Nonequilibrium dynamical mean-field theory of strongly correlated electrons

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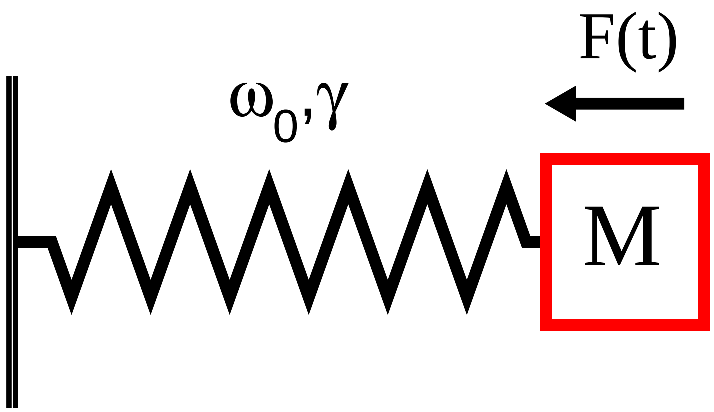
Motivation

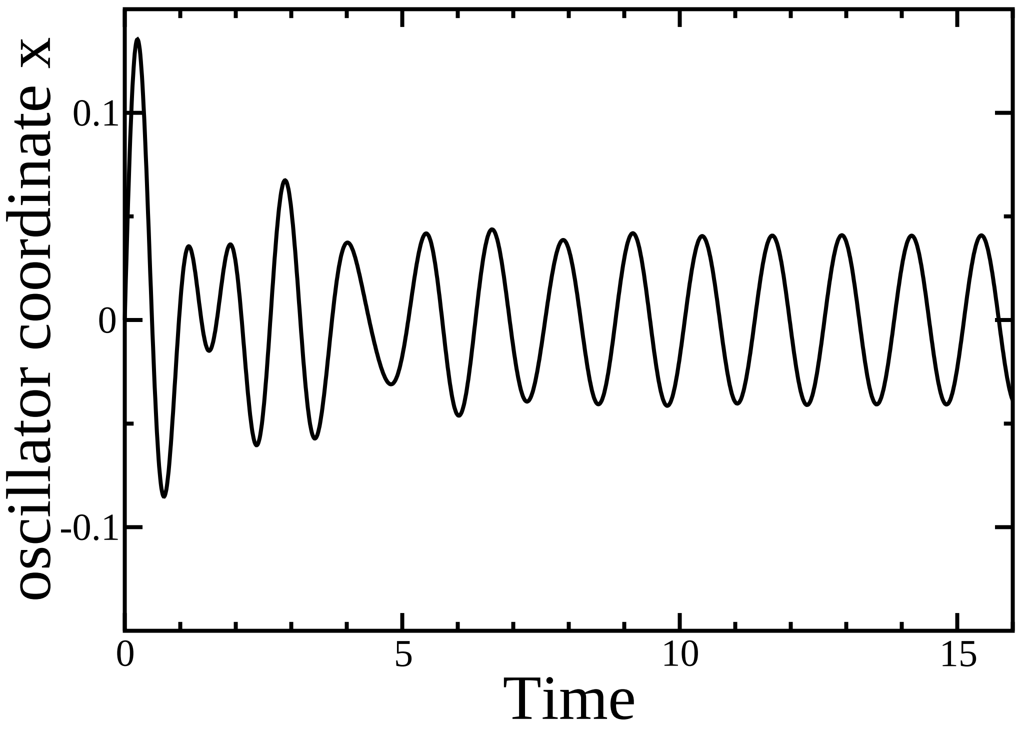
- Most electronic devices have a nonlinear current-voltage relation
- Strongly correlated materials have a great potential to be used in electronic devices due to their tunability
- As devices become smaller, of order or below $100nm$, a potential difference of $1V$ can produce an electric field of order $E \sim 10^5 - 10^6 V/cm$ or higher
- Understanding the nonlinear response of a Mott insulator has been a longstanding unsolved problem
- Modern parallel computers now have sufficient power to solve these problems (total comput. time $\sim 7 \times 10^5$ hours)

Some results for strongly correlated systems

- D=0 (quantum dot), Anderson model, Kondo model
  1. Y. Meir, N.S. Wingreen, D.C. Langreth et al
  2. P. Coleman, C. Hooley et al
  3. N. Andrei, B. Doyon, P. Mehta
- D=1
  1. two-band Hubbard ring, $\mathrm{SrCuO_3}$ (T. Ogasawara et al)
  2. breakdown of the Mott insulator (T. Oka, H. Aoki)
- D=∞
  1. iterated PT for the Hubbard model (H. Monien, P. Schmidt)
  2. nonequilibrium DMFT for the Falicov-Kimball model (J.K. Freericks, V.M. Turkowski, V. Zlatić)

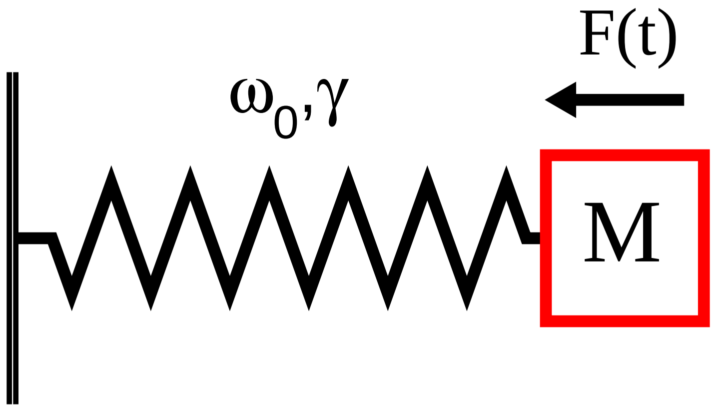
Driven damped harmonic oscillator: an example of a complicated response to an external force

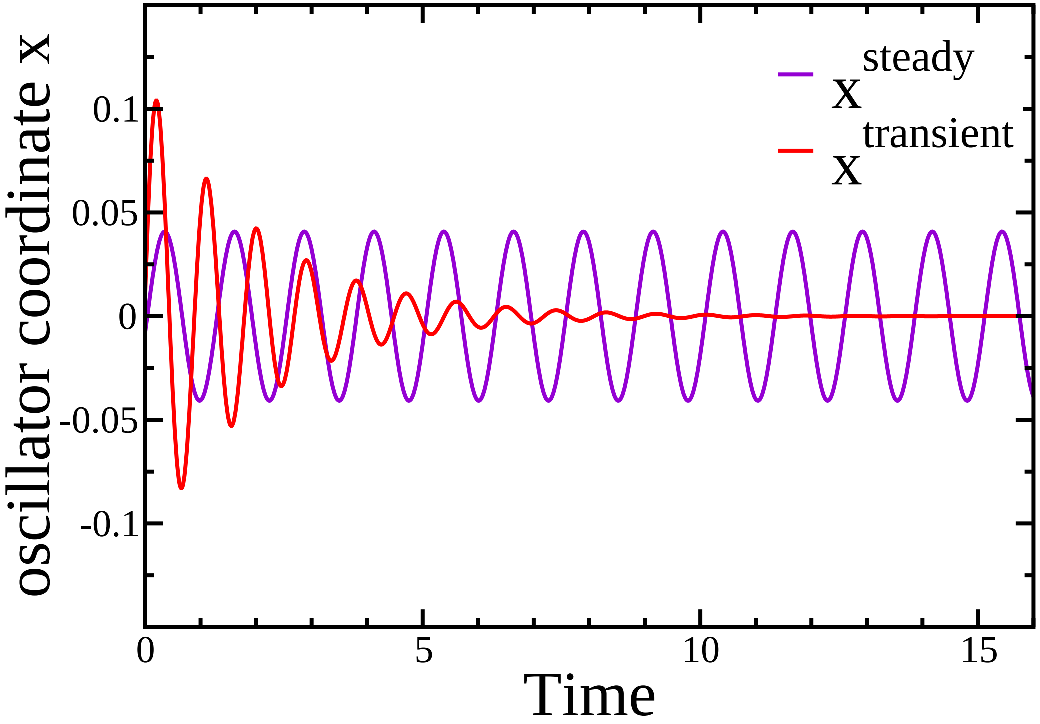




$$\ddot{x}(t) + 2\gamma\dot{x}(t) + \omega_0^2 x(t) = (F_0/M)\sin(\omega t)$$

Driven damped harmonic oscillator: separating out the transient and the steady state response

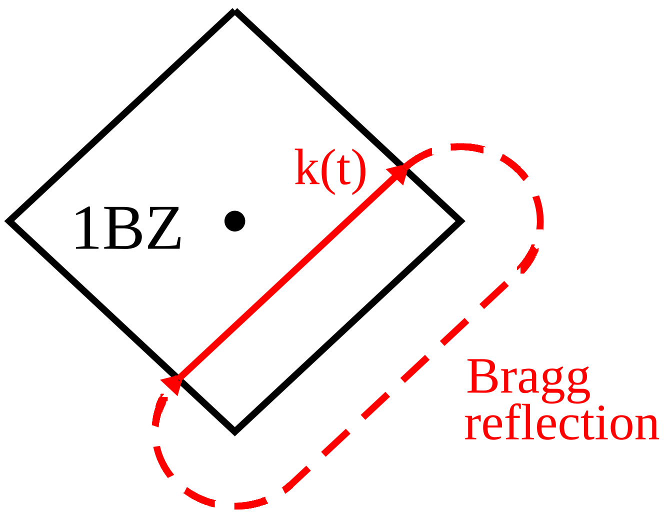




Bloch oscillations (Bloch 1928, Zener 1932)

In a semiclassical picture: $\hbar \frac{d}{dt} k(t) = eE \quad \rightarrow \quad k(t) = eEt/\hbar$

$v(k) = \nabla_k \epsilon(k)$ - the velocity also changes periodically!

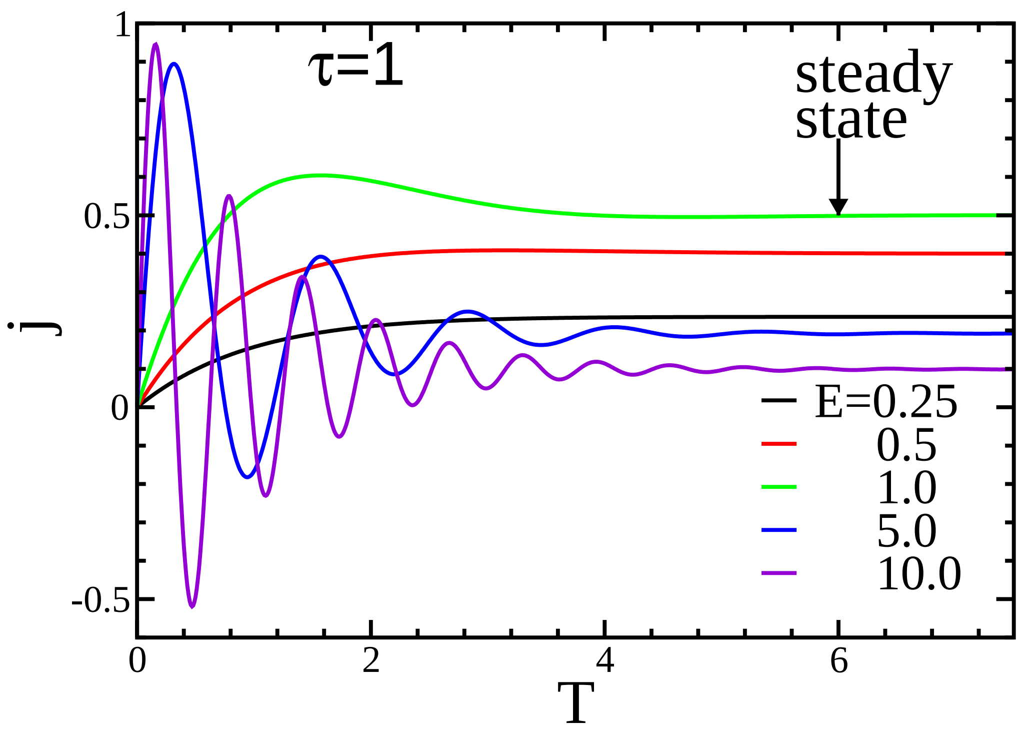


The current is periodic!

- The Bloch oscillations are prevented in realistic bulk materials due to several reasons:
  - the period of the oscillations is much longer than the scattering time: $\tau^{osc} = 2\pi\hbar/(eEa) >> \tau^{scatt} \sim 10^{-12} - 10^{-13} sec$ (requires $E > 10^7 V/cm$)
  - Zener tunneling to higher bands
  - strong Joule heating of the material ($\Delta T \sim \sigma E^2$)
  - Conventional oscilloscopes can't measure the frequencies $\omega > 10^9 Hz$ (typical observable frequencies would be $\omega_{Bloch} > 10^{12} Hz$)
- observed in semiconductor superlattices ($a \sim 10 nm$)

A semiclassical approach: The Boltzmann equation

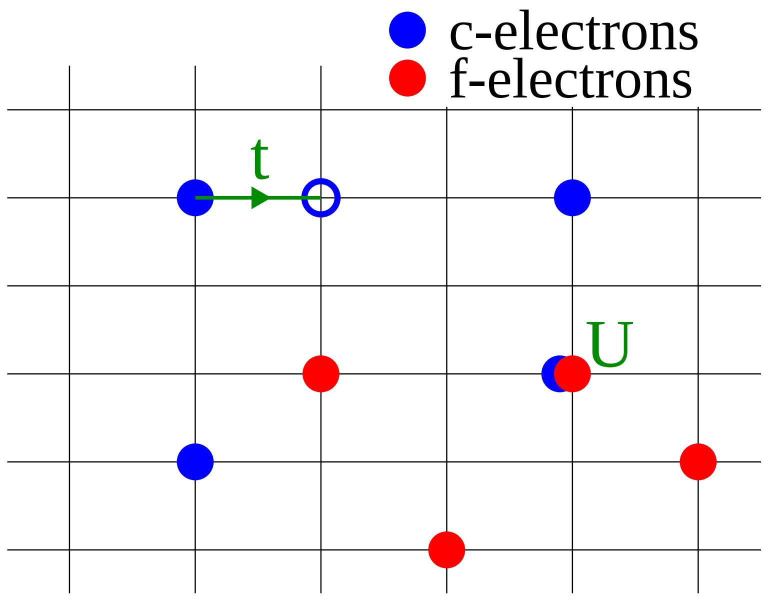
$$\frac{\partial f(\mathbf{k},T)}{\partial T} - \mathbf{E}(T)\frac{\partial f(\mathbf{k},T)}{\partial \mathbf{k}} = -\frac{1}{\tau}[f(\mathbf{k},T) - f_0(\mathbf{k})], \quad E(T) = E\theta(T)$$



The Falicov-Kimball model

Hamiltonian:

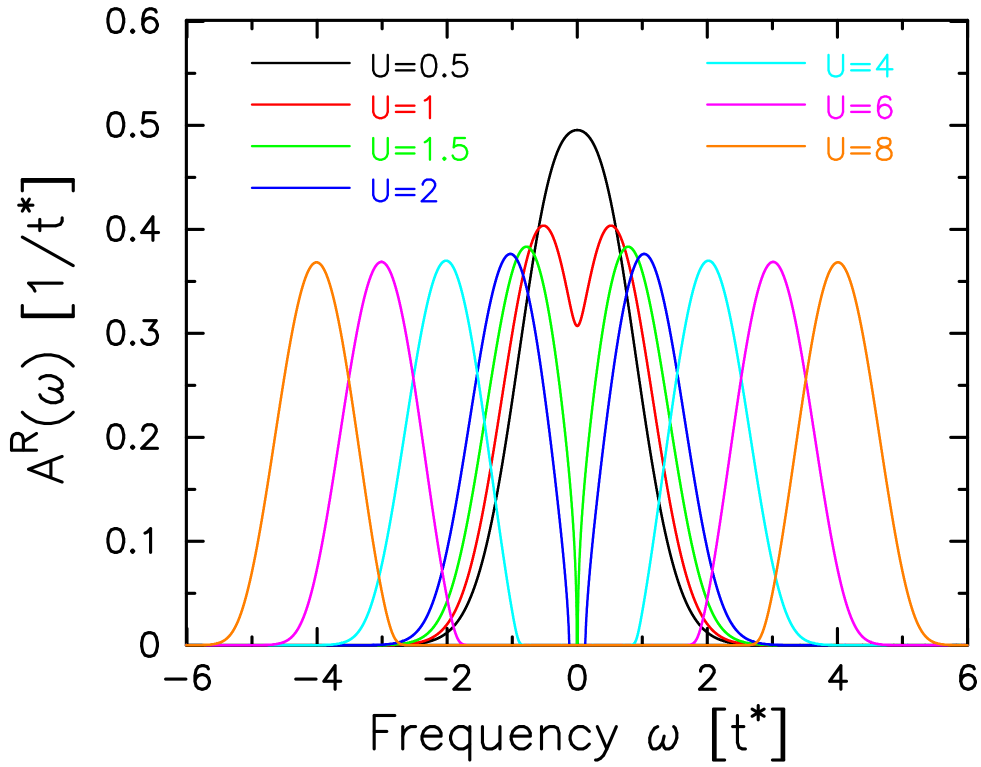
$$\mathcal{H} = -\sum_{<i,j>} t_{ij} c_i^\dagger c_j - \mu \sum_i c_i^\dagger c_i - \mu_f \sum_i f_i^\dagger f_i + U \sum_i f_i^\dagger f_i c_i^\dagger c_i$$



Some equilibrium properties: Mott transition

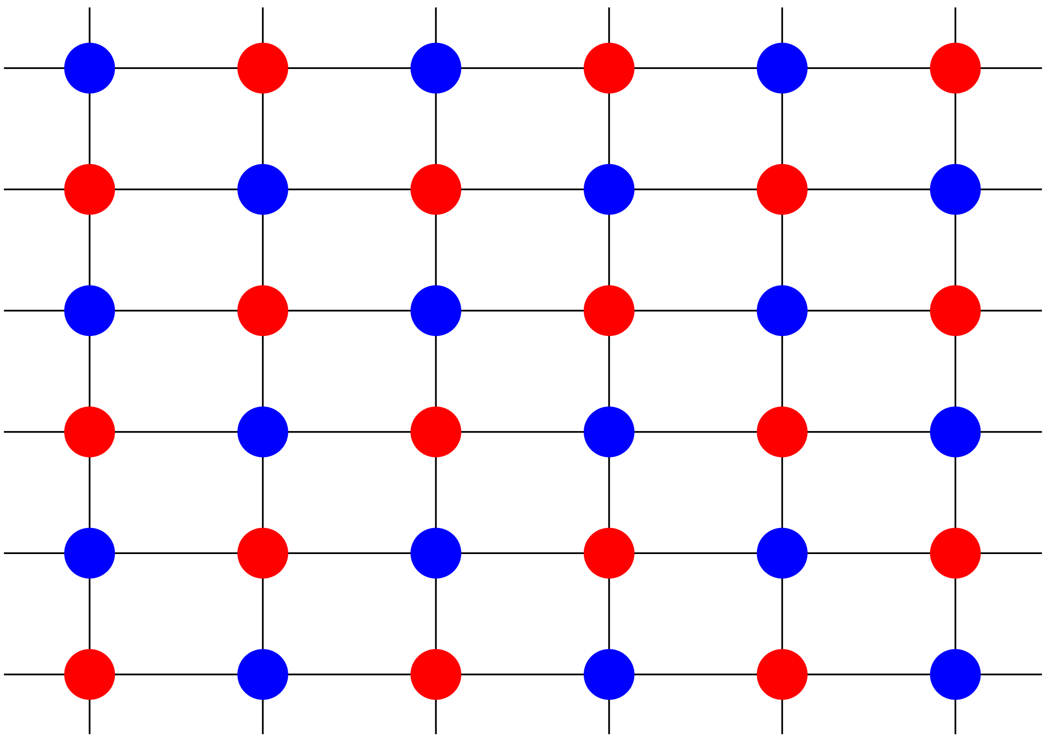
$$n_c + n_f = 1, U = U_c(n_f)$$

($d = \infty$:D.O. Demchenko, A.V. Joura, J.K. Freericks)



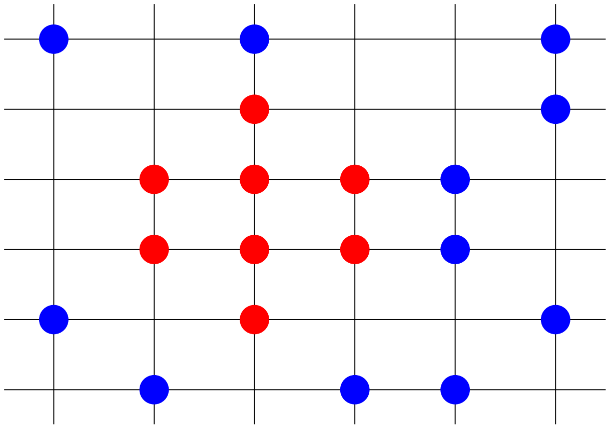
Checkerboard phase

$n_c = n_f = 1/2$, any U (T. Kennedy, E.H. Lieb)

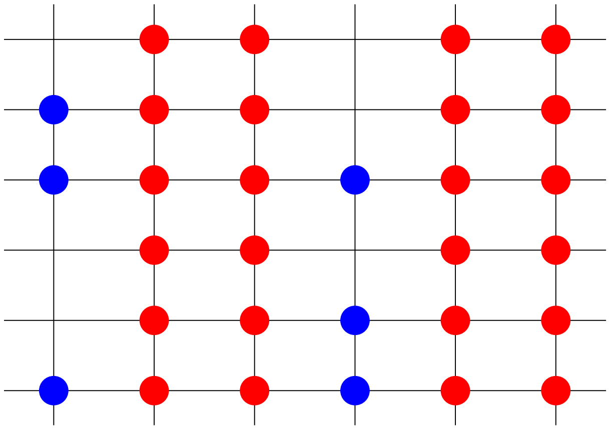


- $n_c, n_f < 1/2$, $U \to \infty$, any d: segregation phases
  (J.K. Freericks, E.H. Lieb, D. Ueltschi)
- large U, $n_c = n_f < 1/2, d = 2$: different stripe arrangements
  (R. Lemański, J.K. Freericks, and G. Banach)
- small U, $n_c + n_f < 1$, $d = 1, 2$: different mixed phases
  (segregation, checkerboard, etc., J.K. Freericks et al; M.-T. Tran)

segregation phase



stripe phase



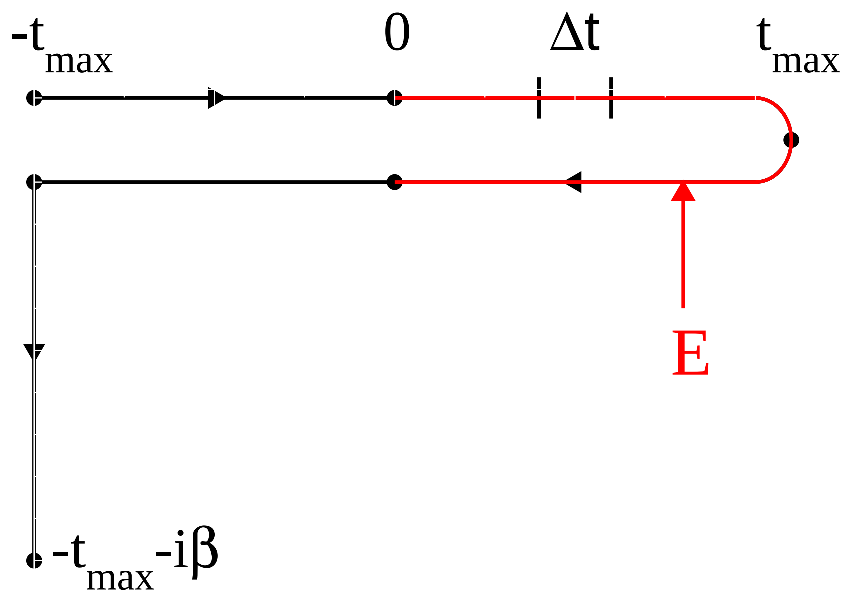
Experimental systems

- Valence-change-transition: $\mathrm{YbInCu_4}$, $\mathrm{EuNi_2(Si_{1-x}Ge_x)_2}$
- System doped through MIT: $\mathrm{Ta_xN}$ (barriers in Josephson junctions)
- Raman scattering experiments in insulators: $\mathrm{SmB_6(?)}$
- Binary alloys
- Modifi ed models: manganites, diluted magnetic semiconductors

Kadanoff-Baym-Keldysh formalism

The Hamiltonian: $\hat{H} = \hat{H}_0 + \hat{H}_{int}(t), \quad \hat{H}_{int}(t < t_0) = 0$

$$\hat{\rho}(\hat{H}_0) = e^{-\beta \hat{H}_0}/\mathrm{Tr}e^{-\beta \hat{H}_0}, \quad G^T(t_1, t_2) = -\frac{i}{\hbar}\langle \mathrm{T}_c c(t_1) c^\dagger(t_2)\rangle$$



The electric fi eld: $\mathbf{E}(\mathbf{r},t) = -\frac{1}{c}\frac{\partial \mathbf{A}(\mathbf{r},t)}{\partial t}$

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

$$H(A) = \sum_{\mathbf{k}} \left[\epsilon\left(\mathbf{k} - \frac{e\mathbf{A}(t)}{\hbar c}\right) - \mu\right] c_{\mathbf{k}}^{\dagger} c_{\mathbf{k}} + U \sum_{\mathbf{p},\mathbf{k},\mathbf{q}} f_{\mathbf{p}+\mathbf{q}}^{\dagger} c_{\mathbf{k}-\mathbf{q}}^{\dagger} c_{\mathbf{k}} f_{\mathbf{p}}.$$

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

Green functions

$$G^R_{\mathbf{k}}(t_1, t_2) = -i\theta(t_1 - t_2)\left\langle \left\{ c_{\mathbf{k}}(t_1), c^\dagger_{\mathbf{k}}(t_2) \right\} \right\rangle, \quad G^<_{\mathbf{k}}(t_1, t_2) = i\left\langle c^\dagger_{\mathbf{k}}(t_2) c_{\mathbf{k}}(t_1) \right\rangle$$

The relative and the average time coordinates:

$$t_{rel} = t_1 - t_2, \quad T = (t_1 + t_2)/2$$

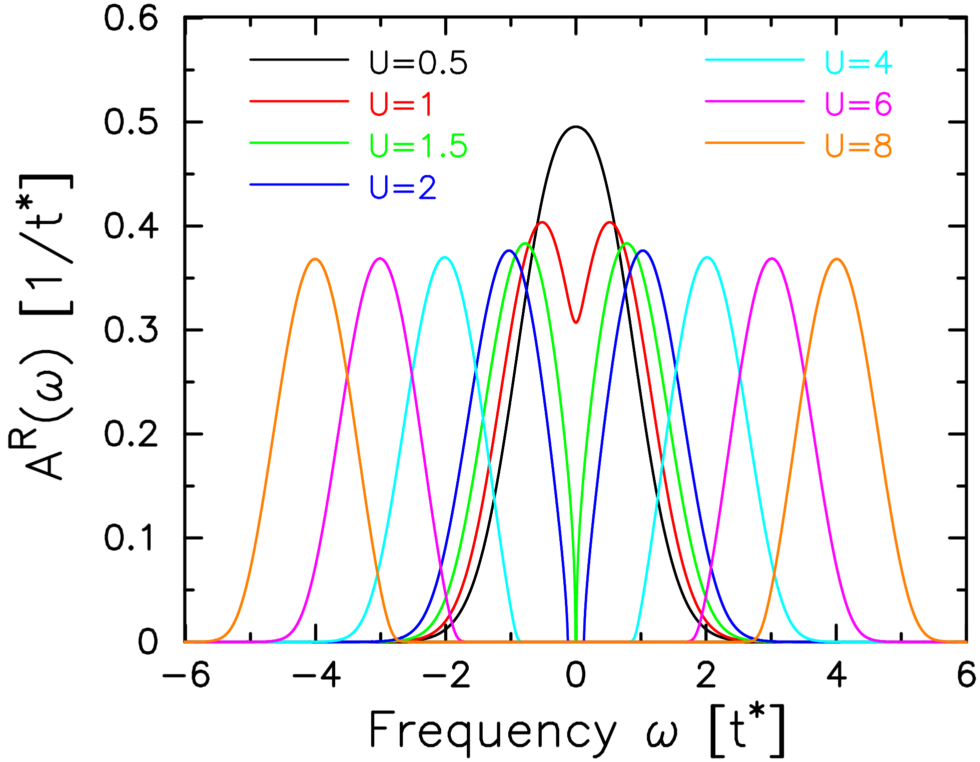
Spectral functions

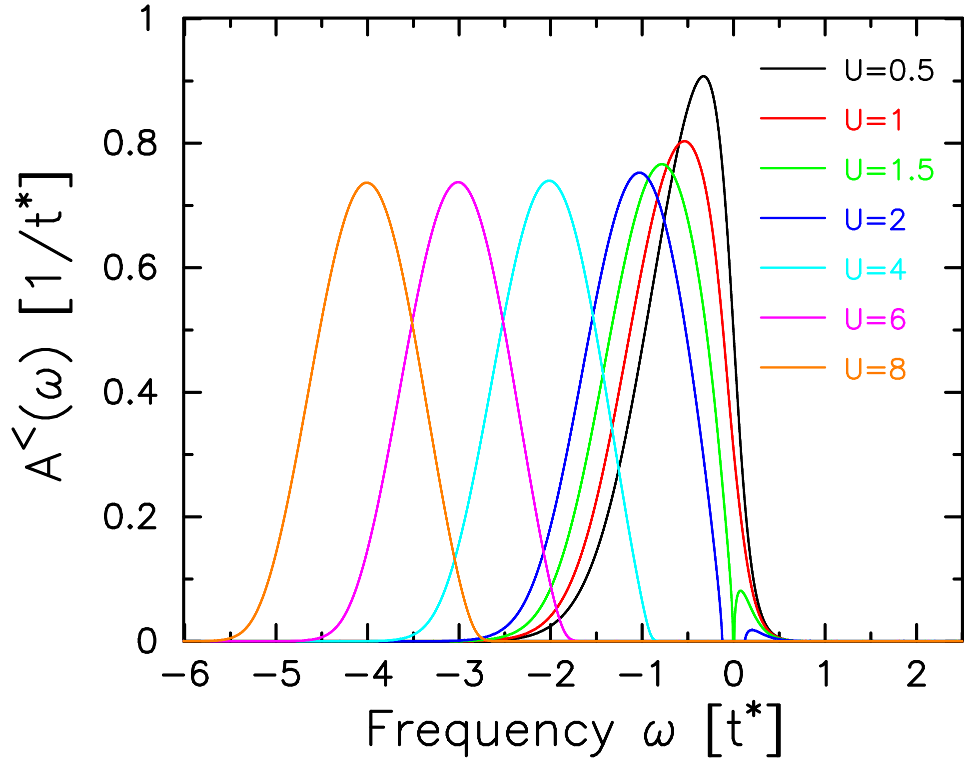
$$A^R_{\mathbf{k}}(T, \omega) = -\int_{-\infty}^{\infty} dt_{rel} e^{i\omega t_{rel}} \left(\frac{1}{\pi}\right) \mathrm{Im} G^R_{\mathbf{k}}(T, t_{rel})$$

$$A^<_{\mathbf{k}}(T, \omega) = \int_{-\infty}^{\infty} dt_{rel} e^{i\omega t_{rel}} \left(\frac{1}{\pi}\right) \mathrm{Im} G^<_{\mathbf{k}}(T, t_{rel})$$

Equilibrium results: Spectral functions

$$\beta = 10$$

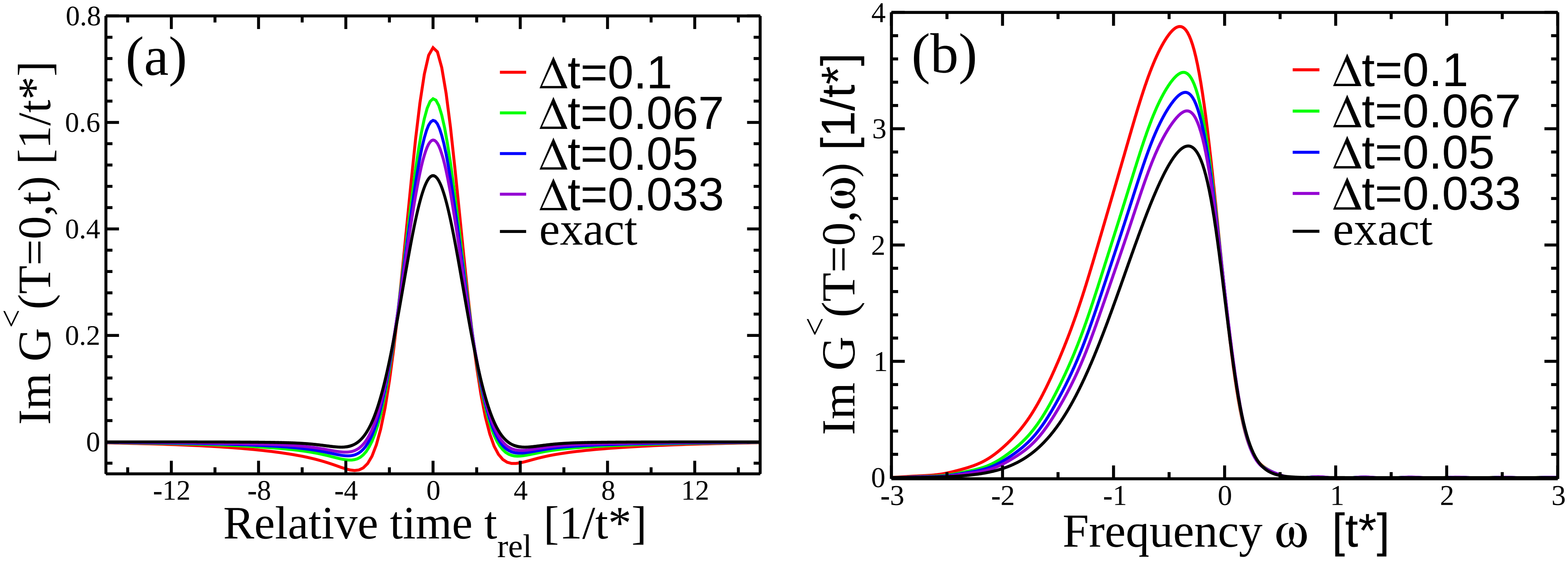




In equilibrium: $A^<(\omega) = 2f(\omega)A^R(\omega)$

Equilibrium results: Nonequilibrium formalism

$U = 0.5$, $\beta = 10$



Spectral function sum rules

$$\mu_n^{R,<}(\mathbf{k},T) = \int_{-\infty}^{\infty} d\omega \omega^n A_{\mathbf{k}}^{R,<}(T,\omega)$$

$$\tilde{\mu}_n^{R,<}(T) = \sum_{\mathbf{k}} \mu_n^{R,<}(\mathbf{k},T)$$

The local moments are time-independent! (except $\tilde{\mu}_1^{<}(T)$)

At $n_c = n_f = \frac{1}{2}$:

$$\int d\omega A^R(T,\omega) = 1, \qquad \int d\omega A^<(T,\omega) = 2n_c$$

$$\int d\omega \omega A^R(T,\omega) = 0$$

$$\int d\omega \omega^2 A^{R,<}(T,\omega) = \frac{1}{2} + \frac{U^2}{4}$$

Equilibrium results: Nonequilibrium formalism

$U = 0.5$, $\beta = 10$

	$\Delta t = 0.1$	$\Delta t = 0.05$	$\Delta t = 0.033$	exact
$\tilde{\mu}_0^R$	1.580785	1.232022	1.144811	1
$\tilde{\mu}_1^R$	0.174040	0.052785	0.030002	0
$\tilde{\mu}_2^R$	1.324976	0.848047	0.737020	0.5625

	$\Delta t = 0.1$	$\Delta t = 0.05$	$\Delta t = 0.033$	exact
$\tilde{\mu}_0^<$	1.480893	1.207662	1.133850	1
$\tilde{\mu}_1^<$	-1.036753	-0.774525	-0.706893	-0.591687
$\tilde{\mu}_2^<$	1.108705	0.777152	0.695791	0.5625

Nonequilibrium moments: Time-dependence

$$U = 0.5,\ \beta = 10,\ E = 1$$

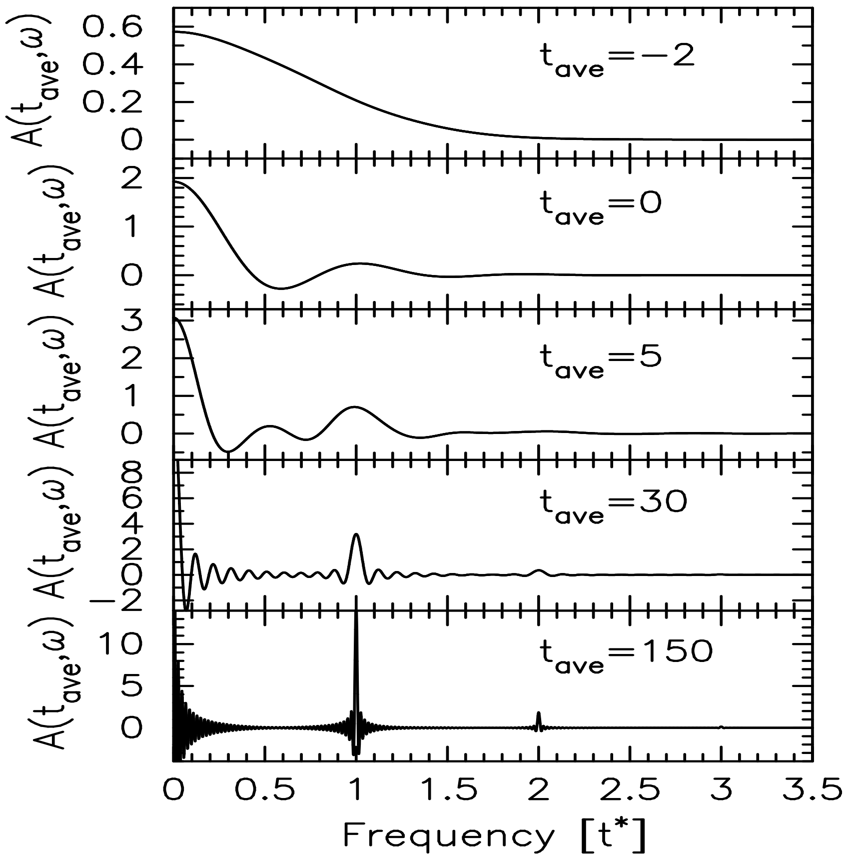
	T=0	T=5	T=15	T=20	exact
$\tilde{\mu}_0^R$	1.0025	1.0088	0.9951	0.9967	1
$\tilde{\mu}_1^R$	0.00665	-0.00054	0.00054	0.00003	0
$\tilde{\mu}_2^R$	0.56155	0.56198	0.55030	0.55112	0.5625

	T=0	T=5	T=15	T=20	exact
$\tilde{\mu}_0^<$	1.0025	1.0098	0.9960	0.9975	1
$\tilde{\mu}_1^<$	-0.5878	0.0042	-0.0454	0.0933	?
$\tilde{\mu}_2^<$	0.5520	0.5666	0.5572	0.5588	0.5625

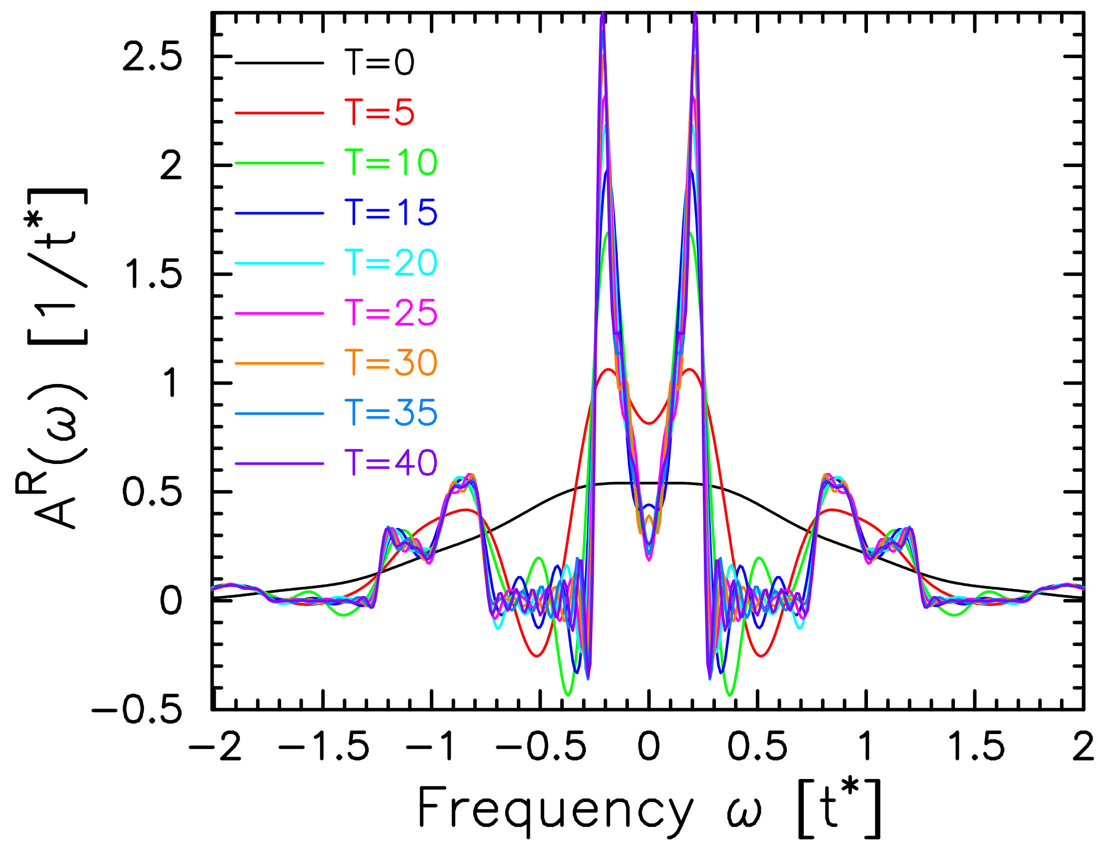
Nonequilibrium results: DOS

$$\beta = 10, E = 1$$

$U = 0$



$U = 0.5$



Time-dependence of the current

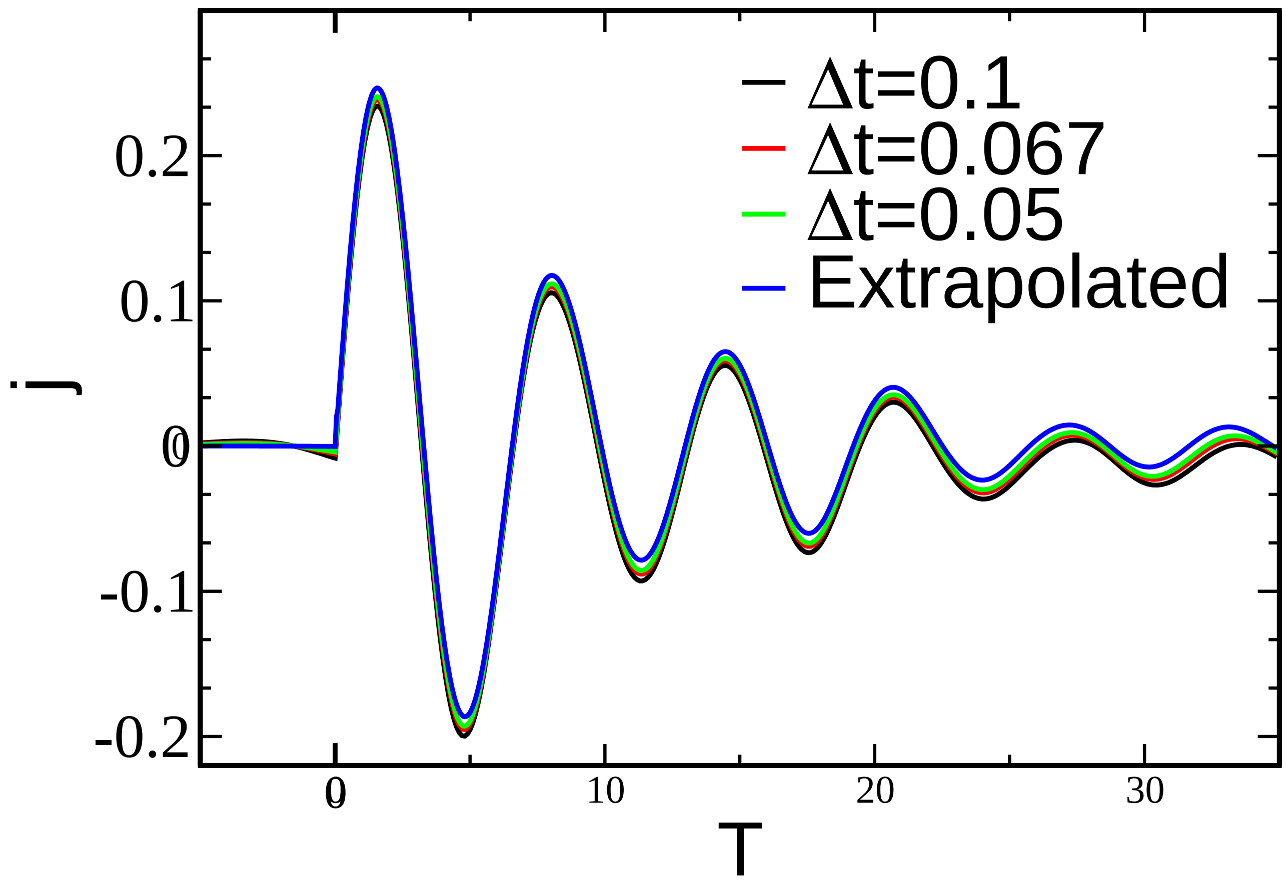
$$j^l(T) = -i\frac{eat^*}{\sqrt{d}}\sum_{\mathbf{k}} \sin\left(k^l a - \frac{eaA^l(T)}{\hbar c}\right) G^<(\epsilon_{\mathbf{k}}, T, T^+)$$

The total current density: $j(T) = \sqrt{d}\, j^l(T)$

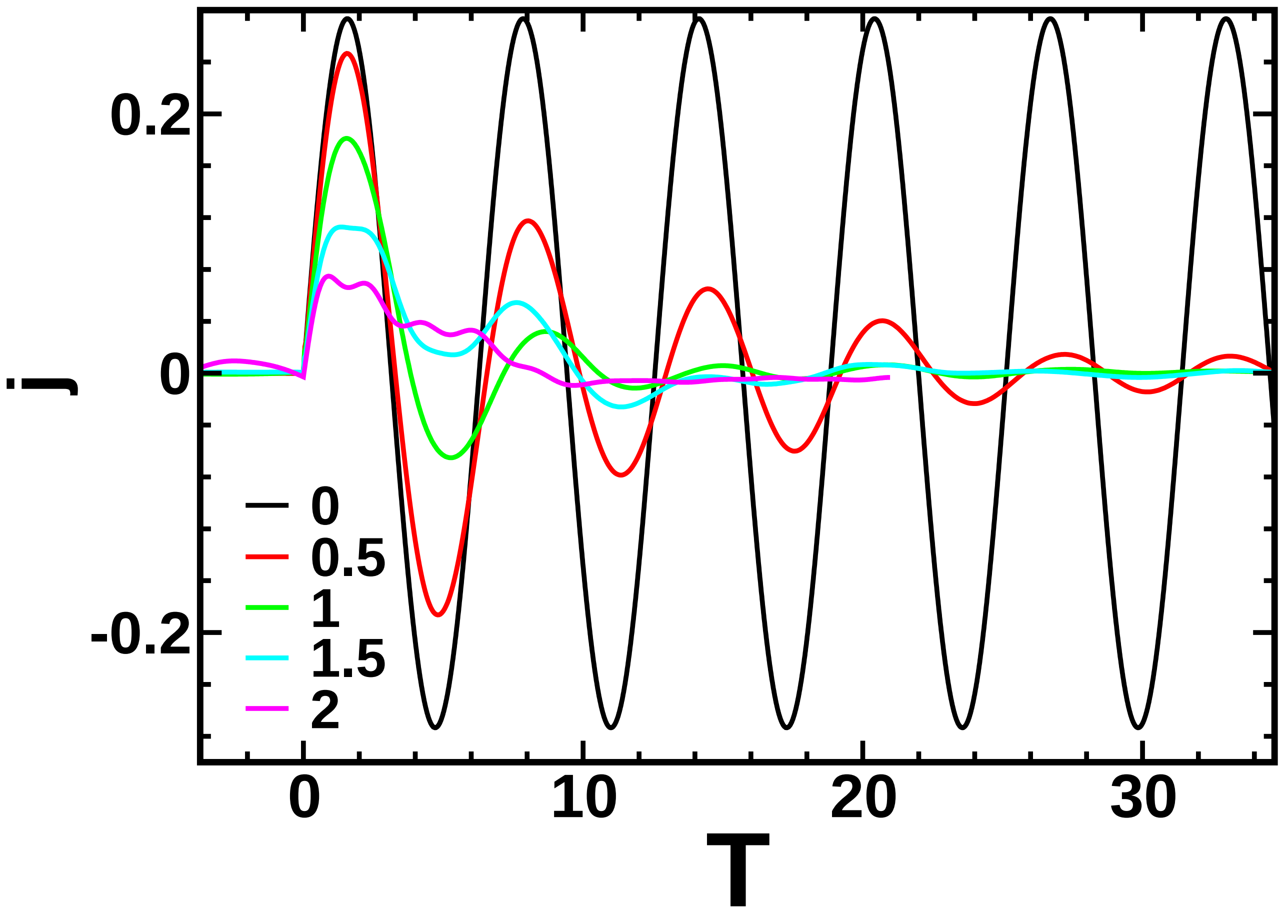
The $U = 0$ case: $j(T) \sim \sin\left(\frac{eaA(T)}{\hbar c}\right) \int d\epsilon \frac{df(\epsilon - \mu)}{d\epsilon} \rho(\epsilon)$

Bloch oscillations (at $A(T) = -EcT$) : $\omega_{Bloch} = eaE/\hbar$

Current: Δt-dependence
$U = 0.5, \beta = 10, E = 1$



Current: U-dependence
$\beta = 10, E = 1$



Conclusions

- A nonequilibrium DMFT formalism for the Falicov-Kimball model in an external time-dependent electric field has been developed
- The time-dependence of $A(\omega)$ and J at different values of U was studied
- The precision of the solution was estimated by comparing the results with the exact equilibrium results obtained by the DMFT in $d = \infty$ and by calculating the spectral moments
- The finite amplitude Wannier-Stark peaks in the DOS and the Bloch oscillations of the current may survive in the case of large E in the steady state regime
- References: V. Turkowski, J.K. Freericks, Phys. Rev. B 71, 085104 (2005); Phys. Rev. B 73, 075108 (2006)