Transient magnetic tunneling mediated by molecular bridge

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This paper extends our recent theoretical study [1] of transient currents through molecular bridges to magnetic tunneling. We calculate the excess magnetic current carried by a molecular bridge shunting the magnetic junction. The system is represented by two ferromagnetic electrodes bridged by a molecular size island with a few discrete electronic levels and a local Hubbard type correlation. The island is linked to the electrodes by tunneling junctions. One of the junctions is permanent, the coupling strength of the other one is assumed to undergo rapid changes modulating the connectivity of the system. The resulting sudden switching events give rise to transient magnetic currents and changes of magnetisation at the island. They depend on the constant galvanic bias between the electrodes. Depending on the time scale of the switching series, the transients are dominated by the initial quantum correlations, or reach the kinetic stage controlled by a simple relaxation mechanism.

We employ the non-equilibrium Green’s functions. The finite-time correlated initial conditions are taken into account using the partitioning-in-time method developed previously [1]. The numerical solution is obtained solving the real-time Dyson equation in the integro-differential form self-consistently. For long time asymptotics, a Generalized Master Equation is matched to the initial stage solution.

Our work: numerical solution of the real-time Dyson equation in the integro-differential form self-consistently to obtain transient changes of magnetisation of the island.

**REFERENCES**


**PRECURSOR EQUATION**

\[ i \frac{d}{dt} G_\sigma(t,t') = \left( \epsilon_b - iU G_\sigma(t,t') \right) G_\sigma(t,t') + \int_0^{t_0} d\tau \Sigma_\sigma^R G_\sigma(t,t') + \int_0^{t_0} d\tau \Sigma_\sigma^A G_\sigma(t,t') \]

\[ \Sigma_\sigma^R = G_\sigma^R \Sigma_\sigma^< G_\sigma^R \]

\[ \Sigma_\sigma^A = G_\sigma^A \Sigma_\sigma^< G_\sigma^A \]

**Test of the GKBA**

Island level occupancies and at a fixed bias 0.5 V as a function of time for Hubbard U=0 eV (left) and U=0.6 eV (right)

To close a precursor equation, GKBA is used (⇒ closed GME eq.)

\[ G_\sigma(t,t') = -G_\sigma^R(t,t') \rho_\sigma(t) + \rho_\sigma(t) G_\sigma^A(t,t') \]