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Effective interaction for correlated electrons with strong electron-phonon coupling

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Electron-electron and electron-phonon interactions in condensed matter systems

1. Strongly coupled electron-phonon systems

Systems, where phonon scale and electron phonon coupling is not small

- Fullerides (doped lattices of fullerenes)

Superconducting at high critical temperatures T_c of 30 - 40°K. *O. Gunnarson*, RMP **69**, 575 (1997)



- Manganites Re_{1-x}A_xMnO₃

Materials with large magnetoresistivity

A.J. Millis, Nature **392**, 147 (2001)





Electron-electron and electron-phonon interactions in condensed matter systems

2. Strongly coupled electron-phonon systems

- Compound Ba_{1-x}K_xBiO₃

Strong coupling to oxygen breathing mode



D.G. Hinks et al., Physica C **162**, 1405 (1989)

Freericks, Jarrel, PRB 50, 6939 (1994)

Electron-electron and electron-phonon interactions in condensed matter systems

- 3. Strongly coupled electron-phonon systems
- Cuprates

Strong coupling to oxygen half breathing mode





O Gunnarsson, O Rösch, J. Phys.: Cond Mat. **20**, 043201 (2008)

Interactions on different energy scales



Theory of conventional superconductivity



Overview

- 1. Phase diagram: competing interactions for the Hubbard Holstein model at half filling
 - Normal state
 - > With symmetry breaking
- 2. Kinks in the nodal dispersion of the copper-oxide superconductors
 - Recent experiments
 - > Theoretical results: phonon kinks in the presence of strong correlations
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Hubbard-Holstein (HH) model

$$H = -t \sum_{i,j,\sigma} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + \text{h.c.}) + U \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} + \omega_0 \sum_{i} b_i^{\dagger} b_i + g \sum_{i} (b_i + b_i^{\dagger}) \left(\sum_{\sigma} \hat{n}_{i,\sigma} - 1\right)$$

Describe coupling to optical phonon in the presence of strong electronelectron repulsion

$$U$$
 vs $\lambda = 2g^2/\omega_0$
Electron scale $W = 2D = 4t$ $ho_0 = rac{2}{\pi D}$

Phonon scale \mathcal{O}_0 renormalized



Dynamical mean field theory (DMFT) and Numerical Renormalisation group (NRG)

Hubbard-Holstein model

Effective Anderson-Holstein model



Competing interactions and phase diagram at half filling



Large d including long range order

Commensurate order on a bipartite lattice

$$H_{\mu} = \sum_{\boldsymbol{k},\sigma} (\varepsilon_{\boldsymbol{k}} c_{\boldsymbol{A},\boldsymbol{k},\sigma}^{\dagger} c_{\boldsymbol{B},\boldsymbol{k},\sigma} + \text{h.c.}) - \sum_{\boldsymbol{k},\sigma} (\mu_{\sigma} c_{\boldsymbol{A},\boldsymbol{k},\sigma}^{\dagger} c_{\boldsymbol{A},\boldsymbol{k},\sigma} + \mu_{-\sigma} c_{\boldsymbol{B},\boldsymbol{k},\sigma}^{\dagger} c_{\boldsymbol{B},\boldsymbol{k},\sigma}) + U \sum_{i} (n_{\boldsymbol{A},i,\uparrow} n_{\boldsymbol{A},i,\downarrow} + n_{\boldsymbol{B},i,\uparrow} n_{\boldsymbol{B},i,\downarrow}),$$

$$A-B \text{ bipartite}$$

We will consider half filling.

Antiferromagnetic order:

$$\Phi_{\rm afm} = (n_{A,\uparrow} - n_{A,\downarrow})/2$$

Charge order:

$$\Phi_{\rm co} = (n_A - 1)/2$$

lattice R

Order parameters weak coupling

Bandwidth W = 4, half filling $\omega_0 = 0.6$



Continuous transition

Order parameters strong coupling

Bandwidth W = 4, half filling $\omega_0 = 0.6$



Discontinuous transition

Phase diagram of the HH model



Bandwith W = 4, half filling $\omega_0 = 0.6$

Role of phonon frequency



Effective mass and quasiparticle interaction in the normal state $z^{-1} = m^{2}$



Bandwith W = 4, half filling $\omega_0 = 0.6$



 $U^r = U$

From two-particle excitations find effective quasiparticle interaction

$$\tilde{U} \sim E_{pp} - 2E_p$$

Take away message for phase diagram at
half filling

 Phase boundaries are largely determined from effective interaction in terms of **bare** parameters

$$U_{\rm eff} = U - \lambda \qquad \lambda = 2g^2/\omega_0$$

- For other quantities this is different
- It appears that interactions are renormalized in a similar way
- Phase diagram has similarity with low dimensional case

JB, AC Hewson, Phys. Rev. B **81**, 235113 (2010) *JB,* EPL **90**, 27001(2010)



- Compound Ba_{1-x}K_xBiO₃



G. Vielsack, W. Weber, PRB **54**, *Liechtenstein et al.*, PRB **44**, 5388 *JB*, EPL **90**, 27001(2010) 6614 (1996) (1991)

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Kinks in nodal dispersion of cuprates

Kinks: abrupt changes in the electronic dispersion relation



Different possible origins of kinks in the dispersion

- Coupling to a phonon mode
 - Lanzara et al., Nature (2001)
 - Cuk et al., PSS (2005)
 - Graf et al., PRL (2008)
- Coupling to spin fluctuations
 - Johnson et al., PRL (2001)
 - Kaminski et al., PRL (2001)
 - Manske et al., PRL (2001)
 - Chubukov et al., PRB (2004)
 - Eschrig, Adv. Phys. (2006)
- Purely caused by electronic correlations
 - Byzcuk et al., Nature Physics (2007)

Case in favour of phonons: Isotope effect for kinks



Spin-fluctuation scenario for kinks and pairing



Combination of inelastic neutron scattering and angle resolved photoemission gives consistent picture for paring and kink

Dahm et al., Nature Phys. 5, $V_{\text{eff}}(\mathbf{Q}, \Omega) = \frac{3}{2} \ \bar{U}^2 \ \chi(\mathbf{Q}, \Omega) \quad \bar{U} = 1.59 \text{ eV}$ 217 (2009)

Peculiar doping dependence of kink position

ARPES spectra and analysis

Doping dependence of kink



97, 017002 (2006)

soften or remain constant with doping

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Kinks through coupling to a bosonic mode



Modelling cuprates as doped Mott insulators



range for phonons

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ho_0 rac{2g^2}{\omega_0}$
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Phonon scale ω_0 renormalized ω_0^r



Dynamical mean field theory (DMFT) and Numerical Renormalisation group (NRG)

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Effective Anderson-Holstein model



Dynamic quantities from the NRG



Spectral density of the Green's function in the Lehmann representation

Equations of motion $\underline{G}_{0}^{-1}(\omega)\underline{G}(\omega) - U\underline{F}(\omega) - g\underline{M}(\omega) = \mathbb{1}_{2}$ $\underline{\Sigma}(\omega) = U\underline{F}(\omega)\underline{G}(\omega)^{-1} + g\underline{M}(\omega)\underline{G}(\omega)^{-1}$



Dispersion for large U (PM-DMFT)



Dispersion for large U (PM-DMFT) and larger λ

$$U/W = 1.5$$
 $\omega_0/W = 0.05$ $n = 0.9$ ^r

Scenario 1: doped Mott insulator



Dispersion for large U (PM-DMFT), larger doping

$$U/W = 1.5$$
 $\omega_0/W = 0.05$ $n = 0.8$



Low energy physics and effective U

Low energy physics can be described by pure Hubbard model with effective *U*

$$U_{\rm eff} = U - \eta \lambda D$$

$$\eta = 2 \omega_0 / U / (1 + 2 \omega_0 / U)$$
 is smal





Effect of phonons visible at higher energy



G. Sangiovanni et al., PRL **95**, 226401 (2005), PRB **73**, 165123 (2006)

Dispersion including AFM correlations (AF-DMFT)

U/W = 1.5 $\omega_0/W = 0.05$ n = 0.9

Scenario 2: doped AFM



Synergistic polaron formation

• Polaron formation enhanced by antiferromagnetic correlations



Peculiar doping dependence of kink position





H. Kordyuk et al, PRL **97**, 017002 (2006)



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Conventional electron-phonon superconductivity

 $\frac{1.04(1+\lambda)}{\lambda - \mu_c^*(1+0.62)}$

 m^{*}/m_{0}

Transition temperature

 $T_c =$

Spectral gap

Dimensionless coupling constant For strong coupling superconductors

 $\Delta_{\rm sp} = 2\omega_0^r e$

 $\lambda \sim 1 - 3$







McMillan, Phys. Rev. **167**, 331 (1968)

Allen, Dynes, Phys. Rev. B **12**, 905 (1975)

Carbotte, Rev. Mod. Phys. **62**, 1027 (1990)

Conventional superconductivity Migdal-Eliashberg theory



Breakdown of Migdal-Eliashberg theory

• Model studies going beyond ME diagrammatics

P Benedetti, R Zeyher, Phys. Rev. B 58, 14320 (1998)

AS Alexandrov, EPL 56, 92 (2001)

D Meyer et al., PRL **89**, 196401 (2002)

M Capone, S Ciuchi, PRL 91, 186405 (2003)

• Indication that ME theory breaks down at intermediate Abstract. — In view of some recent works on the role of vertex corrections in the electronphogoupling strength the important pairs it metal means in the electronphogoupling strength the important pairs it metal means and the solution of the Holstein model and $1/\lambda$ strong-coupling expansion, we argue that the standard Feynman-Dyson perturbation theory by Migdal and Eliashberg with or without vertex corrections cannot be applied if the electron-phonon coupling is strong ($\lambda \ge 1$) at any ratio of the phonon, ω and Fermi, $E_{\rm F}$ energies. In the extreme adiabatic limit ($\omega \ll E_{\rm F}$) of the Holstein model electrons collapse into self-trapped small polarons or bipolarons due to spontaneous translational-symmetry breaking at $\lambda \simeq 1$. With the increasing phonon frequency the region of the applicability of the theory shrinks to lower values of $\lambda < 1$.

Pairing function in conventional superconductivity

Dimensionless coupling constant

$$\lambda = 2 \int_{0}^{\infty} d\omega \ \frac{\alpha^2 F(\omega)}{\omega}$$

Pairing function

Effective parameters dependence on bare parameters (Holstein model)



Procedure to test validity for Migdal Eliashberg theory



Quantitative test of the reliability of Migdal-Eliashberg theory



JB, J Han, O Gunnarsson, cond-mat/1105.2833 (2011)

 $\omega_0 = 0.1t$

Quantitative reliability of Migdal-Eliashberg theory



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Retardation effects as a function of U

 ω_0^r

Spectral gap
$$\Delta_{sp} = 2\omega_0^r e^{-\frac{m^*/m_0}{\lambda - \mu_c^*}}$$
 $\mu_c^* = \frac{\mu_c}{1 + \mu_c \log(\frac{D}{\omega_0})}$
Keep constant $\lambda \simeq 1$
Migdal-Eliashberg (ME)
 $ME z \Sigma (IA)$
 $MFT superconductivity$
is stronger suppressed
 $DMFT superconductivity$
is stronger suppressed
 $MB J Han, O Gunnarsson,$
(2011)

Retardation effects higher order calculation

preliminary results

Terms up to second order

Vertex correction for the electron phonon coupling

Renormalization of the phonon propagator

Terms up to second order in U





JB, J Han, O Gunnarsson, (2011)

 ω_{n_1}

 $-\omega_{n_1}\downarrow$

Retardation effects as a function of U



Summary - 1

- The ground state phase diagram of the Hubbard-Holstein model at half filled for large dimension shows antiferromagnetic and charge order
- The transition line is approximately where the bare effective interaction vanishes
- We find continuous transitions for smaller coupling and larger phonon frequency and discontinuous transitions for larger coupling and smaller phonon frequency
- Find similarities, but also differences with low dimensional results



JB, EPL 90, 27001(2010)

JB, AC Hewson, Phys. Rev. B **81**, 235113 (2010)

AC Hewson, JB, J. Phys. Cond. Mat. **22**, 155602 (2010)

Summary - 2

- From ARPES, in cuprates kink positions in the nodal dispersion show a strong dependence on doping
- Scenario1: DMFT-NRG calculations in PM state with large U we find kink energy larger than phonon energy; understood with effective interaction U changed little by the phonons
- Scenario 2: DMFT-NRG calculations in AF state with large U give kink at phonon energy for comparatively smaller coupling due to cooperative effect
- These scenarios can provide the basis for a situation with similar trends as in experiment



JB, G Sangiovanni, Phys. Rev. B **82**, 184535 (2010)

Summary -3

- We distinguish bare and effective parameters in the electron phonon coupling problem
- Migdal-Eliashberg theory with reliable phonon input is accurate for large couplings if effective phonon scale is small
- Anderson-Morel retardation effects and pseudopotential effect well defined for weak coupling and large band width
- Modification due to higher order effects expected



Thank you for your attention !