Selective bipolaronic Transition in Jahn-Teller Model

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SCES08

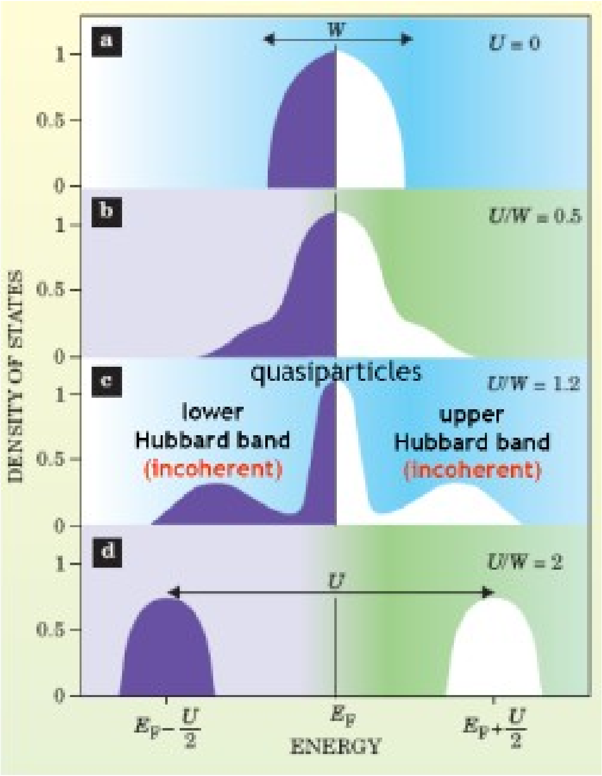
Hubbard Model

$$H = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{+} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

To be more realistic,

- Orbital degrees of freedom
- Relevance of phonon dynamics in strongly correlated electron systems

- Manganese oxide,
- Alkali-doped A_xC_{60} molecular solid.



MODEL AND METHOD

Jahn-Teller model

$$H = H_t + H_{ph} + H_{JT} + H_{e-e} \ ,$$

$$H_t = -\sum_{\langle ij \rangle \gamma\sigma} t_\gamma \left(c^+_{i\gamma\sigma} c_{j\gamma\sigma} + c^+_{j\gamma\sigma} c_{i\gamma\sigma} \right),$$

$$H_{ph} = \Omega_\circ \sum_i \left(a^+_i a_i + b^+_i b_i \right),$$

$$H_{JT} = g \sum_{i\sigma} \left[(n_{i1\sigma} - n_{i1\sigma})(a^+_i + a_i) + (c^+_{i1\sigma} c_{i2\sigma} + c^+_{i2\sigma} c_{i1\sigma})(b^+_i + b_i) \right]$$

Weak-Coupling Perturbation Theory

Up to the second order in g the effective interaction induced by the phonon is proportional to the phonon propagators,

- a-phonon

$$V_{(a)ph}^{eff} = g^2\left(\sum_{\gamma} n_{\gamma\uparrow}n_{\gamma\downarrow} - \sum_{\sigma} n_{1\sigma}n_{2\sigma} - \sum_{\sigma} n_{1\sigma}n_{2\bar{\sigma}}\right)D_a(\omega)$$

- b-phonon

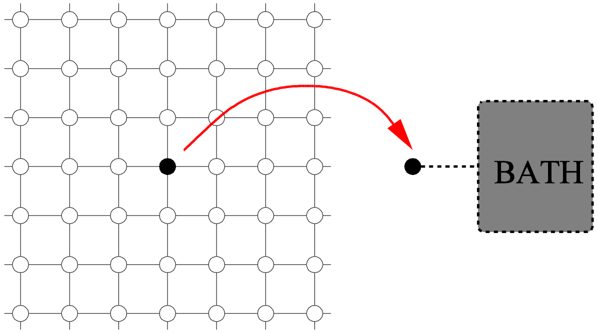
$$V_{(b)ph}^{eff} = -g^2\sum_{\sigma} n_{1\sigma}n_{2\sigma}D_b(\omega)$$
$$-g^2\left((c_{1\uparrow}^{+}c_{1\downarrow}c_{2\downarrow}^{+}c_{2\uparrow} + h.c.) + (c_{1\uparrow}^{+}c_{1\downarrow}^{+}c_{2\uparrow}c_{2\downarrow})\right)D_b(\omega)$$

$$D_a(\omega) = D_b(\omega) = -2\Omega_{\circ}/(\Omega_{\circ}^2 - \omega_{\circ}^2)$$

Dynamical Mean Field Theory (Exact Diagonalization solver)

$$\tilde{\varepsilon}_l, V_l, (l = 1, \ldots, n_s)$$

Impurity Solver



$$G_{imp}(i\omega_n)$$

$$\Sigma_{imp}(i\omega_n) = \left[i\omega_n + \mu - \varepsilon_\circ - \sum_{l=1}^{n_s} \frac{|V_l|^2}{i\omega_n - \tilde{\varepsilon}_l} \right] - G_{imp}^{-1}(i\omega_n)$$

$$G_{loc}(i\omega_n) = \sum_{\mathbf{k}} \left[i\omega_n + \mu - \varepsilon_{\mathbf{k}} - \Sigma_{imp}(i\omega_n) \right]^{-1} \longrightarrow g_{0,new}^{-1}(i\omega_n) = \Sigma_{imp}(i\omega_n) + G_{loc}^{-1}(i\omega_n)$$

$$\left\| g_{0,new}^{-1}(i\omega_n) - \left(i\omega_n + \mu - \varepsilon_\circ - \sum_{l=1}^{n_s} \frac{|V_l|^2}{i\omega_n - \tilde{\varepsilon}_l} \right) \right\|^2$$

Minimization

To analyze the metal-insulator transition

- Quasi-Particle Weights

$$z_i = \frac{1}{1 - \left.\frac{\partial \operatorname{Re}\Sigma_i(\omega)}{\partial \omega}\right|_{\omega=0}} = \frac{1}{1 - \left.\frac{\operatorname{Im}\Sigma_i(i\omega_\circ)}{\omega_\circ}\right|_{\omega_\circ \to 0}}$$

$$z \propto \frac{m}{m^*}$$

- Phonon Displacement Probability Distribution Function

$$P(x) = \langle \psi_\circ | x \rangle \langle x | \psi_\circ \rangle = \sum_{nm} \phi_n(x) \phi_m(x) \langle \psi_\circ | n \rangle \langle m | \psi_\circ \rangle$$

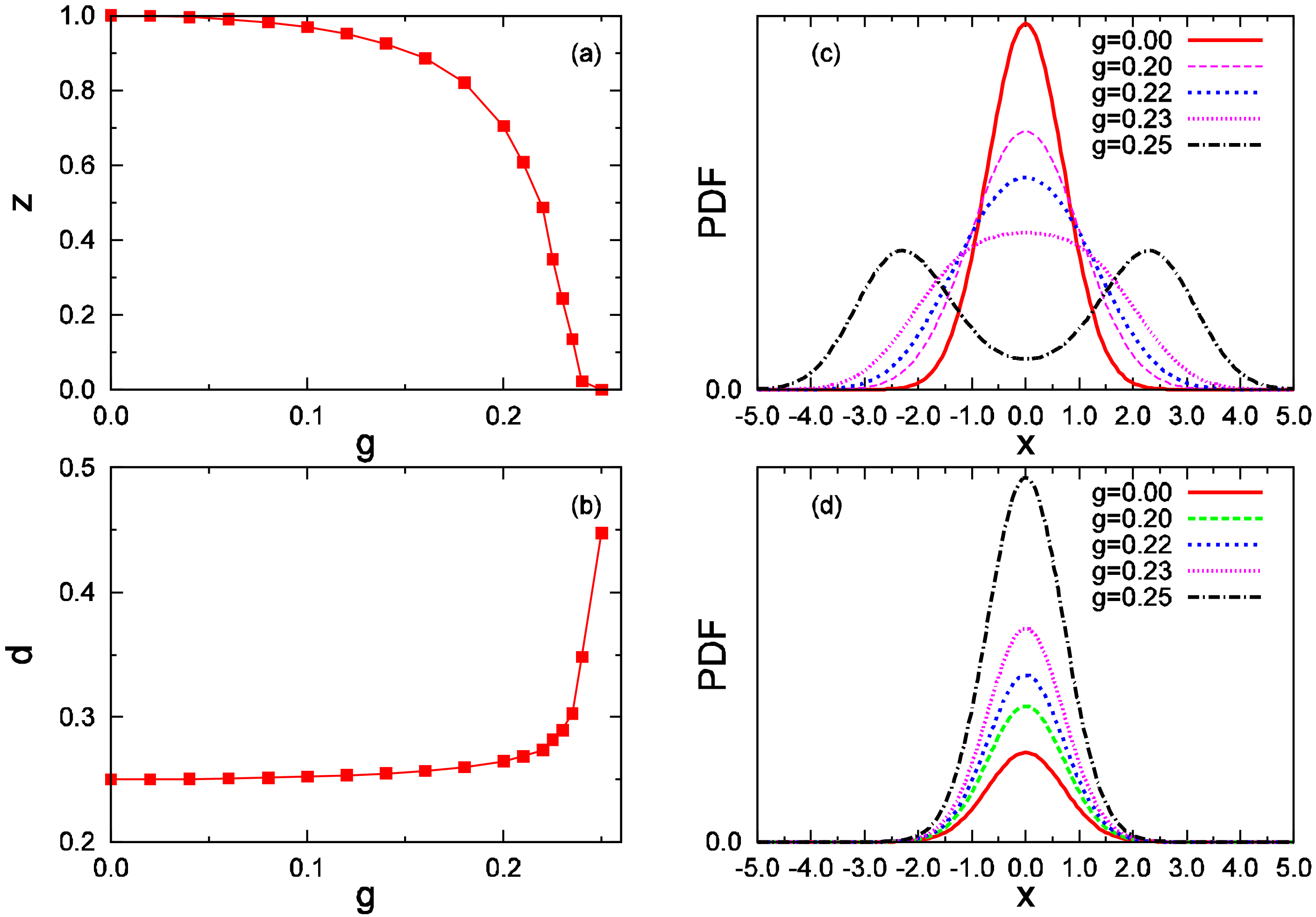
- Double Occupancy

$$d = \langle n_\uparrow n_\downarrow \rangle$$

- Orbital Correlations

$$\langle n_1 n_2 \rangle - \langle n_1 \rangle \langle n_2 \rangle$$

RESULTS (isotropic system)



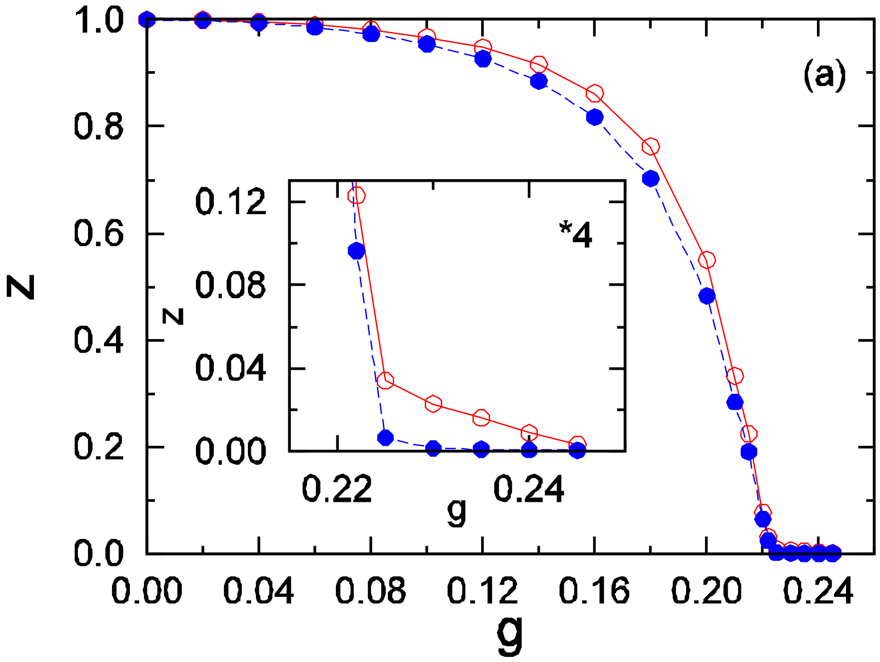
Polaron Formation

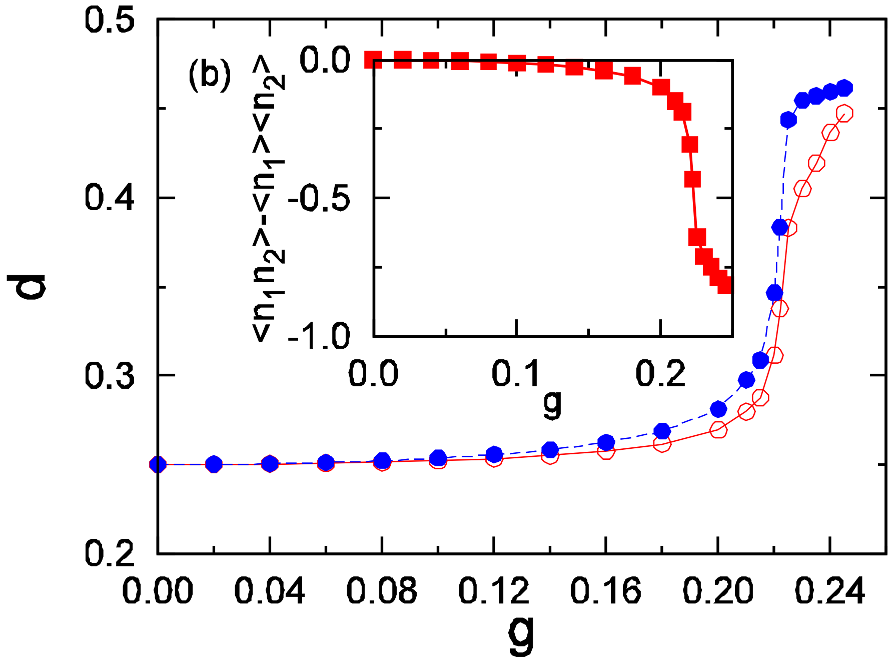
Looks for the minima of the potential $V_{at}(X)$, as if the quantum phonons were classical variables:

$$V_{at}(x) = \frac{1}{2} M\Omega_{\circ}^{2} x^{2} - g\sqrt{2M\Omega_{\circ}}\, nx,$$

- If the site is single occupied ($n = 1$), $x_{at}^{(0)} = g' / K$
- If it is empty ($n = 0$), $x_{at}^{(0)} = 0$
- If the site is double occupied (n=2) $x_{at}^{(0)} = 2g' / K$

RESULTS (anisotropic system)





RESULTS (anisotropic system)