I. NUMERICAL INTEGRATION

The simplest propagation scheme to integrate eq. (**??**) is the Euler integration method where

$$\underline{\rho}(t+dt) = \underline{\rho}(t) + i[\underline{h}^{rt}[\underline{\rho}(t)](t), \underline{\rho}(t)]dt - \underline{I}[\underline{\rho}(t)]dt \tag{1}$$

We want to describe small changes induced by the laser field in the system. To this end we do not directly propagate $\underline{\rho}(t)$ but rather its variation $\Delta\underline{\rho}(t) = \underline{\rho}(t) - \underline{\rho}^{eq}$. This allows us to have a code which is very sensitive to very low changes to the carriers populations and to the creation of weak polarization. In the Eluero scheme this simply amounts in subtracting $\underline{\rho}^{eq}$ on both sides of eq. (1) amd carefully write both $\underline{h}^{rt}[\underline{\rho}(t)]$ and $\underline{I}[\underline{\rho}(t)]$ as explicit functionals of the small changes. In practice $\underline{h}^{rt}[\underline{\rho}(t)]$ is linearized (this is exact for both HF and SEX with equilibrium screening), while, since $\underline{I}[\underline{\rho}(t)] \approx \underline{I}[f_{n\mathbf{k}}(t)]$, the occupations in the valence band are described in terms of holes populations $f^{(h)}_{n\mathbf{k}}$.

Moreover we observe that, during the time propagation, the most time consuming step is the evaluation of the collision integral $\mathrm{Im}[f_{n\mathbf{k}}](t)$. This is also responsible for a smooth dynamics compared to the fast oscillations of the coherent polarization controlled by the l.h.s. of eq. (**??**). This is why the time propagation is also split in two parts: the coherent and the non–coherent evolution. The time step used for both is the smaller required by the coherent evolution, however $\underline{I}[\underline{\rho}(t)] \approx \underline{I}[\underline{\rho}(t_{ref})]$ i.e. it is updated only on a longer time-step. We will discuss below how this is done in practice to respect the particle number conservation.

Let us now focus on the term $[\underline{h}^{rt}(t), \underline{\rho}(t)]dt$. In case the time dependence of $\underline{h}^{rt}(t)$ is smoother compared to the time dependence of $\Delta\underline{\rho}(t)]dt$, the term can be more efficiently replaced with an exponential integrator

$$\underline{\rho}(t+dt) = \underline{U}^{\dagger}(t,dt)\underline{\rho}(t)\underline{U}(t,dt) \tag{2}$$

$$= e^{-i\underline{h}^{rt,\dagger}(t)dt}\underline{\rho}(t)e^{i\underline{h}^{rt}(t)dt}. \tag{3}$$

The implementation is done via a Taylor expansion. This can be acheived either inserting into eq. (3) the indepent expansion of the two exponentials

$$e^{i\underline{h}^{rt,\dagger}(t)dt} \approx 1 + i\underline{h}^{rt,\dagger}(t)dt + i[\underline{h}^{rt,\dagger}(t)]^2 dt^2/2 + \ldots\ , \tag{4}$$

or directly using the expansion of eq. (3)

$$\underline{\rho}(t) + [\underline{h}^{rt}(t), \underline{\rho}(t)]dt + [\underline{h}^{rt}(t), [\underline{h}^{rt}(t), \underline{\rho}(t)]]dt^2/2 + \ldots\ . \tag{5}$$

The two agree up to the order chosen for the exansion however eq. (5) is more accurate, since it does not introduce spurious higher order terms. Moreover it can also be written in terms of $\Delta\underline{\rho}$ resulting in a sensitive scheme. However it is numerically demanding since many matrix matrix multiplications are required at each time step. One of the advantage of the exponential integrator is that it is virtually unitary (with an error decided by the truncation), at variance with the Eulero integrator which is not unitary.

An alternative unitary scheme is available, where the exponential operators are replaced by the

$$\underline{U}(t, dt) = \left[1 + i\underline{h}^{rt,\dagger}(t)dt/2\right] \left[1 - i\underline{h}^{rt,\dagger}(t)dt/2\right]^{-1} \tag{6}$$

It can be seen as an approximation to the implicit Crank–Nicolson approach with $\underline{h}$ always evaluated at time t, defined by the solution of the expression

$$[1 + i\underline{h}(t)dt]\,\underline{\rho}(t + dt) + \underline{\rho}(t + dt)\,[1 - i\underline{h}(t)dt] = [1 - i\underline{h}(t)dt]\,\underline{\rho}(t) + \underline{\rho}(t)\,[1 + i\underline{h}(t)dt]\,. \tag{7}$$

Again the solution of eq. (2) cannot be easely written in a sensitive way. Instead the direct solution of eq. (7) can be easily formulated in a sensitive way. However its solution is non trivial. Two options are available. The first via a diagonalization of $\underline{h}$ which makes the solution simple; however in the diagonalization process numerical sensitivity is lost again. The second is obtained rewriting the equation using super–indexes where commutators become matrix vector multiplications; it is numerically very sensitive but also much slower than all other approaches.