Quantum transport studies in Kadanoff-Baym approach

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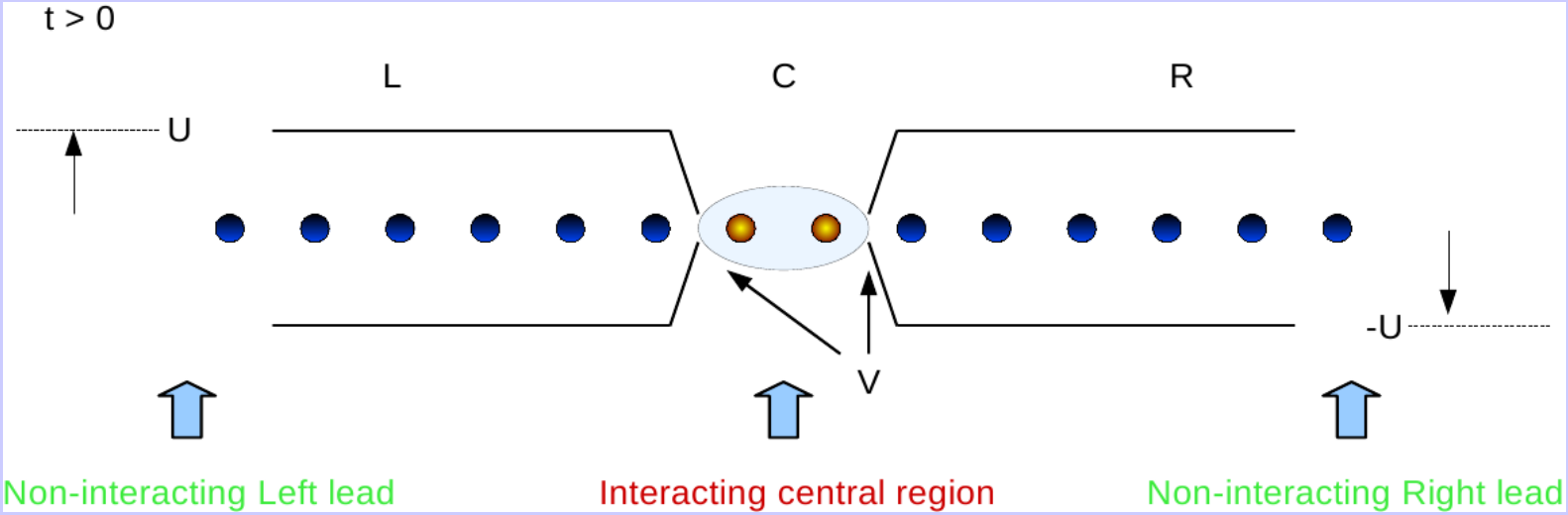
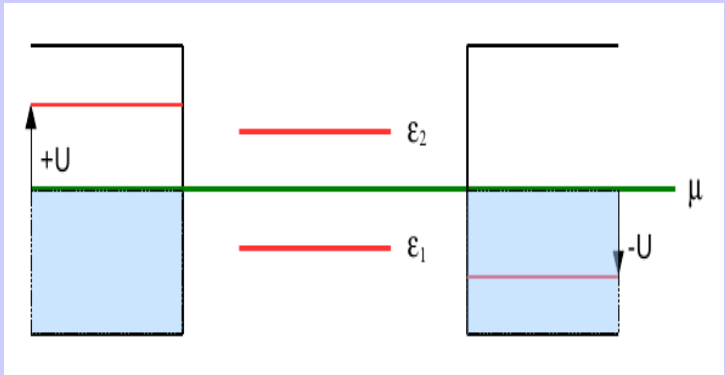
Model

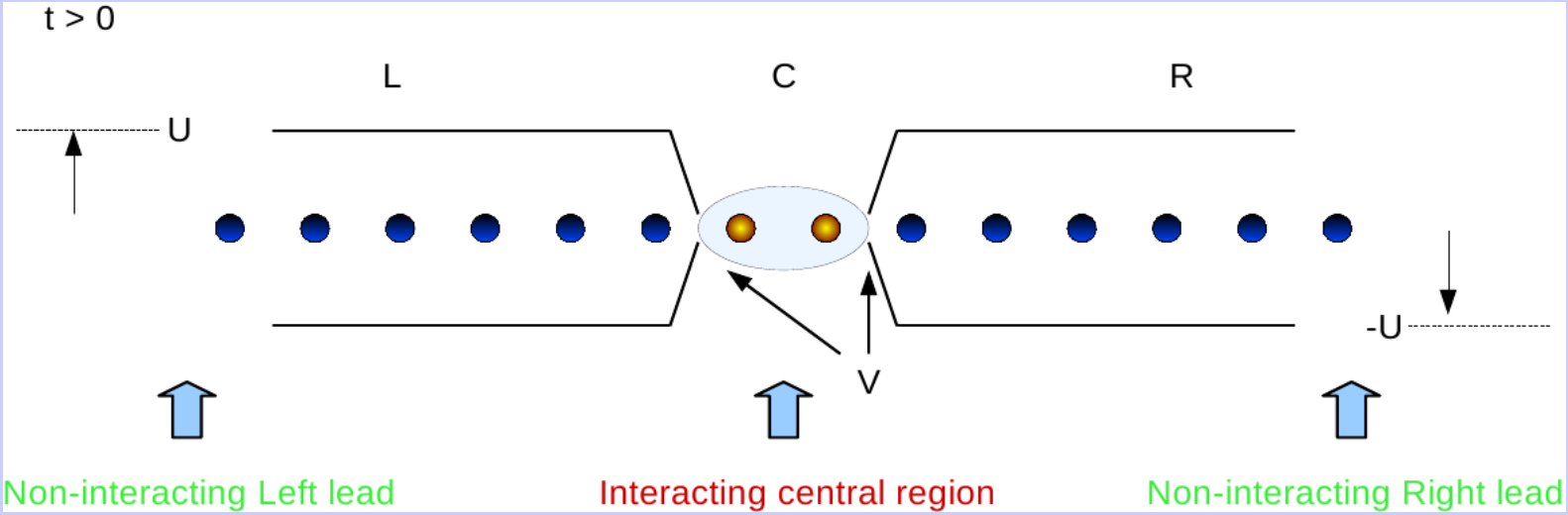


Hamiltonian

$$\hat{H}(t) = \sum_{ij,\sigma\alpha} [t_{ij}^{\alpha} + \delta_{ij} U_{\alpha}(t)] \hat{c}_{i\sigma\alpha}^{\dagger} \hat{c}_{j\sigma\alpha} + \sum_{ij,\sigma} t_{ij} \hat{d}_{i\sigma}^{\dagger} \hat{d}_{j\sigma} + \frac{1}{2} \sum_{ij,\sigma\sigma'} v_{ij} \hat{d}_{i\sigma}^{\dagger} \hat{d}_{j\sigma'}^{\dagger} \hat{d}_{j\sigma'} \hat{d}_{i\sigma} + \sum_{ij,\sigma\alpha} V_{i,j\alpha} [\hat{d}_{i\sigma}^{\dagger} \hat{c}_{j\sigma\alpha} + \hat{c}_{j\sigma\alpha}^{\dagger} \hat{d}_{i\sigma}]$$



KB -equations



Equation of motion for the Green function

$$\left[i\partial_z - \mathbf{h}(z)\right]\mathcal{G}(z,z') = \delta(z,z')\mathbf{1} + \int_\gamma \left[\mathbf{\Sigma}_{\mathrm{MB}}(z,\bar{z}) + \mathbf{\Sigma}_{\mathrm{em}}(z,\bar{z})\right]\mathcal{G}(\bar{z},z')d\bar{z}$$

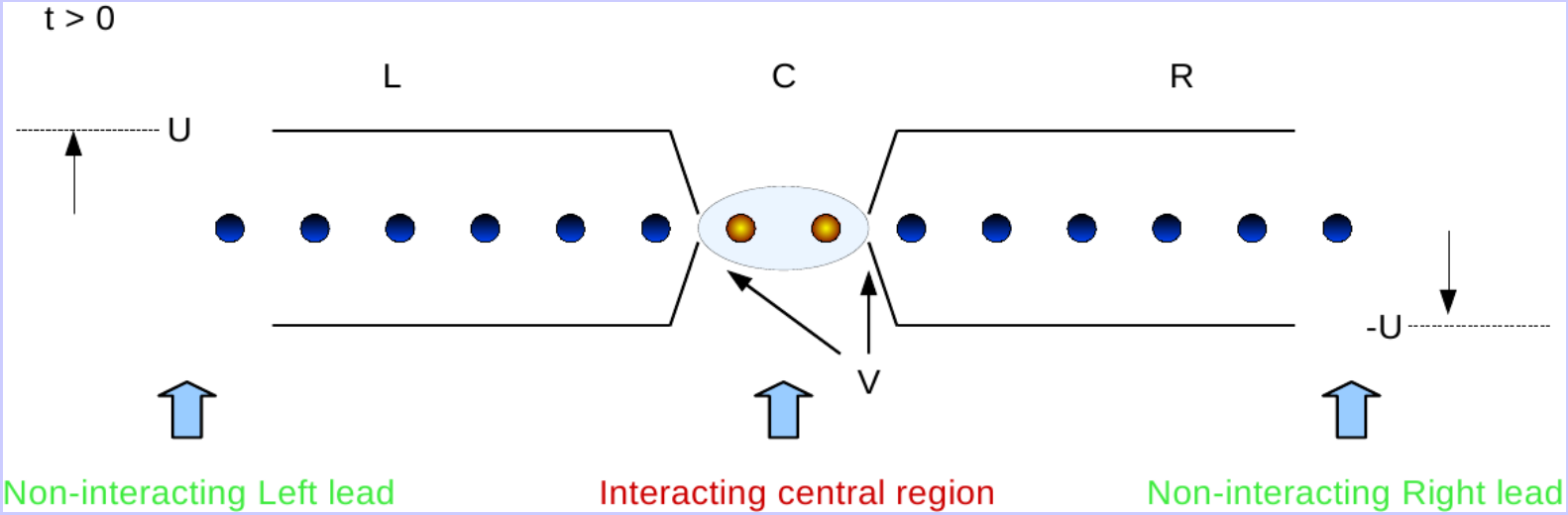
Number of particles in lead α

$$\mathrm{N}_\alpha(t) = -i\mathcal{G}^<_{\alpha\alpha}(t,t)$$

Current

$$\mathrm{I}_\alpha(t) = \frac{dN_\alpha(t)}{dt}$$

Embedding self-energy



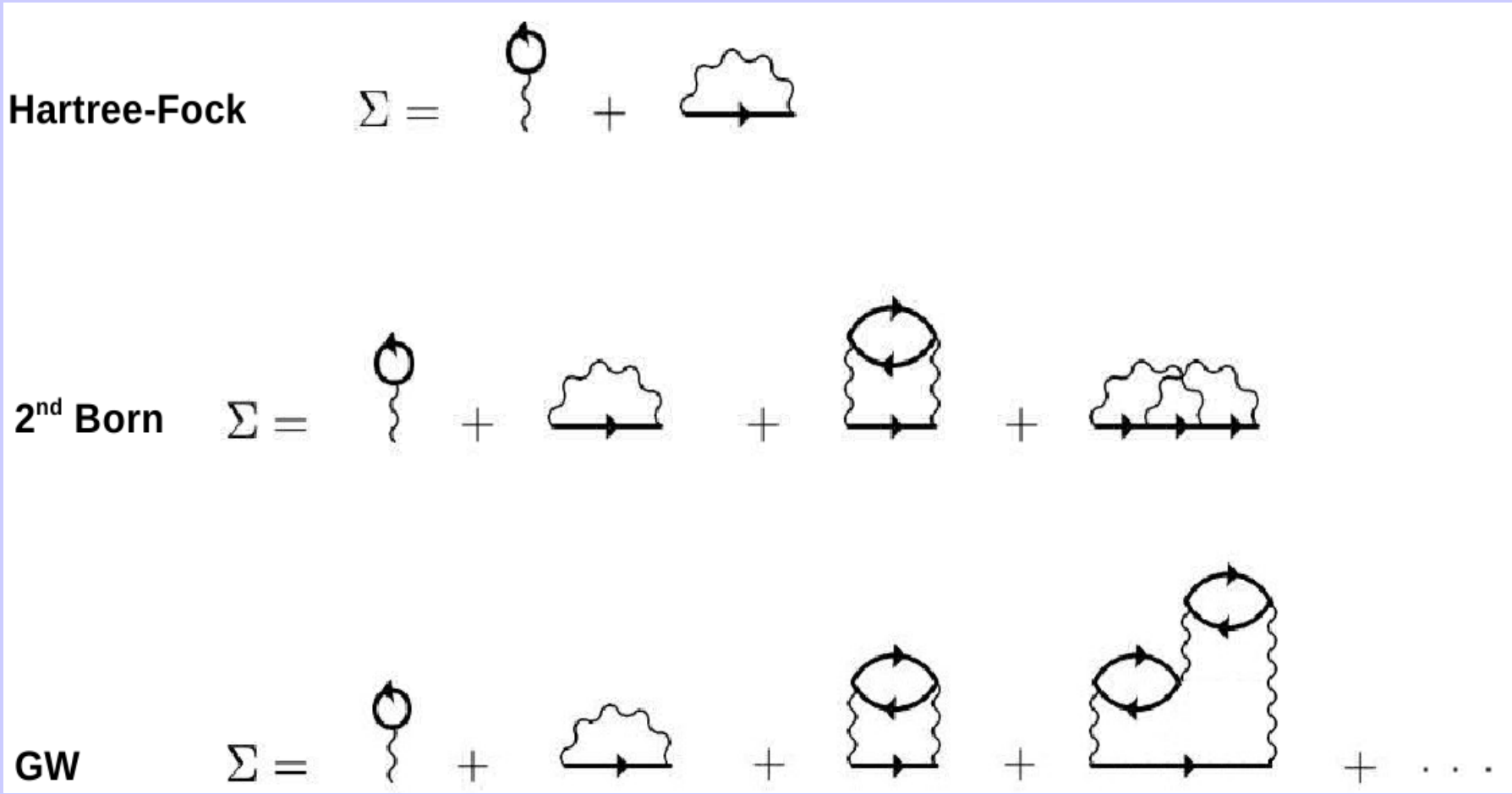
Embedding self-energy

$$\Sigma^{>}_{ij,\alpha,\mathrm{em}}(t_1,t_2) = ie^{-i\int_{t_2}^{t_1} dt\, U_\alpha(t)} \int \frac{d\epsilon}{2\pi} (f(\epsilon)-1)\Gamma_{ij,\alpha}(\epsilon) e^{-i\epsilon(t_1-t_2)}$$

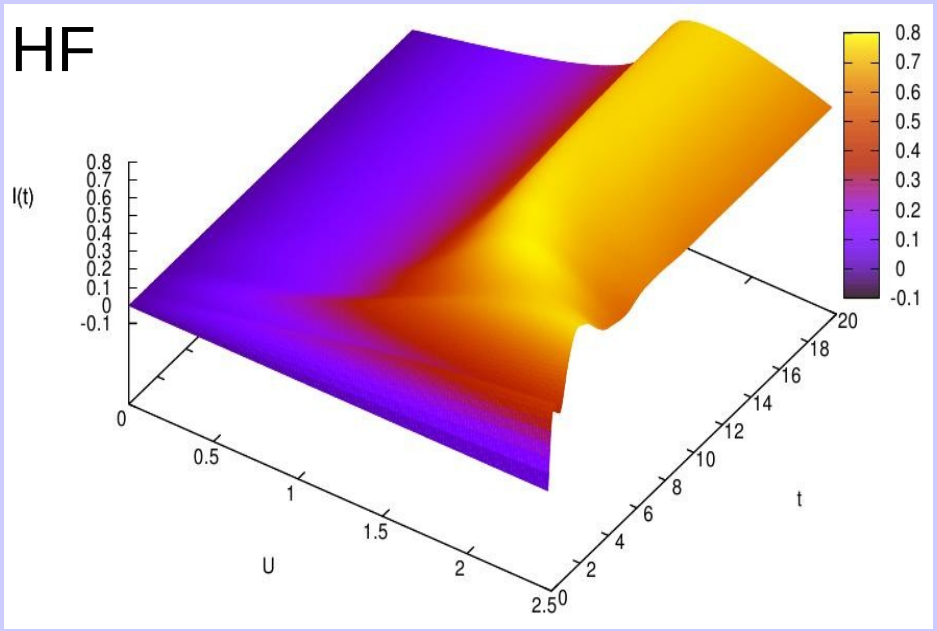
$$\Sigma^{<}_{ij,\alpha,\mathrm{em}}(t_1,t_2) = ie^{-i\int_{t_2}^{t_1} dt\, U_\alpha(t)} \int \frac{d\epsilon}{2\pi} f(\epsilon)\Gamma_{ij,\alpha}(\epsilon) e^{-i\epsilon(t_1-t_2)}$$

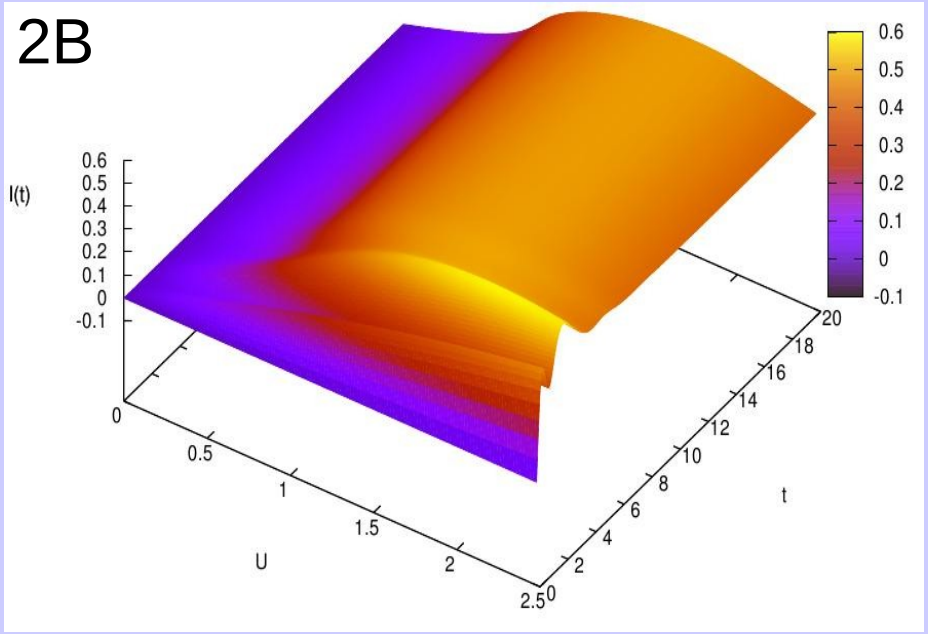
with $\Gamma_{ij,\alpha}(\epsilon) = 2\pi \sum_k V_{i,k\alpha} V_{k\alpha,j}\, \delta(\epsilon - \epsilon_{k\alpha})$

Approximations for many-body self energy

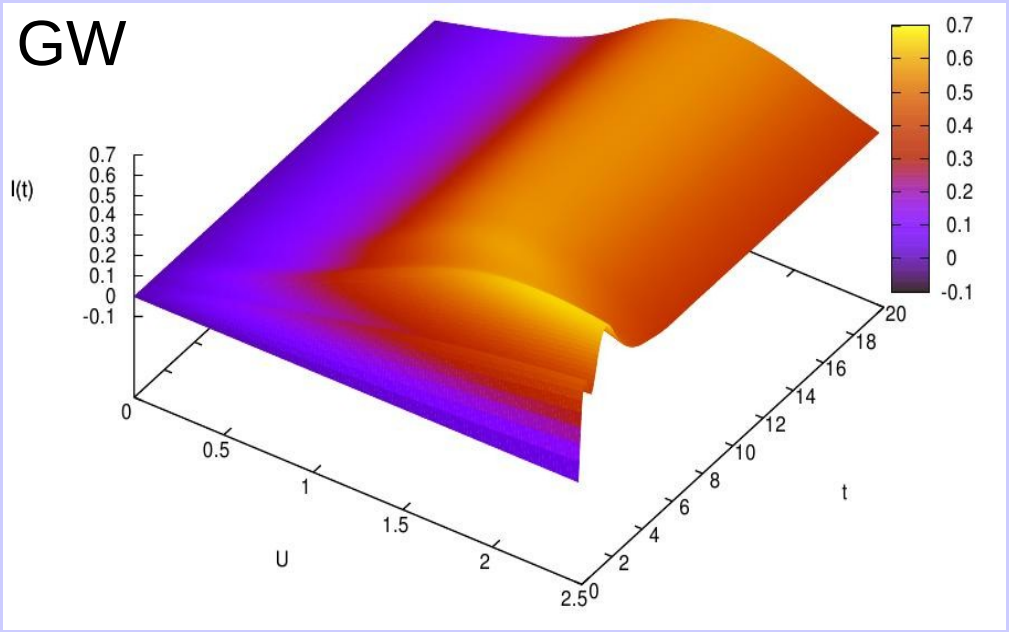


Results

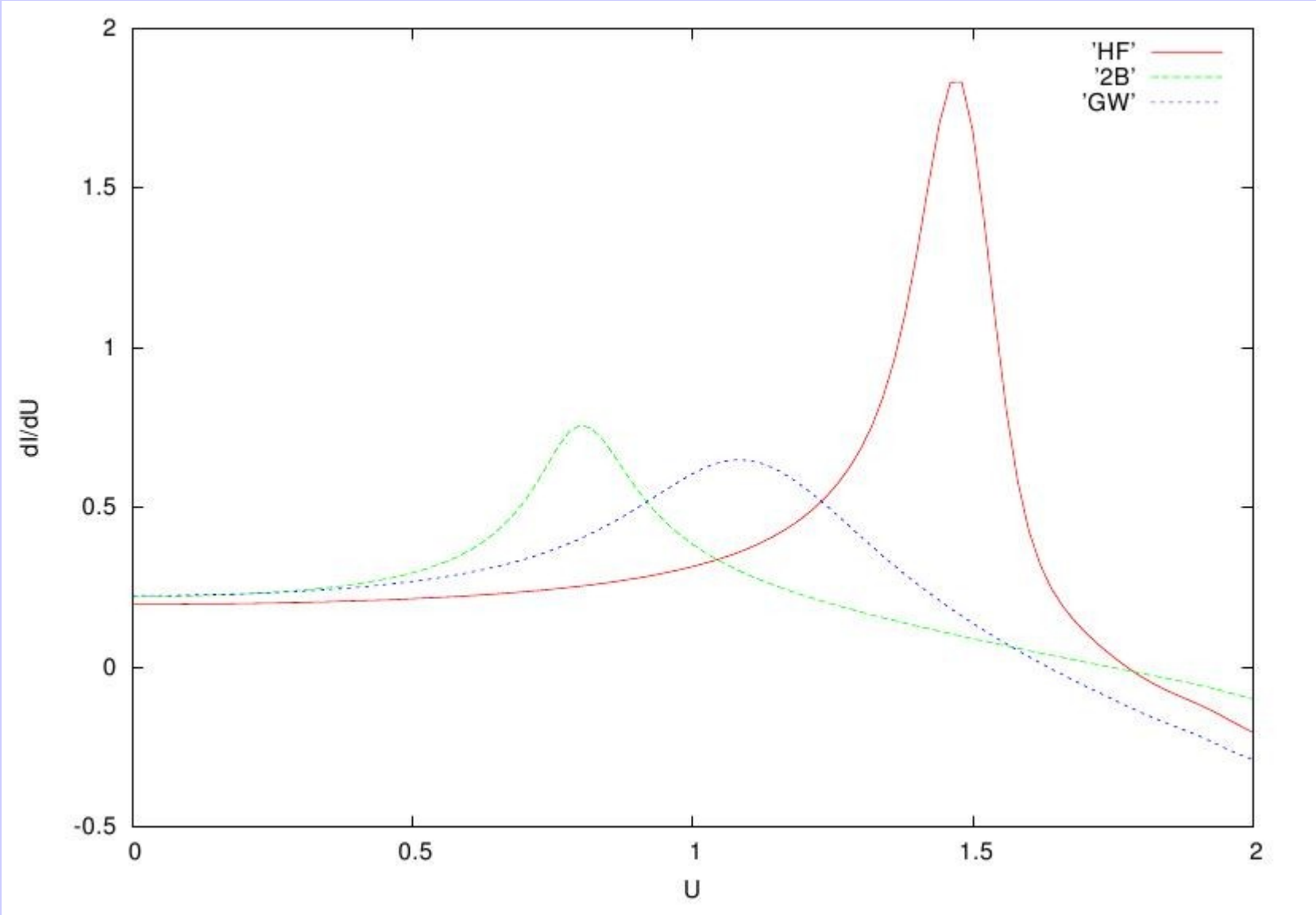




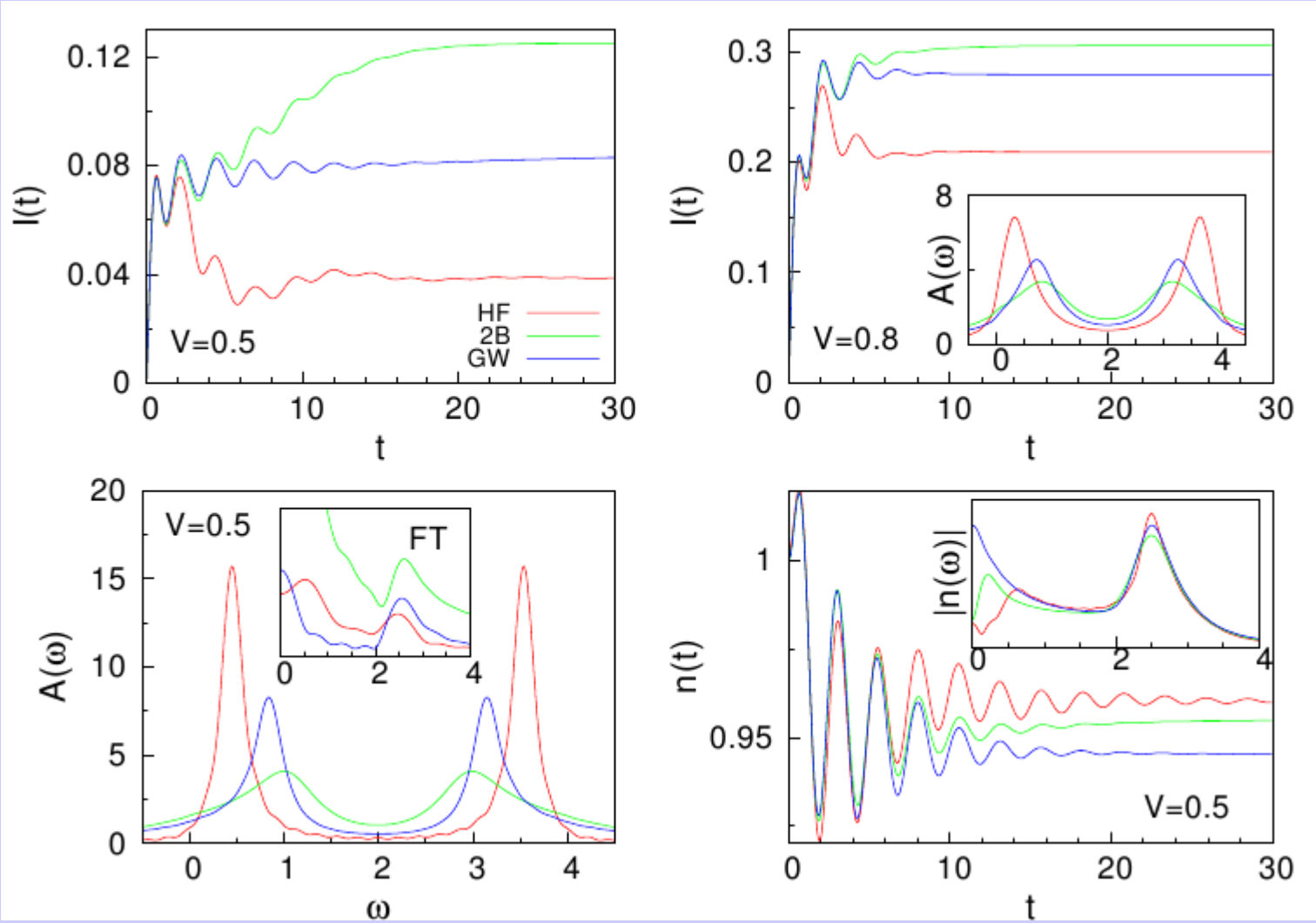
V=1.0



Results

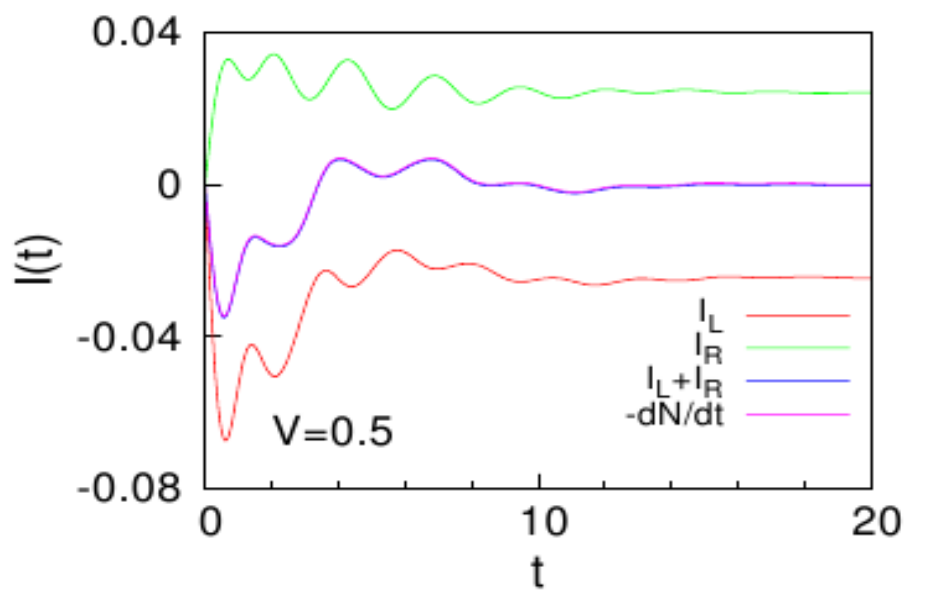


Results

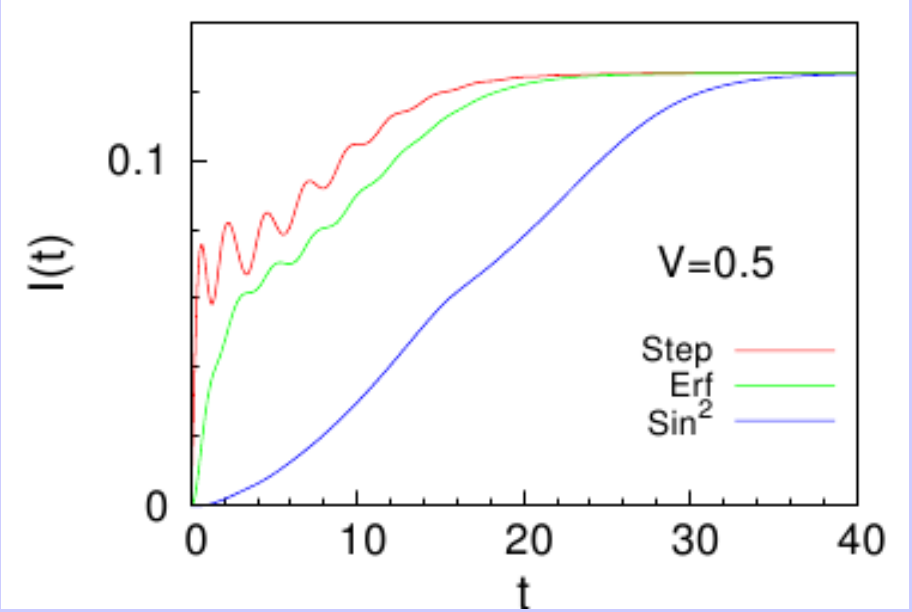


Results

Particle number conservation



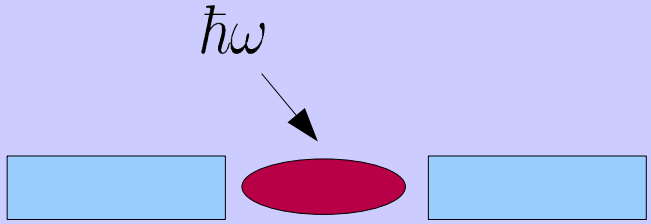
Different switch-on of bias



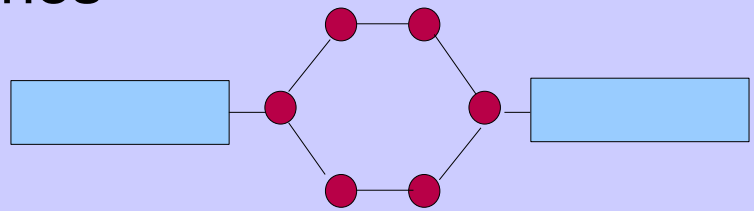
Applications / To do's / Visions

Bound state oscillations

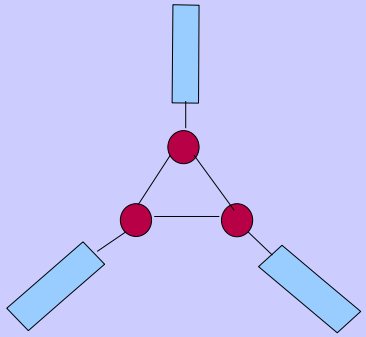
Optical properties



Long atom chains & different geometries



Multiple terminals



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Audience

Thank you!