Schema of how to do in experiment

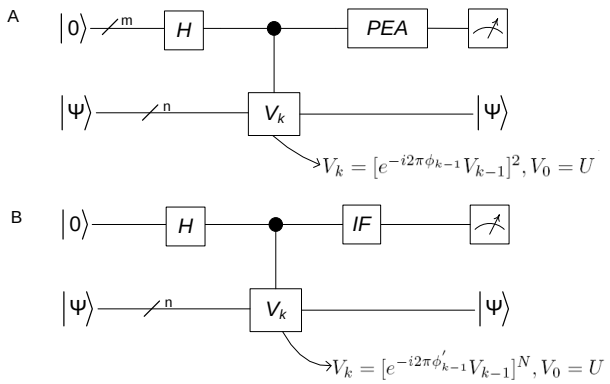

FIG. 1: Schemes to calculate the ground energy of molecules.(A) the schematic diagram of Aspuru-Guzik's proposal. (b) the diagram of our modified schema. PEA is phase estimate algorithm and IF is Interferometer. both the schemes should be iterated for many times and for each iteration the energy is calculated with a few bits of precision

the overall formula is

$$V_k = [e^{-i2\pi\phi'_{k-1}}V_{k-1}]^N, V_0 = U$$

Note that

1.ϕ is the overall real phase we are to measure

2.ϕ_k^{exp} is the value we get in the experiment in the kth iteration.

3.ϕ_k^{real} is the real value in the kth iteration that we are to measure. so $\phi = \phi_0^{real}$

4.$\phi_{errbound} = 0.014$ is the error bound which means $|\phi_k^{real} - \phi_k^{exp}| \leq \phi_{errbound}$.

5.$\phi'_k = max\{\phi_k^{exp} - \phi_{errbound}, 0\}$ is the value we use to generate the operator V_{k+1} in the $k+1$-th iteration.

6.in our experiment, $N = 8$.

so in the first iteration,

$$V_0 = U;$$

in the second iteration,

$$\begin{aligned} V_1 &= [e^{-i2\pi\phi'_0}V_0]^8 && (1)\\ &= U^8 * e^{-i2\pi(\phi'_0*8)} && (2)\\ \phi'_0 &= max\{\phi_0^{exp} - \phi_{errbound}, 0\} && (3)\end{aligned}$$

in the third iteration,

$$\begin{aligned} V_2 &= [e^{-i2\pi\phi'_1}V_1]^8 && (4)\\ &= [e^{-i2\pi\phi'_1}U^8 * e^{-i2\pi(\phi'_0*8)}]^8 && (5)\\ &= U^{64} * e^{-i2\pi(\phi'_0*64)}e^{-i2\pi(\phi'_1*8)} && (6)\\ \phi'_1 &= max\{\phi_1^{exp} - \phi_{errbound}, 0\} && (7)\end{aligned}$$

So for all the iterations

$$\begin{aligned} V_k &= U^{8^k} * \prod_{j=0}^{k-1} e^{-i2\pi(\phi'_j*8^{k-j})} && (8)\\ \phi'_k &= max\{\phi_k^{exp} - \phi_{errbound}, 0\} && (9)\end{aligned}$$

CAUTION: THE iteration number k starts from 0, not 1!!!!