Electric field-driven dissipative dimer-Hubbard model

Latest results and current draft

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Model Hamiltonian

$$\boxed{\begin{aligned} H = & -t \sum_{<ij>a\sigma} (c^\dagger_{ia\sigma} c_{ja\sigma} + \text{H. c.}) - t^\perp \sum_{i\sigma} (c^\dagger_{i1\sigma} c_{i2\sigma} + \text{H. c.}) + \\ & + U \sum_{ia} c^\dagger_{ia\uparrow} c_{ia\uparrow} c^\dagger_{ia\downarrow} c_{ia\downarrow} - E \sum_{ia\sigma} x_i c^\dagger_{ia\sigma} c_{ia\sigma} + \\ & + \sum_{ia\sigma\alpha} \left(-\gamma \left(b^\dagger_{ia\sigma\alpha} c_{ia\sigma} + \text{H. c.} \right) + \epsilon_\alpha b^\dagger_{ia\sigma\alpha} b_{ia\sigma\alpha} \right) \\ & \sigma = \uparrow, \downarrow \quad \text{and} \quad a = 1, 2 \quad \text{(orbital)} \end{aligned}}$$

Square lattice: $\epsilon(\boldsymbol{k}) = -2t(\cos k_x + \cos k_y)$

Bonding (B) / anti-bonding (A) basis:

$$c^\dagger_{i\sigma B} = \left(c^\dagger_{i\sigma 1} + c^\dagger_{i\sigma 2} \right) / \sqrt{2}, \quad c^\dagger_{A\sigma} = \left(c^\dagger_{i\sigma 1} - c^\dagger_{i\sigma 2} \right) / \sqrt{2}$$

DMFT equations

Lattice Dyson equations:

$$\begin{aligned} G^R_{B,A}(\omega,k_y) &= \left[\omega-\epsilon(k_y)\mp t^{\perp}-\Sigma^R_{B,A}(\omega)-t^{\shortparallel 2}F^R_{totB,A}(\omega,k_y)\right]^{-1}, \\ G^K_{B,A}(\omega,k_y) &= |G^R_{B,A}(\omega)|^2\left[\Sigma^K_{B,A}(\omega)+t^{\shortparallel 2}F^K_{totB,A}(\omega,k_y)\right]. \end{aligned}$$

Impurity problem:

$$\begin{aligned} \mathcal{G}^R_{0B,A}(\omega) &= \left[G^R_{B,A}(\omega)^{-1}+\Sigma^R_{UB,A}(\omega)\right]^{-1}, \\ \mathcal{G}^K_{0B,A}(\omega) &= |\mathcal{G}^R_{0B,A}(\omega)|^2\left[\frac{G^K_{B,A}(\omega)}{|G^R_{B,A}(\omega)|^2}-\Sigma^K_{UB,A}(\omega)\right]. \end{aligned}$$

$\Sigma(\omega)\equiv\Sigma_U(\omega)+\Sigma_{th}(\omega)$,
$\Sigma^R_{th}(\omega)=-i\Gamma$, $\Sigma^K_{th}(\omega)=-2i\Gamma\tanh\left(\frac{\omega}{2T}\right)$.

Parameters

Table 1: Typical values of the DHM parameters for VO_2[1]

	t	$t^{\perp}$	U	Γ	T
eV	0.25	0.3	2.5	(0.002)	0.0025
Normalized units	1	1.2	10	(0.008)	0.01

[1] O. Nájera et al. "Multiple crossovers and coherent states in a Mott-Peierls insulator". In: *Phys. Rev. B* 97 (4 Jan. 2018), p. 045108. DOI: *10.1103/PhysRevB.97.045108*. URL: *https://link.aps.org/doi/10.1103/PhysRevB.97.045108*.

Definitions

- Density of states:

$$\rho(\omega) = -\frac{1}{\pi}\mathrm{Im}G^R_{loc}(\omega)$$

- Distribution function:

$$f(\omega) = \frac{1}{2}\left(1 - \frac{1}{2}\frac{\mathrm{Im}G^K_{\mathrm{loc}}(\omega)}{\mathrm{Im}G^R_{\mathrm{loc}}(\omega)}\right)$$

.

(with $G_{loc}(\omega) = \frac{1}{2}\left(G_B(\omega) + G_A(\omega)\right)$)

- Effective temperature

$$T^2_{eff} = \frac{6}{\pi^2}\int \omega\left[f(\omega) - \Theta(-\omega)\right] d\omega,$$

- Electrical current

$$J = \int d\omega \int dk_y \left\{j_B[\boldsymbol{G}_B(\omega, k_y), \boldsymbol{F}_B(\omega, k_y)] + j_A[\boldsymbol{G}_A(\omega, k_y), \boldsymbol{F}_A(\omega, k_y)]\right\} \tag{1}$$

Equilibrium

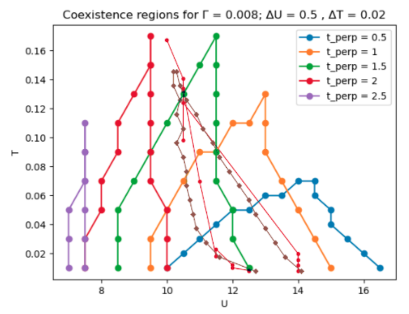

Figure 1: Shape of coexistence region for varying $t^{\perp}$. Presence of positive tilting of IMT lines.

$\rightarrow$ Tilting is inverted by $t^{\perp} \neq 0$

$\rightarrow$ This is due to the nature of the insulating state (localized spin vs. singlet)

Metallic states

- Quasiparticle peak is split between the two bands

$\rightarrow$ Split given (close to $\omega = 0$) by effective $t^{\perp}$:

$$t^{\perp}_{\mathit{eff}} = Z\left(t^{\perp} \pm \mathrm{Re}\, \Sigma^{R}_{B,A}\Big|_{\omega=0}\right), \quad \text{with} \quad Z = \left(1 - \frac{\partial \mathrm{Re}\Sigma^{R}_{B,A}}{\partial\omega}\bigg|_{\omega=0}\right)^{-1}$$

- $\rho(\omega)$ and $f(\omega)$ match very well to equilibrium states at $T = T_{\mathit{eff}}$

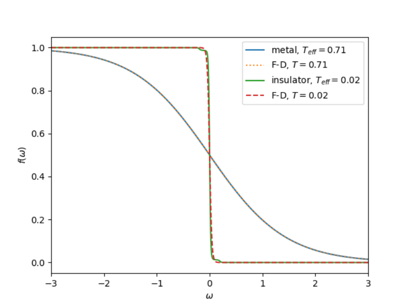

Figure 2: $t^{\perp} = 1$, $U = 10$, $\Gamma = 0.008$, $T = 0.01$, $E = 0.02$.

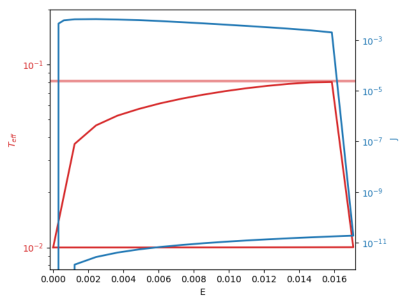

Figure 3: $t^{\perp} = 1$, $U = 13.5$, $\Gamma = 0.008$, $T = 0.01$.

Insulating states

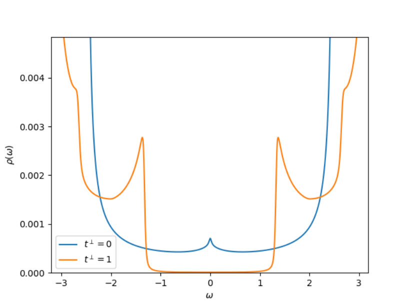

Figure 4: Gap in the density of states. $U = 13.5$, $\Gamma = 0.008$, $T = 0.01$.

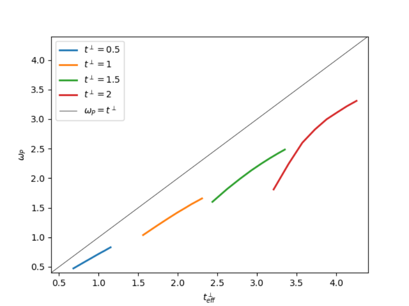

Figure 5: $U = [11, 18]$, $\Gamma = 0.008$, $T = 0.01$.

(Also remember: spurious IPT peaks at $\pm\omega_P/2$ for higher T.)

Non-equilibrium insulator

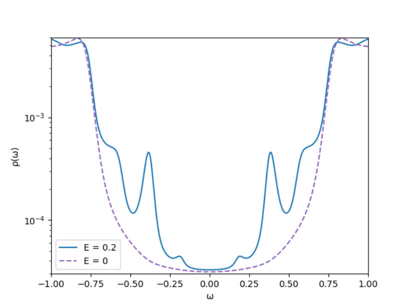

Figure 6: $t^{\perp} = 1$, $U = 10$, $\Gamma = 0.008$, $T = 0.01$.

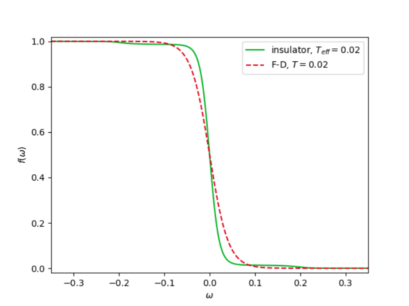

Figure 7: $t^{\perp} = 1$, $U = 10$, $\Gamma = 0.008$, $T = 0.01$, $E = 0.02$.

$\rightarrow$ Landau-Zener copies in the gap at intervals given by E;

$\rightarrow$ Accompanying step-like structure in $f(\omega)$.

Non-equilibrium IMT

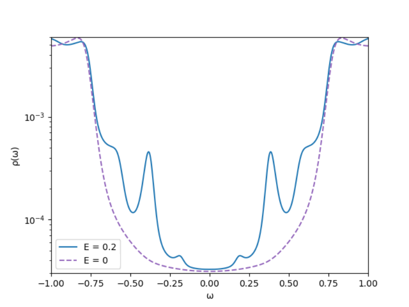

Figure 8: $t^{\perp} = 1$, $U = 10$, $\Gamma = 0.008$, $T = 0.01$.

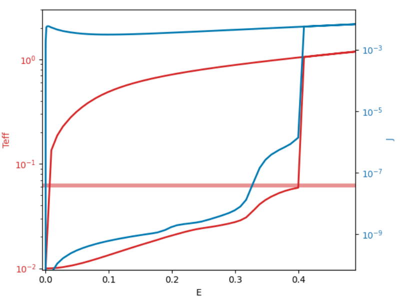

Figure 9: $t^{\perp} = 1$, $U = 10$, $\Gamma = 0.008$, $T = 0.01$.

$\rightarrow$ Transition still happens at equilibrium critical temperature;

$\rightarrow E^{IMT} \gg E^{MIT}$.

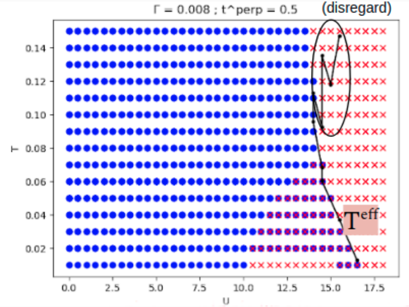

Figure 10: T_{eff}^{MIT} line matches equilibrium MIT line (same for IMT but not pictured).

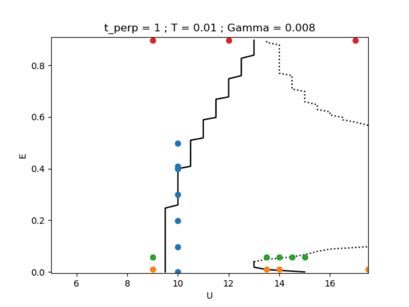

Figure 11: $t^{\perp} = 1$, $\Gamma = 0.008$, $T = 0.01$. 'Open/soft' coexistence region MIT borders.