, S are the density and overlap matrices. $\Gamma_{A,\mu} = \Gamma_A K_\mu$ is just the product of an element specific constant and a shell specific constant, for our purposes the element is always carbon and the shell is either the first or second in GFN2 thus we have 2 numbers $\Gamma_{\text{Carbon},1(2)}$ henceforth referred to as $\mathit{\Gamma}_{1(2)}$.

Let us first rewrite the inner expression a bit given our new definition and knowledge of the atoms we are working with.

$$\sum_{\mu\in A}(q_{A,\mu})^3\Gamma_{A,\mu} = \sum_{\mu=1}^{2}(q_{A,\mu})^3\mathit{\Gamma}_\mu \tag{2}$$

We now need a unitary which computes this function on a given state $|q_{A,\mu}\rangle|\Gamma_\mu\rangle|0\rangle \rightarrow |q_{A,\mu}\rangle|\Gamma_\mu\rangle|(q_{A,\mu})^3\mathit{\Gamma}_\mu\rangle$. Consider having access to the following addition (multiplication) unitary $|A\rangle|B\rangle \rightarrow |A\rangle|A+(*)B\rangle$ as well as the unitary taking $|A\rangle \rightarrow |A^2\rangle$. We can now apply the following to get our desired unitary.

$$\text{MULT}^\dagger_{x,y}\text{SQR}^\dagger_x\text{MULT}^\dagger_{x,y}\text{ADD}_{y,z}\text{MULT}_{x,y}\text{SQR}_x\text{MULT}_{x,y}\,|q_{A,\mu}\rangle_x\,|\Gamma_\mu\rangle_y\,|0\rangle_z \tag{3}$$

$$=\text{MULT}^\dagger_{x,y}\text{SQR}^\dagger_x\text{MULT}^\dagger_{x,y}\text{ADD}_{y,z}\text{MULT}_{x,y}\text{SQR}_x\,|q_{A,\mu}\rangle_x\,|\Gamma_\mu q_{A,\mu}\rangle_y\,|0\rangle_z \tag{4}$$

$$=\text{MULT}^\dagger_{x,y}\text{SQR}^\dagger_x\text{MULT}^\dagger_{x,y}\text{ADD}_{y,z}\text{MULT}_{x,y}\,|(q_{A,\mu})^2\rangle_x\,|\Gamma_\mu q_{A,\mu}\rangle_y\,|0\rangle_z \tag{5}$$

$$=\text{MULT}^\dagger_{x,y}\text{SQR}^\dagger_x\text{MULT}^\dagger_{x,y}\text{ADD}_{y,z}\,|(q_{A,\mu})^2\rangle_x\,|(q_{A,\mu})^3\Gamma_\mu\rangle_y\,|0\rangle_z \tag{6}$$

$$=\text{MULT}^\dagger_{x,y}\text{SQR}^\dagger_x\text{MULT}^\dagger_{x,y}\,|(q_{A,\mu})^2\rangle_x\,|(q_{A,\mu})^3\Gamma_\mu\rangle_y\,|(q_{A,\mu})^3\Gamma_\mu\rangle_z \tag{7}$$

$$=\text{MULT}^\dagger_{x,y}\text{SQR}^\dagger_x\,|(q_{A,\mu})^2\rangle_x\,|\Gamma_\mu q_{A,\mu}\rangle_y\,|(q_{A,\mu})^3\Gamma_\mu\rangle_z \tag{8}$$

$$=\text{MULT}^\dagger_{x,y}\,|q_{A,\mu}\rangle_x\,|\Gamma_\mu q_{A,\mu}\rangle_y\,|(q_{A,\mu})^3\Gamma_\mu\rangle_z \tag{9}$$

$$=|q_{A,\mu}\rangle_x\,|\Gamma_\mu\rangle_y\,|(q_{A,\mu})^3\Gamma_\mu\rangle_z \tag{10}$$

$$\tag{11}$$

This circuit to compute the inner sum in E^{Γ} could be called $E^{\Gamma}_{i\ (x,y,z)}$. Let us say we are given the following state

$$\bigotimes_A(|q_{A,1}\rangle_a\,|q_{A,2}\rangle_b)\otimes(|\Gamma_1\rangle_c\,|\Gamma_2\rangle_d\,|0\rangle_e)$$

we can now apply $\prod_a E^{\Gamma}_{i\ (a,c,e)}\prod_b E^{\Gamma}_{i\ (b,d,e)}$ to get

$$\bigotimes_A(|q_{A,1}\rangle_a\,|q_{A,2}\rangle_b)\otimes(|\Gamma_1\rangle_c\,|\Gamma_2\rangle_d\,|0\rangle_e) \rightarrow \bigotimes_A(|q_{A,1}\rangle_a\,|q_{A,2}\rangle_b)\otimes(|\Gamma_1\rangle_c\,|\Gamma_2\rangle_d\,|E^{\Gamma}\rangle_e)$$