Excitonic condensation in the mass imbalance extended Falicov–Kimball model

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1 INTRODUCTION

- The condensation of excitons with significantly different masses of electrons and holes in semimetallic or semiconducting systems is currently topical issue in condensed matter physics [1–2].
- In the theoretical side, the most promising candidate to describe the electron-hole system nowadays is the Extended Falicov-Kimball model (EFKM) [3-4].
- In the current work, the mass imbalance EFKM taking into account the electron-phonon correlations is investigated by using the unrestricted Hartree-Fock approximation (UHFA).
- Signature of the excitonic condensate or the excitonic insulator (EI) state at zero temperature is examined.

2 THEORETICAL APPROACH

- Hamiltonian of the EFKM with phonon and the electron-phonon interaction reads

$$\mathcal{H}=\sum_{\mathbf{k}}\varepsilon_{\mathbf{k}}^{c}c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}+\sum_{\mathbf{k}}\varepsilon_{\mathbf{k}}^{f}f_{\mathbf{k}}^{\dagger}f_{\mathbf{k}}+\omega_0\sum_{\mathbf{q}}b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}}$$

$$+\frac{U}{N}\sum_{\mathbf{k},\mathbf{k'},\mathbf{q}}c_{\mathbf{k+q}}^{\dagger}c_{\mathbf{k'}}f_{\mathbf{k'-q}}^{\dagger}f_{\mathbf{k}}+\frac{g}{\sqrt{N}}\sum_{\mathbf{k},\mathbf{q}}\left(c_{\mathbf{k+q}}^{\dagger}f_{\mathbf{k}}\left(b_{-\mathbf{q}}^{\dagger}+b_{\mathbf{q}}\right)+\mathrm{H.c}\right)$$

where $\varepsilon_{\mathbf{k}}^{c/f}=-t^{c/f}\left(\cos \mathrm{k}_x-\cos \mathrm{k}_y\right)+\epsilon^{c/f}-\mu$ (setting $t^c=1$ and $\epsilon^c-\epsilon^f=2$).

- In the frame work of UHFA, $\mathcal{H}$ can be simplified as

$$\mathcal{H}_{HF}=\sum_{\mathbf{k}}\bar{\boldsymbol{\varepsilon}}_{\mathbf{k}}^{c}c_{\mathbf{k}}^{\dagger}c_{\mathbf{k}}+\sum_{\mathbf{k}}\bar{\boldsymbol{\varepsilon}}_{\mathbf{k}}^{f}f_{\mathbf{k}}^{\dagger}f_{\mathbf{k}}+\delta\sum_{\mathbf{k}}\left(c_{\mathbf{k+q}}^{\dagger}f_{\mathbf{k}}+\mathrm{H.c}\right)$$

$$+\omega_0\sum_{\mathbf{q}}b_{\mathbf{q}}^{\dagger}b_{\mathbf{q}}+\sqrt{\boldsymbol{N}}\boldsymbol{h}\left(b_{-\mathbf{q}}^{\dagger}+b_{-\mathbf{q}}\right)\boldsymbol{\delta}_{\mathbf{q},\mathbf{0}}$$

that can be diagonalized.

- The excitonic condensate order parameter

$$\delta=\frac{g}{\sqrt{N}}\langle b_{-\mathbf{q}}^{\dagger}+b_{\mathbf{q}}\rangle\boldsymbol{\delta}_{q,0}-\frac{U}{N}\sum_{\mathbf{k}}\langle c_{\mathbf{k}}^{\dagger}f_{\mathbf{k}}\rangle$$

- The real part of the optical conductivity

$$\sigma(\omega)=\frac{\pi e^2}{\omega N}\sum_{\mathbf{k}}\left(v_{\mathbf{k}}^{f}-v_{\mathbf{k}}^{c}\right)^2\xi_{\mathbf{k}}^2\eta_{\mathbf{k}}^2\left[n_F\left(E_{\mathbf{k}}^1\right)-n_F\left(E_{\mathbf{k}}^2\right)\right]$$

$$\times\left\{\delta\left(\omega-E_{\mathbf{k}}^2+E_{\mathbf{k}}^1\right)-\delta\left(\omega-E_{\mathbf{k}}^1+E_{\mathbf{k}}^2\right)\right\}$$

REFERENCES

[1] S. Conti, D. Neilson, F. M. Peeters, A. Perali, *Condens. Matter,* 5, 22, 2020.

[2] S. Saberi-Pouya, S. Conti et al, *Phys. Rev. B,* 101, 140501(r), 2020.

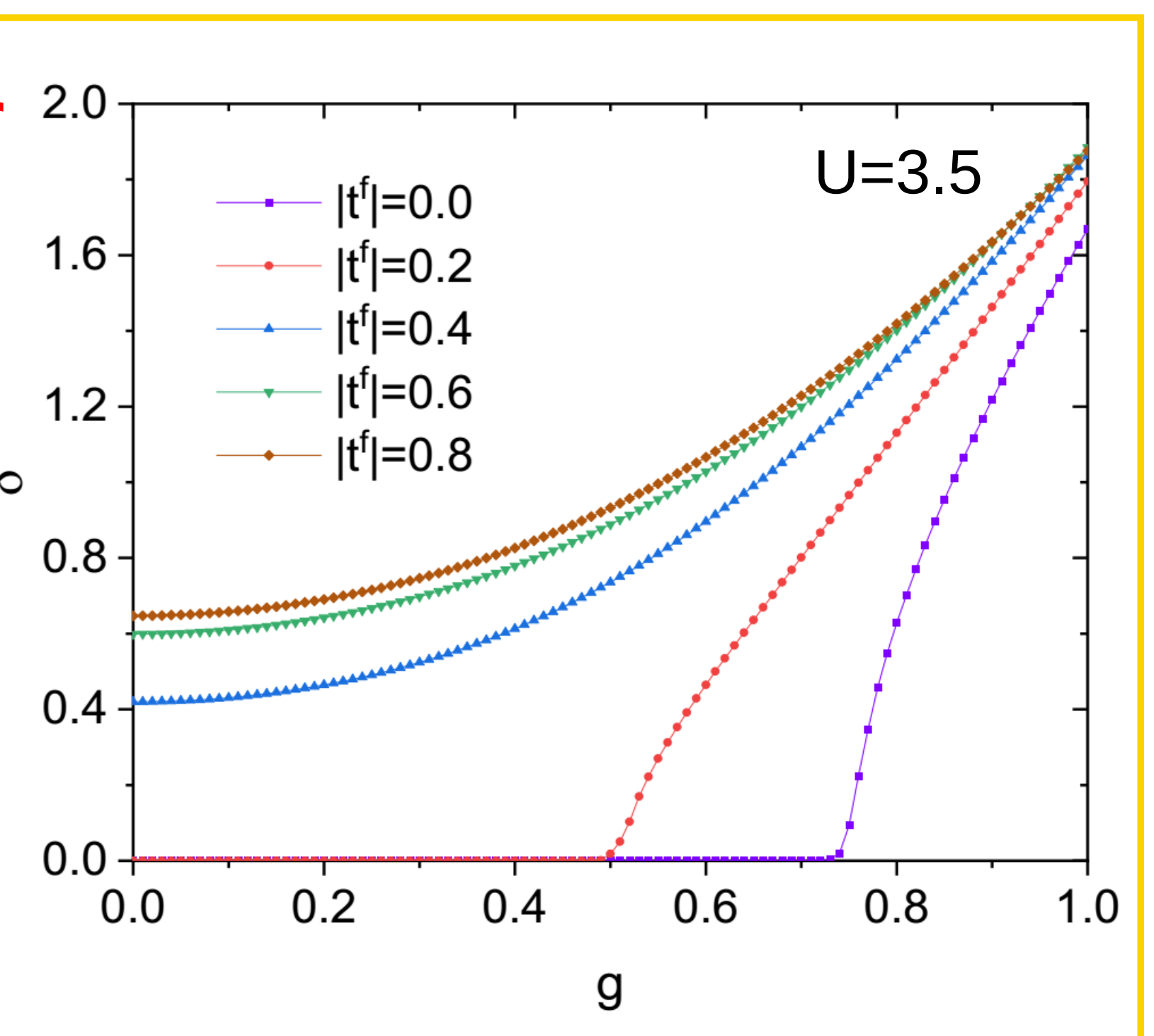
[3] B. Zenker et al, *Phys. Rev. B*, 81: 115122, 2010.

[4] D. Ihle et al, *Phys. Rev. B*, 78: 193103, 2008.

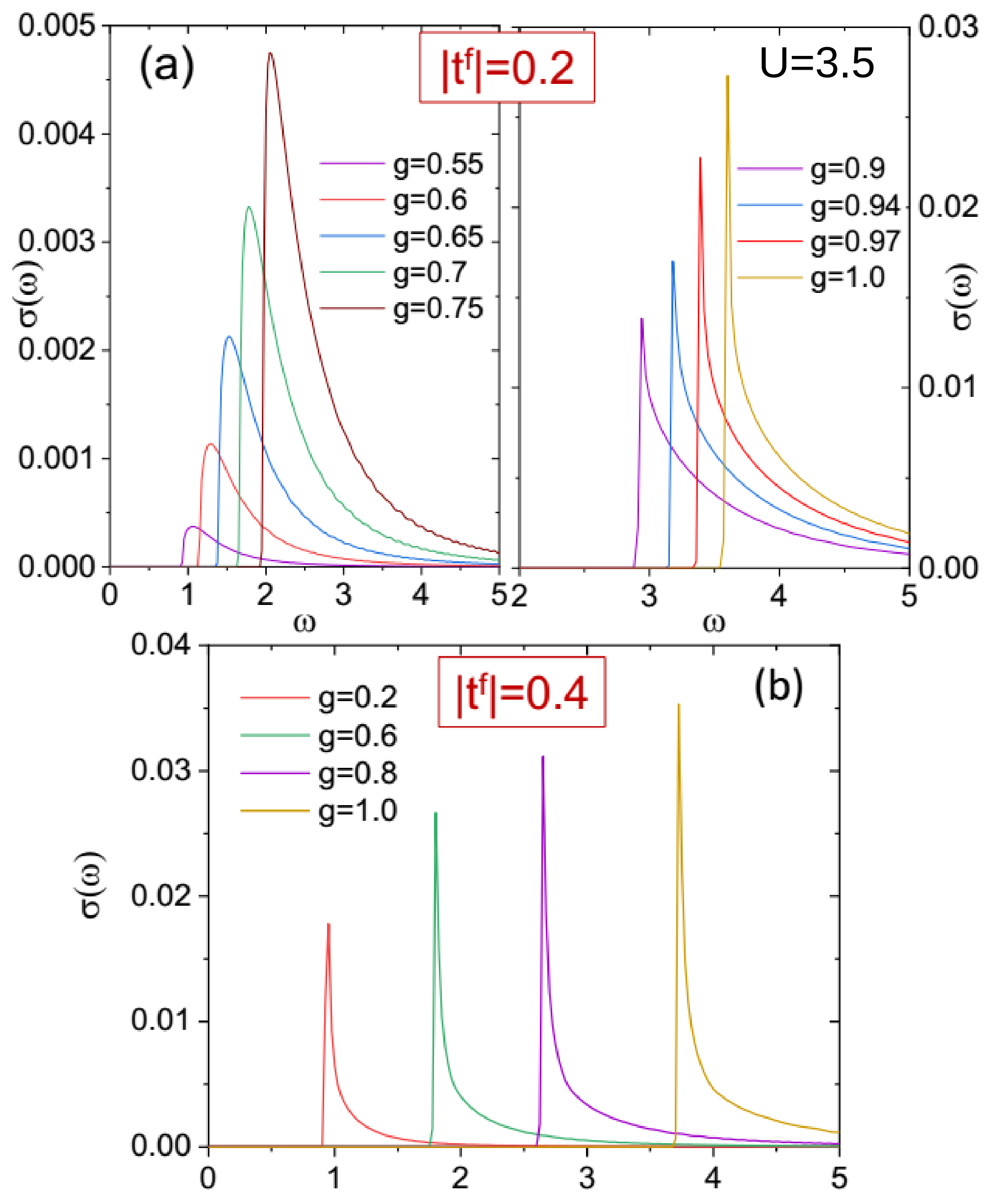
3 NUMERICAL RESULTS

Excitonic condensate order parameter

- $|t^f|=0$ (large mass imbalance) excitonic condensation state stabilizes only at a small regime of g.
- Increasing $|t^f|$, the EI can be found even at g = 0

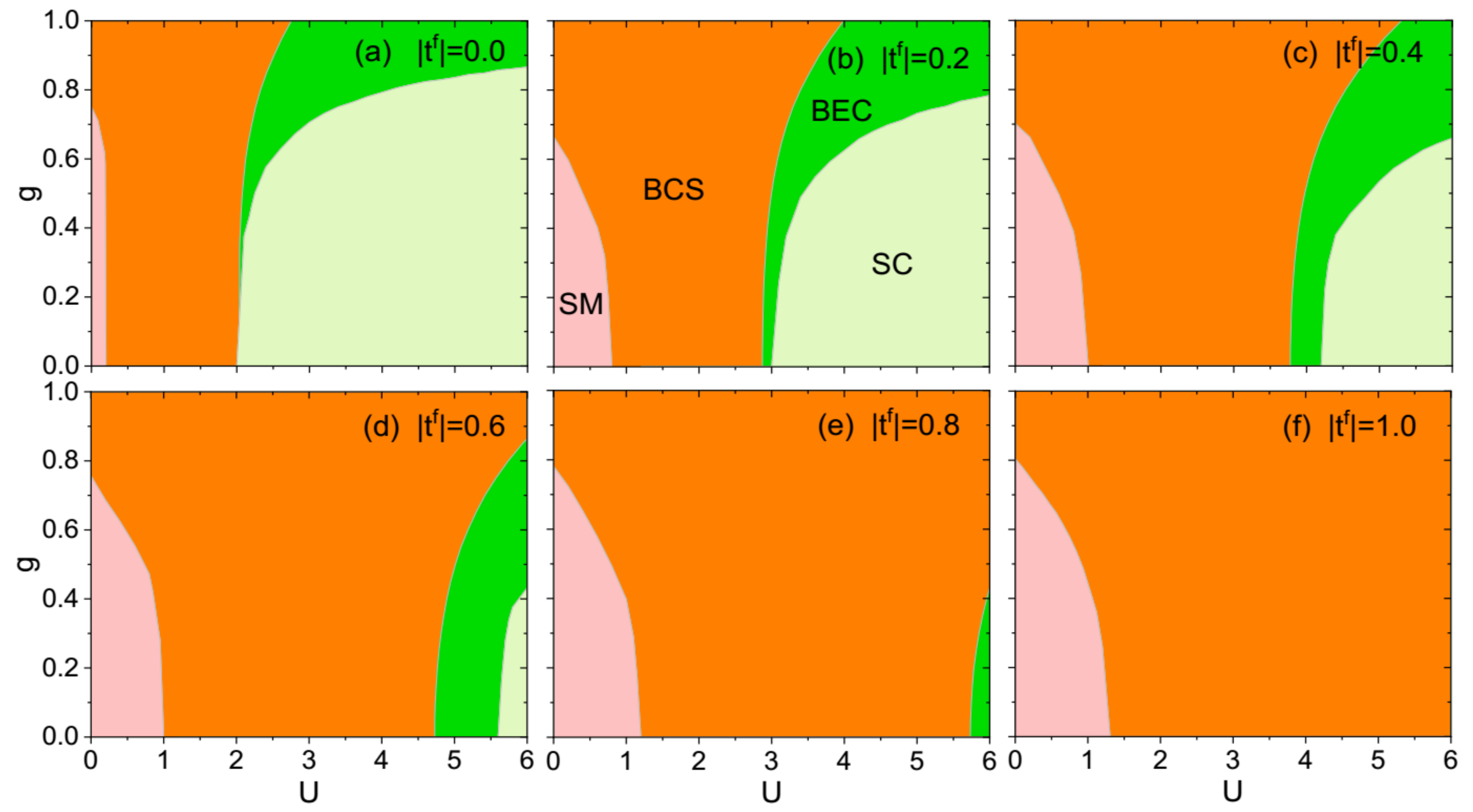


The optical conductivity



- σ(ω) shows the sharp peak at ω = 2δ, exhibiting the stability of the excitonic condensation state
- $|t^f|=0.2$: Intermediate g: the blunter peak of σ(ω) at low frequency indicates the BEC excitonic condensate.
- $|t^f|=0.2$ with large g or $|t^f|=0.4$ (decreasing mass imbalance): σ(ω) shows sharper peak and system stabilizes in BCS excitonic condensation state.

Phase diagram



- The BCS-BEC crossover of the condensation state can be found in case of large mass imbalance.
- The BEC type of the condensate then disappears and one finds the simultaneous transition of the BCS condensate to the semimetal (SM) and then semiconducting (SC) state by lowering the mass imbalance.
- Increasing g leads to the extension of the BEC excitonic condensate, specifically for the large mass imbalance.

4 CONCLUSIONS

- By lowering the mass imbalance and increasing electron-phonon coupling, the excitonic condensed state becomes stabilized, indicated by the right shift of the optical spectrum.
- BCS-BEC crossover of the excitonic insulator state can be found in the case of large mass imbalance. Increasing the electron-phonon coupling leads to the extension of BEC excitonic condensate.