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BI-/POLARON FORMATION AND OPTICAL CONDUCTIVITY IN THE HOLSTEIN-HUBBARD MODEL

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The polaron formation at finite densities is studied in the Holstein-Hubbard model transformed, by a modified Lang-Firsov transformation, to a polaron Hamiltonian. In a variational approach, an effective polaronic Hubbard model is derived, where squeezing effects are taken into account. The correlations are treated in the slave-boson saddle-point approximation. Including charge- and magnetically ordered states the phase diagram is calculated, and a self-trapping transition from light to heavy polarons is found. The optical conductivity of heavy polarons reveals correlation-induced structures. By a Schrieffer-Wolff transformation up to second order in the residual polaron-multiphonon interaction, an effective polaron model is derived, where for a polaronic attraction an on-site bipolaron model is obtained.

The (bi) polaron formation in strongly coupled electron-phonon systems was suggested to play an essential role also in high-T_c superconductors, e.g., for the explanation of the midinfrared optical absorption.[1] Thereby, the study of finite-density and strong correlation effects is of particular importance. We consider the Holstein-Hubbard model

$$\mathcal{H} = \mathcal{H}_{Hubbard} + \mathcal{H}_{e-ph} + \mathcal{H}_{ph} \,. \qquad (1)$$

$\mathcal{H}_{e-ph} = -\sqrt{\varepsilon_p\, \hbar\omega_0}\sum_{i\sigma}(b_i^\dagger + b_i)\, n_{i\sigma}$ is the coupling to a dispersionless phonon mode (ω_0). Treating the polaron formation by a variational approach, we perform the modified variational Lang-Firsov transformation $\tilde{\mathcal{H}} = e^S \mathcal{H} e^{-S}$, $S = \sqrt{\varepsilon_p/\hbar\omega_0}\sum_i(b_i^\dagger + b_i)[n + \gamma(n_i - n)]$ and obtain the polaron Hamiltonian

$$\tilde{\mathcal{H}} = \overline{\mathcal{H}}^0 - t \sum_{\langle i,j\rangle\sigma} (\Phi_{ij} - \overline{\Phi}_{ij})\, c_{i\sigma}^\dagger c_{j\sigma} + \mathcal{H}_{ph} + \mathcal{H}_\gamma \,, \qquad (2)$$

$$\overline{\mathcal{H}}^0 = -\tilde{\varepsilon}_p \sum_i n_i - \rho t \sum_{\langle i,j\rangle\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \tilde{U}\sum_i n_{i\uparrow} n_{i\downarrow} \,,$$

where $\Phi_{ij} = \exp\{\gamma\sqrt{\varepsilon_p/\hbar\omega_0}\,(b_i - b_i^\dagger + b_j^\dagger - b_j)\}$, $\tilde{\varepsilon}_p = \varepsilon_p[\gamma(2-\gamma)+2(1-\gamma)^2 n]$, $\tilde{U} = U - 2\varepsilon_p\gamma(2-\gamma)$, $\rho = \overline{\Phi}_{ij}$, and $\mathcal{H}_\gamma \propto (\gamma - 1)$ is given in Refs. 2,3.

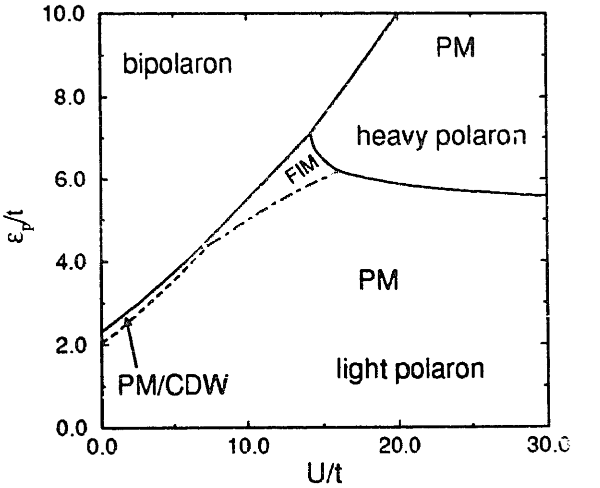

Figure 1. Phase diagram at $\hbar\omega_0/t = 0.8$, $n = 0.7$.

Including charge-density wave (CDW) and magnetically ordered, e.g. ferrimagnetic (FIM), states and taking the average of $\tilde{\mathcal{H}}$ over the transformed squeezed phonon state $\exp\{\alpha\sum_i(b_i^\dagger b_i^\dagger - b_i b_i)\}|0\rangle$, we obtain an effective polaronic model $\mathcal{H}_{eff}^0$ ($\rho = \exp(-\varepsilon_p\gamma^2\tau^2/\hbar\omega_0)$, $\tau^2 = e^{-4\alpha}$).[2] Here, we present the phase diagram (Fig. 1), where the Hubbard correlations are treated in the slave-boson saddle-point approximation. In the non-dimerized paraphase we get

$$\mathcal{H}_{eff}^0 = \overline{\mathcal{H}}^0 + \frac{\hbar\omega_0}{4}(\tau^2 + \tau^{-2})N \,. \qquad (3)$$

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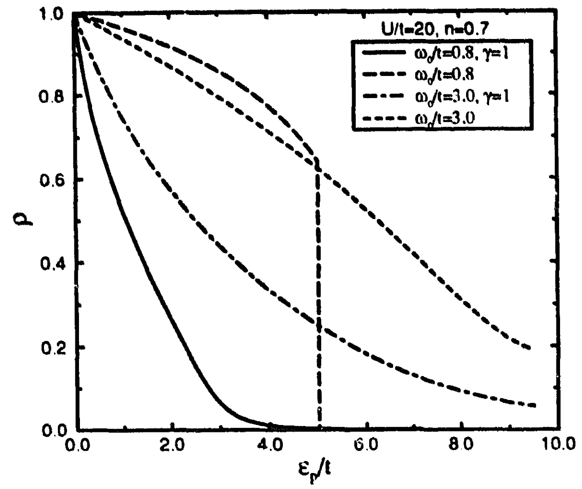

Figure 2. Polaron band narrowing ρ.

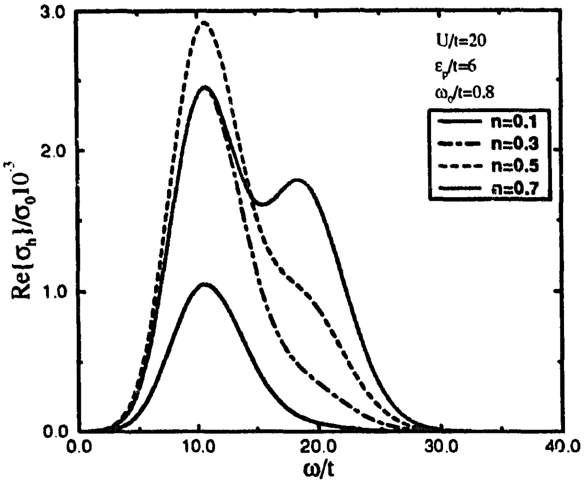

Figure 3. Polaron hopping conductivity.

Minimizing the ground-state energy with respect to τ^2 and γ, for low enough ω_0 the band narrowing ρ (Fig. 2) reveals a self-trapping transition from light ($\rho \lesssim 1$) to heavy polarons ($\rho \ll 1$) at coupling strengths of about the half-bandwidth. If (unlike Ref. 3) only τ^2 is varied ($\gamma \equiv 1$), we get a non-abrupt transition. With increasing polaron repulsion the transition is shifted to lower couplings (Fig. 1) due to the increasing correlation-induced carrier localization, and the effective polaron mass below the transition is enhanced.

Calculating from (2) the optical hopping conductivity of heavy polarons to lowest order in ρt and neglecting squeezing, we obtain the $T = 0$ absorption spectrum[3]

$$\mathrm{Re}\{\sigma_h\} \propto \frac{\rho^2}{\omega\omega_0}\{2n(1-n)B(\omega)+n^2 B(\omega-\tilde{U}/\hbar)\}\,, \quad (4)$$

$$B(\omega) = (2\varepsilon_p/\hbar\omega_0)^{\frac{\omega}{\omega_0}}\,\Gamma^{-1}(1+\omega/\omega_0)$$

shown in Fig. 3. With increasing n, the peak near $2\varepsilon_p$ (also known from single-polaron theories) increases, and the structure at about U due to polaron transitions with the creation of doubly occupied sites becomes visible. For smaller U values, only one absorption maximum may appear which broadens and shifts to higher energies with increasing n.[3]

Here, we extend our approach to the polaron formation by taking into account the residual polaron-multiphonon interaction (in the Hubbard interband terms of (2)) and perform a Schrieffer-Wolff transformation up to second order. Averaging over the squeezed phonon state and taking $\gamma \equiv 1$ we obtain the effective polaron model

$$\tilde{\mathcal{H}}_{eff} = \mathcal{H}^0_{eff} - \frac{2(\rho t)^2}{\tilde{U}}(1-\rho^2)\sum_{\langle i,j\rangle} C_i^\dagger C_j + \frac{2t^2}{\tilde{U}}(1-\rho^2)\sum_{\langle i,j\rangle}\left(\mathbf{S}_i\mathbf{S}_j - \frac{1}{4}n_i n_j\right) \quad (5)$$

with $\tilde{U}$ in $\mathcal{H}^0_{eff}$ replaced by $\tilde{U}' = \tilde{U} + 8t^2(1-\rho^2)/\tilde{U}$. The pair transfer ($C_i^\dagger = c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger$) and superexchange terms are due to virtual transitions to unpaired and paired polarons, respectively. Projecting (5), for $\tilde{U} < 0$, onto the subspace of empty and double occupancy, we get the bipolaron model

$$\mathcal{H}_b = -\varepsilon_b \sum_i N_i + t_b \sum_{\langle i,j\rangle} C_i^\dagger C_j + V \sum_{\langle i,j\rangle} N_i N_j\,, \quad (6)$$

where $N_i = C_i^\dagger C_i$, $t_b = 2(\rho t)^2(1-\rho^2)/|\tilde{U}|$, $\varepsilon_b = |\tilde{U}'| + 2\varepsilon_p$, and $V = 2t^2(1-\rho^2)/|\tilde{U}|$ is the bipolaron intersite repulsion The analysis of (5) and (6) is under study.

REFERENCES

1. X. X. Bi and P. C. Eklund, Phys. Rev. Lett. **70**, 2626 (1993).
2. U. Trapper *et al.*, Z. Phys. B **93**, 465 (1994).
3. H. Fehske *et al.*, Z. Phys. B **94**, 91(1994).