Non-equilibrium properties of a Mott insulator in an external electric field

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1 Motivation

- Most electronic devices (transistors, Josephson junctions etc.) have a nonlinear current-voltage relation.
- Devices become smaller, of order or below $100nm$. A potential difference of $1V$ produces an electric field $E \sim 10^7 V/cm$ for nanometer scaled devices.
- High density energy short time pulsed laser experiments, fields $E \sim 10^{10} V/cm$. It is important to study the relaxation to equilibrium.
- Some strongly correlated materials, for example inorganic semi-conductor Sr_2CuO_3, have a strong potential for high bit-rate all-optical switching.
- The Falicov-Kimball model was applied to describe some experimental systems, e.g. $YbInCu_4$, $EuNi_2(Si_{1-x}Ge_x)_2$, Ta_xN, and SmB_6, in equilibrium.
- It is important to generalize the solution on the non-equilibrium case.

2 The Falicov-Kimball model

The Hamiltonian:

$$\mathcal{H} = -\sum_{<i,j>} t_{ij} c_i^\dagger c_j + U \sum_i w_i c_i^\dagger c_i.$$

(A. Georges et al, Rev. Mod. Phys. **68**, 13 (1996), J.K. Freericks, V. Zlatic, Rev. Mod. Phys. **75**, 1333 (2003)).

Electric field:

$$\mathbf{E}(\mathbf{r},t) = -\frac{1}{c}\frac{\partial \mathbf{A}(\mathbf{r},t)}{\partial t}.$$

The Peierls substitution:

$$t_{ij} \to t_{ij} \exp\left[-\frac{ie}{\hbar c}\int_{\mathbf{R}_i}^{\mathbf{R}_j} \mathbf{A}(\mathbf{r},t) d\mathbf{r}\right].$$

The vector potential: $\mathbf{A}(t) = A(t)(1, 1, ..., 1)$.

The free electron spectra:

$$\epsilon_{\mathbf{k}} = -2t \sum_l \cos\left[a\left(k^l - \frac{eA^l(t)}{\hbar c}\right)\right]$$

is proportional to

$$\epsilon(\mathbf{k}) = -t^* \sum_l \cos(ak^l)/\sqrt{d}$$

and

$$\bar{\epsilon}(\mathbf{k}) = -t^* \sum_l \sin(ak^l)/\sqrt{d}.$$

$t = t^*/2\sqrt{d}$ in the limit $d \to \infty$.

Two energy density of states:

$$\rho_2(\epsilon, \bar{\epsilon}) = \frac{1}{\pi t^{*2} a^d} \exp\left[-\frac{\epsilon^2}{t^{*2}} - \frac{\bar{\epsilon}^2}{t^{*2}}\right]$$

(P.Schmidt, Diplome thesis, University of Bonn, 2002).

3 Main equations

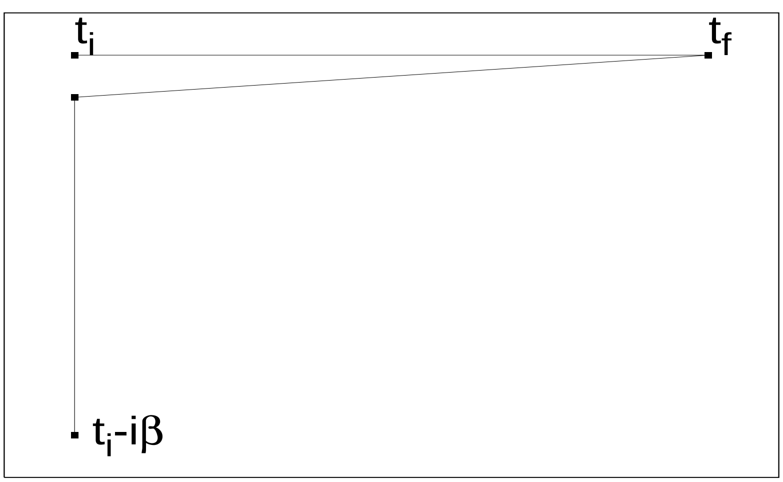
$$g = \int d\epsilon \int d\bar{\epsilon} \rho_2(\epsilon, \bar{\epsilon}) \left[g_0^{-1}(\epsilon, \bar{\epsilon}) - \Sigma \right]^{-1} \quad (1)$$

$$\lambda = g_{imp}^{-1} - g^{-1} - \Sigma \quad (2)$$

$$g = \frac{1 - w_1}{g_{imp}^{-1} - \lambda} + \frac{w_1}{g_{imp}^{-1}[\mu \to \mu - U] - \lambda} \quad (3)$$

$$\Sigma = g_{imp}^{-1} - g^{-1} - \lambda \quad (4)$$

The Kadanoff-Baym time contour:



4 Equilibrium results

The relative t and the average T time variables:

$$t = t_1 - t_2, \quad T = (t_1 + t_2)/2.$$

The lesser self-energy:

$$\Sigma^<(\omega, T) = \int dt e^{i\omega t} \Sigma^<(T + t/2, T - t/2).$$

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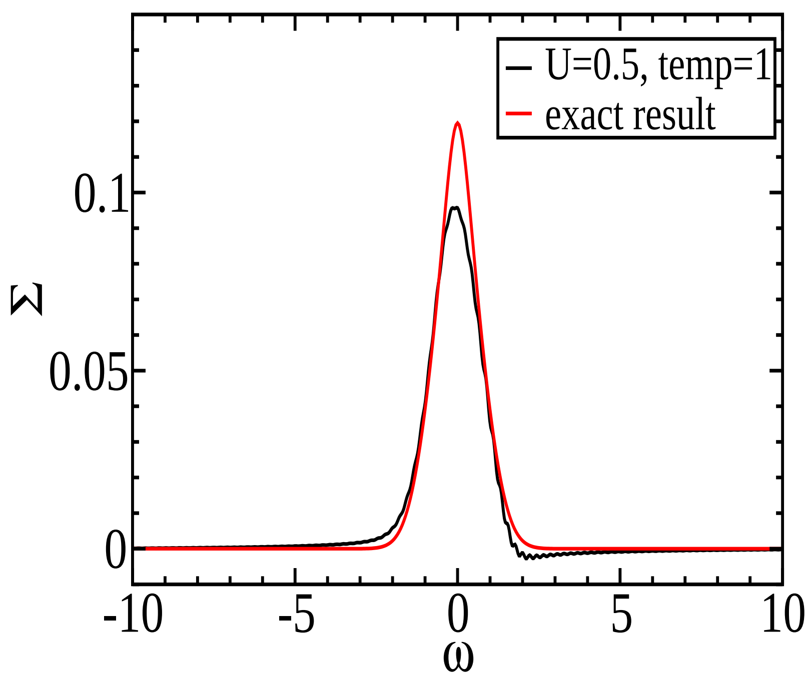
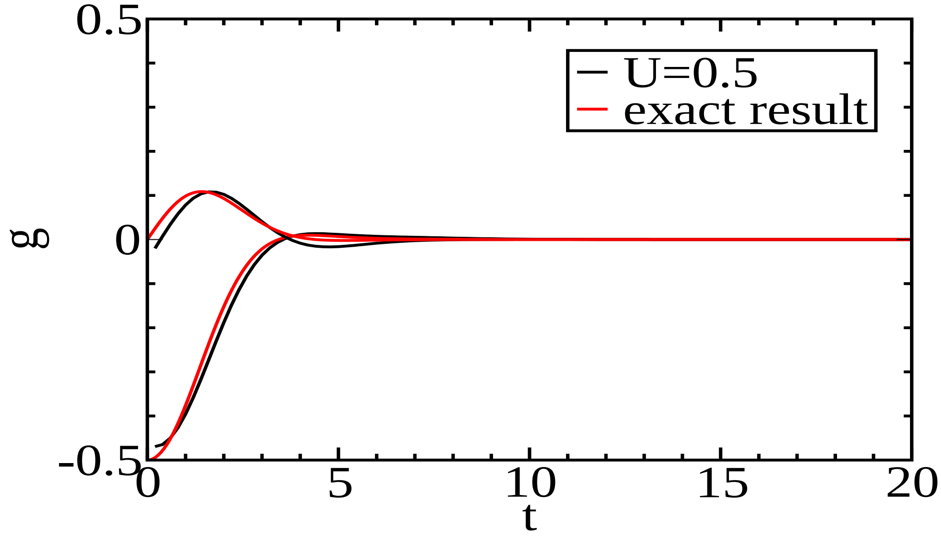
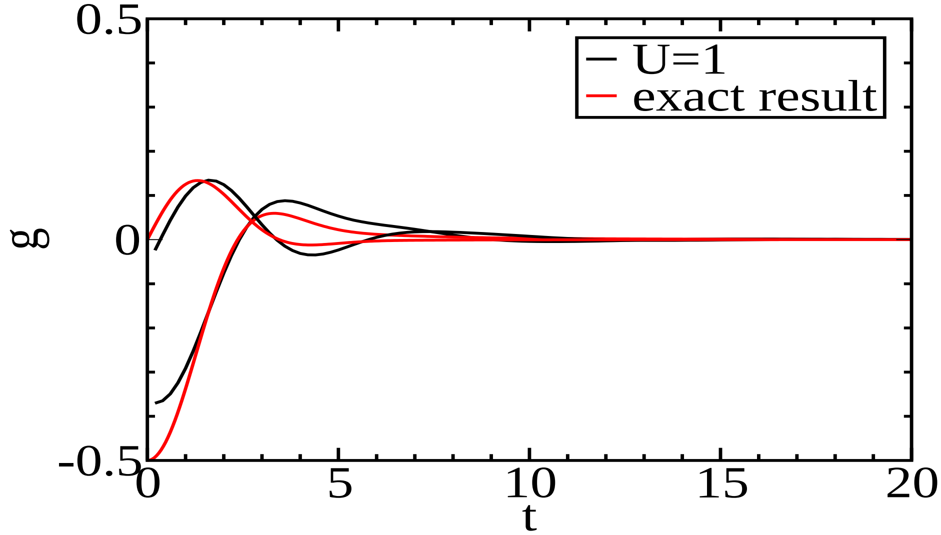


Lesser Green's function, U=0.5, β=1



Lesser Green's function, U=1, β =1



5 Time-dependence of the current

The current density $j^l(T)$ is:

$$-i\frac{eat^*}{\sqrt{d}}\sum_{\mathbf{k}}\sin\left(k^l a - \frac{eaA^l(T)}{\hbar c}\right)g(\epsilon_{\mathbf{k}}, T, T^+).$$

The total current density:

$$j(T) = \sqrt{d}j^l(T)$$

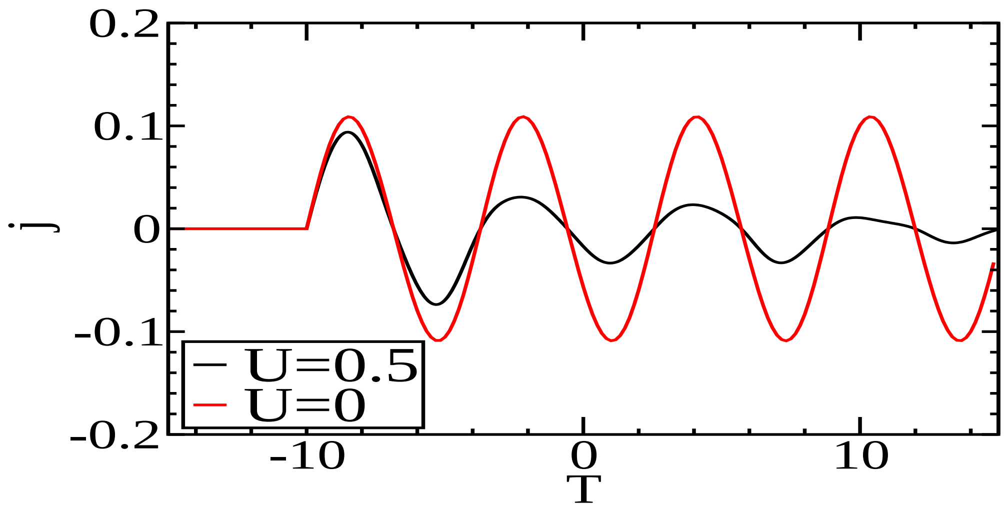
In the non-interacting limit:

$$j(T) \sim \sin\left(\frac{eaA(T)}{\hbar c}\right)\int d\epsilon\frac{df(\epsilon-\mu)}{d\epsilon}\rho(\epsilon)$$

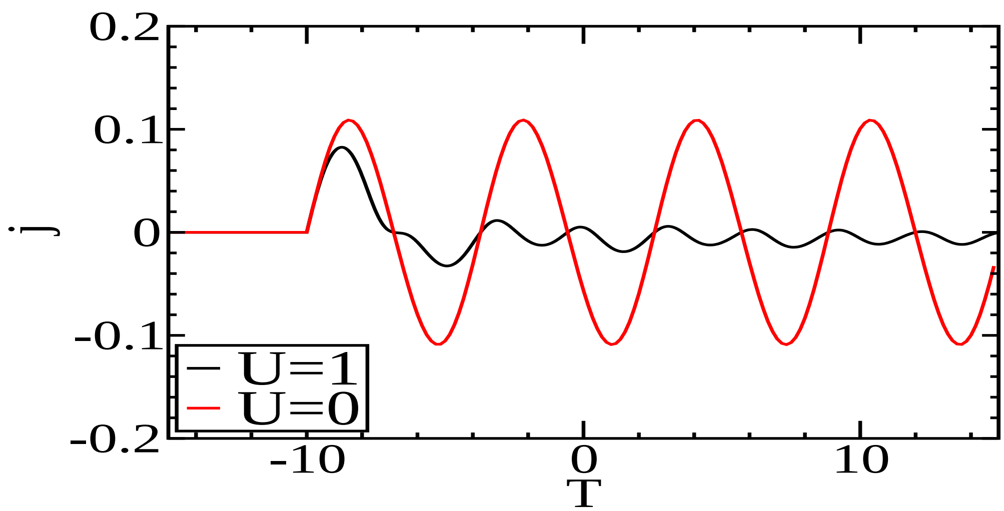
In the static case $A(T) = -EcT$ one gets the Bloch oscillations:

$$\omega_{Bloch} = eaE/\hbar.$$

Current, U=0.5, β=1, E=1



Current, U=1, β=1, E=1



6 Conclusions

- A method which allows to analyze non-equilibrium properties of the Falicov-Kimball model in $d = \infty$ in an external time-dependent electric field has been developed.
- The precision of the solution was estimated by comparing the results with the exact equilibrium results obtained by the DMFT in $d = \infty$.
- The time-dependence of the current density at different values of the on-site repulsion U was studied in the case when the constant electric field is switched on at some moment of time.
- It has been shown that the Bloch oscillations of the current density, which take place in the non-interacting case, can also survive in the case of large U when E is strong.