**Charge and Energy Transport through Quantum Dots**

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**Motivation**

- Interaction is expected to strongly modify transport properties of molecular or nanoscale systems.
- Numerically exact methods (e.g., td-DMRG [1]) are exceedingly time consuming and often restricted to single or few-site systems.
- Analytical solutions are rare and limited to very special cases [2].

⇒ Apply Hartree-Fock (HF) approximation to non-equilibrium transport and benchmark results with exact methods.

**Spinless Fermion Model**

Hamiltonian of the central molecule

\[ \hat{H}_C = -t_0 (\hat{c}^{\dagger}_{a+1} \hat{c}_a + h.c.) + U \left( \hat{n}_{a+1} - \frac{1}{2} \right) \left( \hat{n}_a - \frac{1}{2} \right) \]

Charge current

\[ \hat{I} = i e t' (\hat{c}^{\dagger}_{a+1} \hat{c}_a - h.c.) \]

Density matrix

\[ \hat{\rho}_0 = Z^{-1} e^{-\beta E_m (\hat{H}_L - \mu \hat{N}_L) + \beta \hat{C}\hat{C} - \beta \beta (\hat{H}_R - \mu \hat{N}_R)} \]

\[ \hat{\rho}(t) = e^{-iHt} \hat{\rho}_0 e^{iHt} \]

Equal-time Green’s function

\[ G_{lm}(t) = \langle \hat{c}^{\dagger}_{m} \hat{c}_{n} \rangle = \text{Tr}[\hat{\rho}(t) \hat{c}^{\dagger}_{n} \hat{c}_{m}] = I(t) \]

**How to Treat Interaction?**

**A) Hartree-Fock approximation**

\[ \hat{n}_1 \hat{n}_{1+1} = \langle \hat{n}_1 \rangle \hat{n}_{1+1} + \langle \hat{n}_{1+1} \rangle \hat{n}_1 - \langle \hat{c}^{\dagger}_{1+1} \hat{c}_1 \rangle \langle \hat{c}^{\dagger}_{1+1} \hat{c}_1 \rangle - \langle \hat{c}^{\dagger}_{1} \hat{c}_{1+1} \rangle \langle \hat{c}^{\dagger}_{1} \hat{c}_{1+1} \rangle \]

**B) Hubbard-Stratonovich transformation**

Trotter breakup

\[ e^{-iHt} = \left( e^{-i(\hat{T}/2 + \hat{V} + \hat{T}/2)\Delta t} \right)^M \approx \left( e^{-i\hat{T}\Delta t/2} e^{-i\hat{V}\Delta t} e^{-i\hat{T}\Delta t/2} \right)^M \]

Auxiliary Ising field [3]

\[ e^{-iU(\hat{n}_1 - 1/2)(\hat{n}_{1+1} - 1/2)\Delta t} = \frac{1}{2} e^{-iU\Delta t/4} \sum_{\sigma = \pm 1} e^{-i\alpha(\hat{n}_1 - \hat{n}_{1+1})\Delta t} \]

**I-V Characteristics and Transmission**

- Left figure: I-V characteristics for several values of the interaction \( U, \beta = 8/t_0 \) and \( t' = 0.5t_0 \). HF (lines) vs. Hubbard-Stratonovich (symbols).
- Right figure: HF transmission coefficient \( T(E) \) against the energy \( E \) for different values of \( U \) and zero voltage \( V \).

⇒ Landauer formula

\[ I = \frac{e}{\hbar} \int dE T(E,V)[f_L(E) - f_R(E)] \]

with

\[ f_{L,R}(E) = \left( 1 + e^{E - \mu_{L,R}} \right)^{-1} \]

**Time-Dependent Currents**

- Current as function of time for \( \beta = 8/t_0, t' = 0.5t_0 \), and various values of \( U \). HF (lines) vs. Hubbard-Stratonovich (symbols).
- Left figure: \( V = t_0/e \), right figure: \( V = 4t_0/e \).
- Arrows indicate HF results for infinitely long leads.

**Summary**

- The HF approximation is a computationally cheap and versatile approach to calculate I-V characteristics of correlated systems at finite temperatures.
- For a simple spinless fermion model, the HF data agree reasonably well with available exact results, with the exception of the large voltage regime.
- Generalization to larger systems, temperature gradients, interacting leads, and energy or heat transport is straightforward.

**References**