Time-dependent quantum transport in the Kadanoff-Baym approach

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Method

Kadanoff-Baym equations:

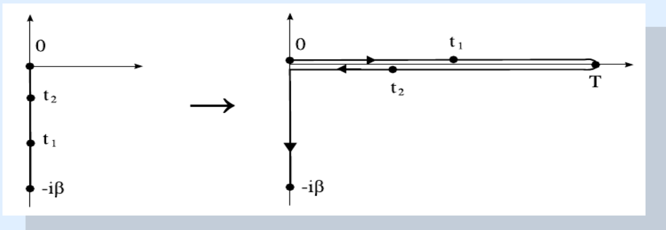
Equation of motion for the Green function

$$[i\partial_z - h(z)]G(z,z') = \delta(z,z') + \int_c d\bar z[\Sigma_{\mathrm{MB}}(z,\bar z) + \Sigma_{\mathrm{emb}}(z,\bar z)]G(\bar z,z')$$

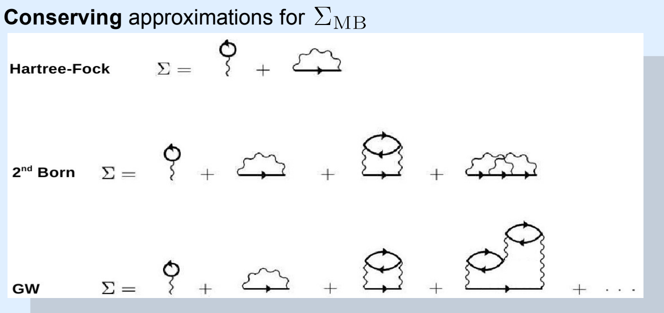
many-body effects

Effects from the leads (embedding)

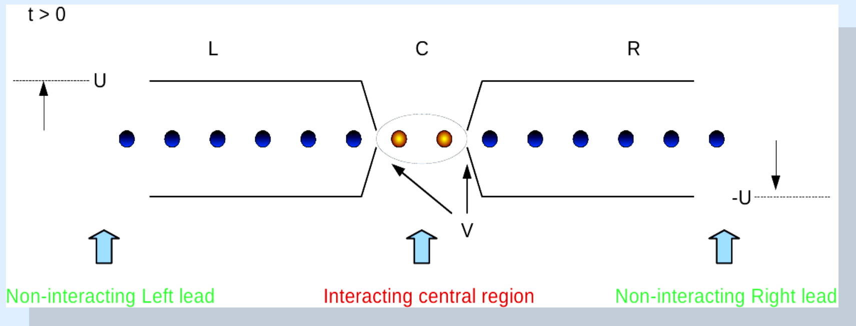
Keldysh-contour



Conserving approximations for Σ_{MB}



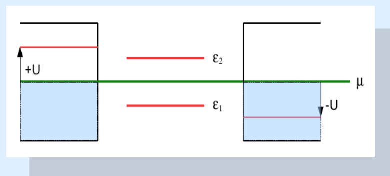
Model



Hamiltonian for the whole system

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

Level view of the biased system



Spectral function

$$A(T,\omega) = -\mathrm{Tr}\,\mathrm{Im}\int \mathrm{d}t\, e^{i\omega t}[G^> - G^<](T+\frac{t}{2}, T-\frac{t}{2})$$

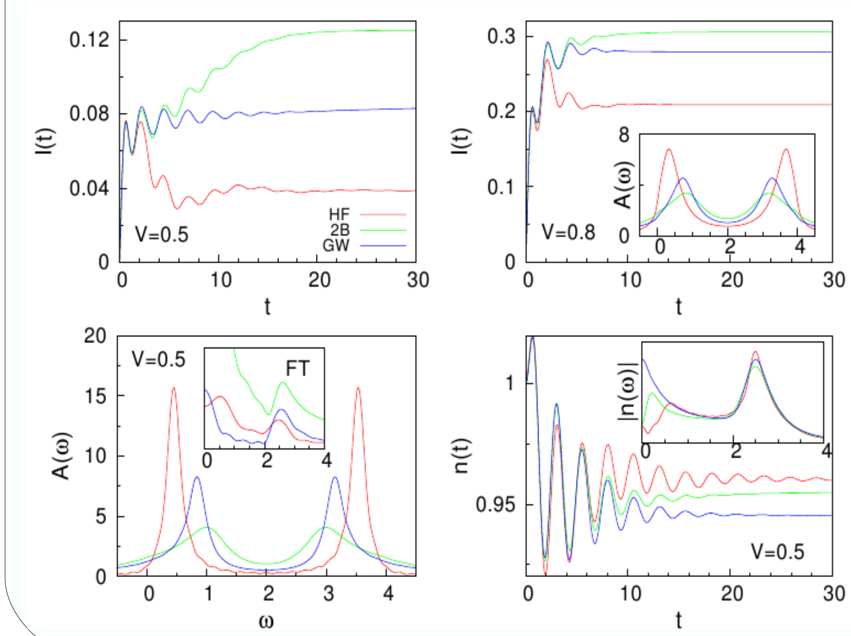
$$T = (t_1+t_2)/2 \qquad t = t_1 - t_2$$

Current in lead α is obtained from

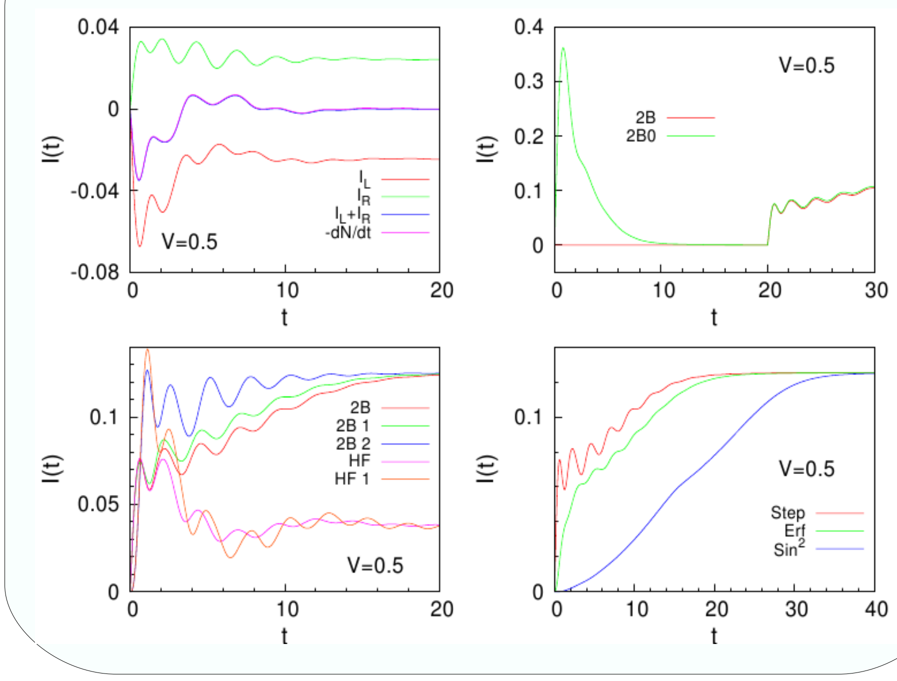
$$I_\alpha(t) = -2\mathrm{Re}\,\mathrm{Tr_C}[G^< \cdot \Sigma^A_{\alpha,\mathrm{emb}} + G^R \cdot \Sigma^<_{\alpha,\mathrm{emb}} + G^\rceil \star \Sigma^\lceil_{\alpha,\mathrm{emb}}](t,t)$$

Initial correlations and memory

Transients and spectral structure



Initial correlations and memory



Conclusions

- The KB equations provide a powerful tool to study correlated quantum transport in real time
- The method allows for inclusion of many-body correlations while satisfying important conservation laws
- Many-body interactions have large effects on steady-state and transient currents
- The temporal features in the transients and density distributions were analyzed in detail and related to level structure displayed in the spectral functions
- The memory terms have a large effects on the time-dependent currents
- Provides benchmark results for TDDFT-QT
- KB equations offer a way to construct **conserving** xc-functionals with **memory** in TDDFT [U.von Barth,N.E.Dahlen,R.van Leeuwen and G.Stefanucci, Phys.Rev.B **72**, 235109 (2005)]

References

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