PROPERTIES OF EXCITON AND EXCITON-POLARON: EXACT NUMERIC SOLUTION. A.S. Mishchenko^{1,2}, N. Nagaosa^{1,3}, N.V. Prokof'ev⁴, B.V. Svistunov², and E.A. Burovski²

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We developed a Monte Carlo method of calculation of Green function in imaginary times which is free from systematic errors for the case of quasiparticle in a boson bath [1,2]. A novel procedure of analytic continuation [1], which is free from systematic errors, provides a tool for study of optical spectra of quasiparticles. Our method does not rely on the specific form of the quasiparticle dispersion and properties of boson bath.

As a specific examples we consider Frohlich [1] and Holstein polaron. Calculating within free from approximation approach the current-current correlation function and making the numeric analytic continuation we obtain exact data for the optic response of polarons.

We generalize the method to get a precise numeric solution of the irreducible two-body problem and apply it to excitons in solids [3,4]. Our method does not rely on the specific form of the electron and hole dispersion laws and is valid for any attractive electron-hole potential. We establish limits of validity of the Wannier (large radius) and Frenkel (small radius) approximations, present accurate data for the intermediate radius excitons, and give evidence for the charge transfer nature of the monopolar exciton in mixed valence materials.

Finally, we discuss generalization of the method to the case of exciton in phonon field and extend the technique for the t-J model [5] to the case of interaction of the hole with optical phonons.

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- Description of the techniques of exact generation of Matsubara Green function of the quasiparticles in bosonic bath.
- Description of the exact method of analytic continuation to the real energies.
- Generalization of the technique to two-particle Green function: exciton.
- Several application of the technique: Rashba-Pekar exciton, charge-transfer exciton.
- Magical number '4' for Fröhlich polaron. Lehman function and optical response.
- Further generalization: quasiparticle in two bosonic bathes. t-J model in phonon field.

Quasiparticle in the boson bath: Fröhlich polaron and Rashba-Pekar exciton

$$H = H_{\epsilon} + H_{\rm pb} + H_{\rm e-ph} \; . \label{eq:H}$$

Quasiparticle dispersion:

$$H_{
m e} = \sum_{f k} arepsilon({f k}) \, a_{f k}^{\dagger} a_{f k} \; .$$

Boson dispersion:

$$H_{_{\mathrm{ph}}} = \sum_{\mathbf{q}} \omega_{\mathbf{q}} b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} \; .$$

Quasiparticle-boson interaction:

$$H_{\mbox{\tiny e-ph}}\,=\,\sum\limits_{{\bf k},{\bf q}}\,V({\bf q})\,\left(b_{\bf q}^{\dagger}-b_{-{\bf q}}\right)\,a_{{\bf k}-{\bf q}}^{\dagger}a_{{\bf k}}$$

Although presented technique is suitable for arbitrary dispersion of quasiparticle, arbitrary dispersion of phonons and valid for arbitrary vortex of quasiparticle-boson interaction, I'll show the results for the continuous model

$$\varepsilon(\mathbf{k}) = k^2/2; \quad \omega_{\mathbf{q}} = 1.$$

in two specific cases.

I. Fröhlich polaron (long-range interaction):

$$V_{FR}(\mathbf{q})\,=\,i\,\left(2\sqrt{2}lpha\pi
ight)^{1/2}\,rac{1}{q}\,.$$

II. Exciton-polaron (short-range interaction):

$$V_{EX}(\mathbf{q}) = V_{FR}(\mathbf{q}) \left\{ \frac{1}{[1 + (p_e a_B q/2)^2]^2} - \frac{1}{[1 + (p_h a_B q/2)^2]^2} \right\}.$$

Here $p_{e,h} = m_{e,h}/(m_e + m_h)$ and a_B is the Bohr radius.

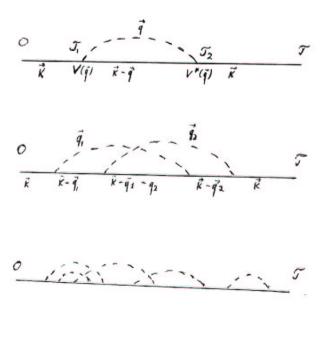
Diagrammatic Feinman expansion for Matsubara Green function

Expansion can be transformed into a series of **positively definite** integrals with ever increasing number of integration variables.

$$G(\mathbf{k},\tau) = \sum_{n=0,2,4,...,\tau}^{\infty} \int_{\tau}^{0} d\tau_{n} \int_{\tau_{n}}^{0} d\tau_{n-1} \dots \int_{\tau_{2}}^{0} d\tau_{1} \times \int_{\tau_{1}}^{0} d\mathbf{q}_{2} \dots \int d\mathbf{q}_{n/2} |V(\mathbf{q}_{1})|^{2} |V(\mathbf{q}_{2})|^{2} \dots |V(\mathbf{q}_{n/2})|^{2} \times G^{(0)}(\mathbf{k},\tau_{1}-0)G^{(0)}(\mathbf{k}-\mathbf{q}_{1},\tau_{2}-\tau_{1})\dots G^{(0)}(\mathbf{k},\tau-\tau_{n-1}) \\ D(\mathbf{q}_{1},\tau'-\tau_{1})\dots D(\mathbf{q}_{1},\tau_{n}-\tau'')$$

Here

$$G^{(0)}(\mathbf{k},\tau) = \exp\{-(\varepsilon(\mathbf{k})-\mu)\tau\}; \ D(\mathbf{q},\tau) = \exp\{-\omega_{\mathbf{q}}\tau\}$$



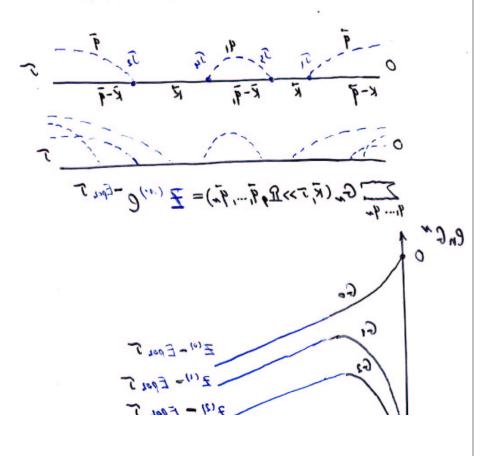
$$G_{N}(\mathbf{k},\tau,\mathbf{q}_{1},...,\mathbf{q}_{N}) = \langle \operatorname{vac} \mid b_{\mathbf{q}_{N}}(0)...b_{\mathbf{q}_{1}}(0)a_{\mathbf{p}}(0)a_{\mathbf{p}}^{\dagger}(\tau)b_{\mathbf{q}_{1}}(\tau)_{\mathbf{t}_{\mathbf{t}_{\mathbf{t}}}^{\dagger}}b_{\mathbf{q}_{N}}(\tau)^{\dagger} \mid \operatorname{vac} \rangle$$

Where

$$\mathbf{p} = \mathbf{k} - \sum_{j=1}^{N} \mathbf{q}_{j}$$

This gives both energy and phonon distribution of the quasiparticle

 $G_N(\mathbf{k},\tau \gg \Omega, \mathbf{q}_1,...,\mathbf{q}_N) = \mid \phi_N(\mathbf{k},\mathbf{q}_1,...,\mathbf{q}_N) \mid^2 e^{-F_{pol}(\mathbf{k})}$



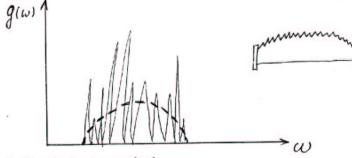
$$f = \frac{1}{16ktronjx} + \frac{1}{1$$

Spectral density $g(\omega)$.

$$g_{\mathbf{k}}(\omega) = \sum_{\nu} \delta(\omega - E_{\nu}(\mathbf{k})) |\langle \nu | a_{\mathbf{k}}^{\dagger} | \mathrm{vac} \rangle|^{2}$$

$$G(au)=\int_{0}^{\infty}g(\omega)e^{-\omega au}d\omega$$

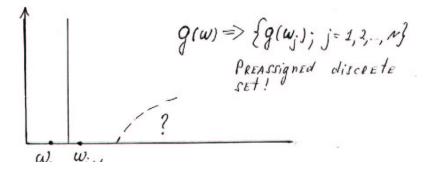
This equation is "ill-defined" problem and solution is difficult due to "saw-tooth" instability.



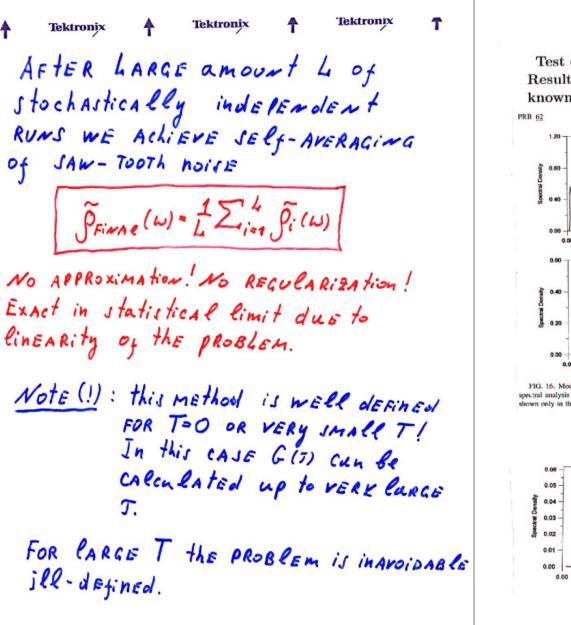
1. Regularization method.

$$+\int_0^\infty F(g(\omega),g'(\omega),g''(\omega))$$

2. Maximal Entropy method.

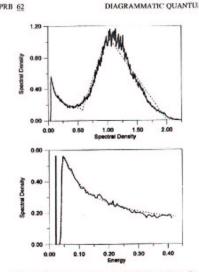


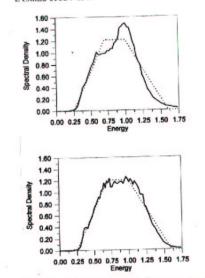
WE PARAMETRISE the spectral \$ \$(w) FUNCTION GIW, BY A JET OF RECTANGULARS: $C = \{\{h_t, W_t, C_t\}; t = 1, ..., K\}$ 62 It how = 1 (1) he, We, Ct are continuous VARIABLES (2) K is not fixed WE START FROM RANdomLA ChosEN INITIAL CONFIGURATION C AND PERFORM stochAstically RANdom minimization of the MEASURE $\int \frac{\int \hat{G}(T) - \hat{G}(T)}{\int \int T} dT \quad \hat{G}(T) = \int \hat{g}(\omega) \hat{e}$ 1 K is not Fixed during minimization DROCEDURE All initial configurations C are are statistically in dependent.
 (3) Each final optimal configuration



Test of the spectral analysis.

Results, which follow, can not be obtained by any other known method.





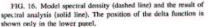
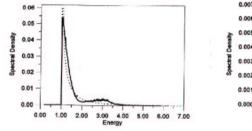


FIG. 17. The model spectrum (dashed lines) and results of spectral analysis (solid lines) for $\eta = 10^{-2}$ (upper panel) and $\eta = 10^{-3}$ (lower panel).



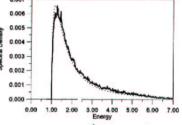
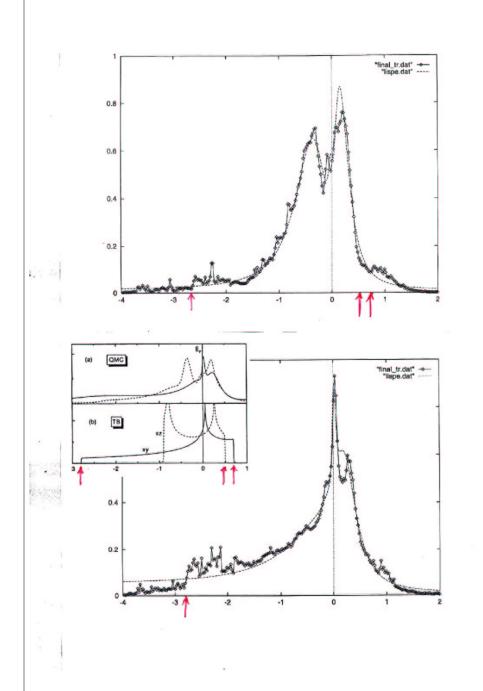
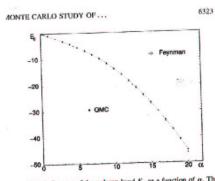
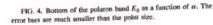


FIG. 13. The comparison of the numeric results (solid lines) and the perturbation-theory curves (dashed lines) for the spectral density of Fröhlich model with $\alpha = 0.05$ (upper panel) and the short-range interaction model with $\alpha = 0.05$ and $\kappa = 1$ (lower panel).



Fröhlich polaron.





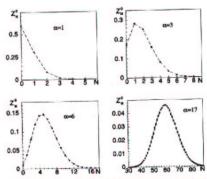


FIG. 7. Partial contributions of N-phonon states to the polaron ground state for various values of α . Error bars are shown, but are typically smaller than the point size. (The dushed lines are to guide the eye.)

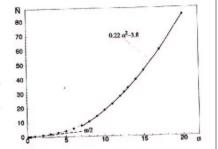


FIG. 8. The average number of phonons in the polaron ground state as a function of α . Filled circles are the MC data (calculated to the relative accuracy better than 10^{-3}), the dashed line is the perturbation theory result (4.1), and the solid line is the parabolic fit for the strong coupling limit.

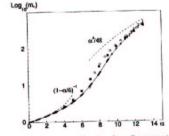
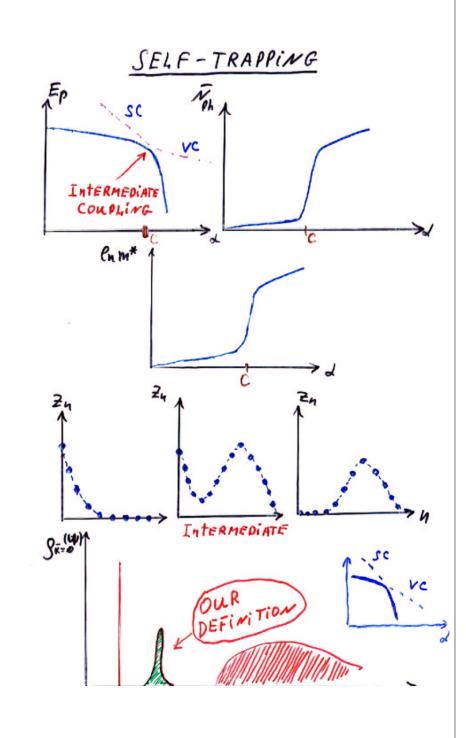
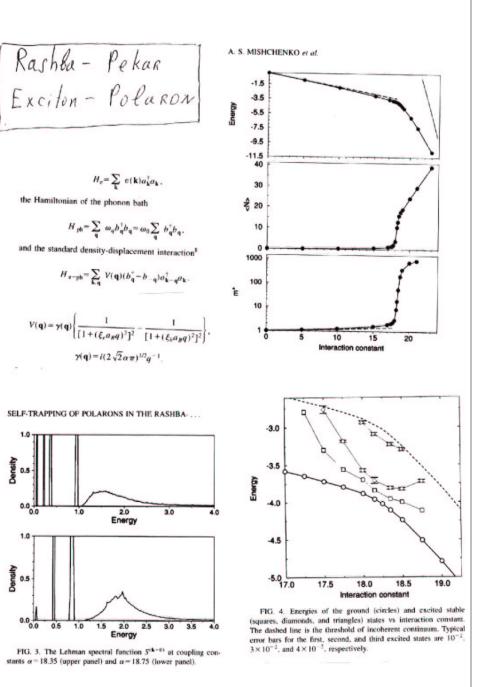


FIG. 5. Effective mass as a function of coupling parameter. Our MC data (circles interpolated by solid line; error bars are shown, but for $\alpha < 9$ they are smaller than the point size, and as small as $10^{-3}m_{+}$ for $\alpha < 6$) are compared with perturbation theory and strong-coupling-limit results (dashed lines), Feynman's approach (squares), and Feranchuk *et al.* variational approach (diamonds).



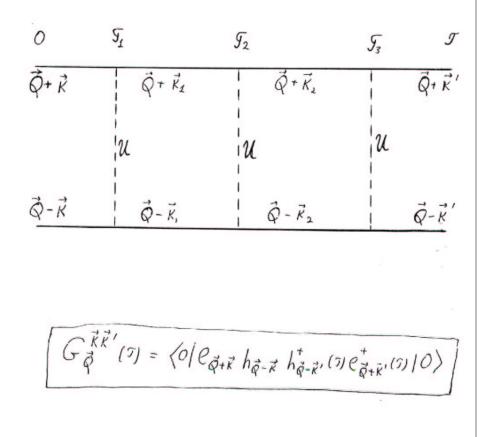


PRL, vol. 87, p. 186402 (1001) E. Burrovski. Diagrammatic expansion for Coulomb ladder.

$$H_0 = \sum_{\mathbf{k}} \varepsilon_c(\mathbf{k}) e_{\mathbf{k}}^{\dagger} e_{\mathbf{k}} + \sum_{\mathbf{k}} \varepsilon_v(\mathbf{k}) h_{\mathbf{k}} h_{\mathbf{k}}^{\dagger}, \qquad (1)$$

$$H_{\rm e-h} = -N^{-1} \sum_{\mathbf{p}\mathbf{k}\mathbf{k}'} \mathcal{U}(\mathbf{p}, \mathbf{k}, \mathbf{k}') e^{\dagger}_{\mathbf{p}+\mathbf{k}} h^{\dagger}_{\mathbf{p}-\mathbf{k}'} h_{\mathbf{p}-\mathbf{k}'} e_{\mathbf{p}+\mathbf{k}'}.$$
 (2)

Here $e_{\mathbf{k}}$ ($h_{\mathbf{k}}$) is the electron (hole) annihilation operator, $\varepsilon_{c}(\mathbf{k})$ ($\varepsilon_{v}(\mathbf{k})$) is the conduction (valence) band dispersion law, N is the number of lattice sites, and $\mathcal{U}(\mathbf{p}, \mathbf{k}, \mathbf{k}')$ is an attractive interaction potential.



Intermediate radius exciton.

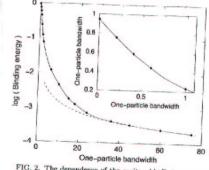


FIG. 2. The dependence of the exciton binding energy on the bandwidth $E_e = E_e$. Statistical errors are less than $5 \cdot 10^{-3}$ in relative units. The dashed line corresponds to the Wannier model. The solid line is the cubic spline, the derivatives at the right and left ends being fixed by the Wannier limit and perturbation theory, respectively. Insert: the initial part of the plot.

(a)

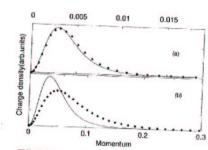
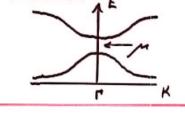


FIG. 3. The momentum dependence of the charge density $|\xi_{pk}(g.s.)|^2 k^3$ for $E_e = E_v = 60$ (a) and $E_e = E_u = 10$ (b). Solid lines are the Wannier model result. Statistical errors are typically of order 10-4.



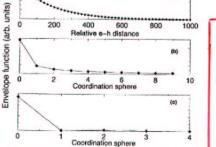
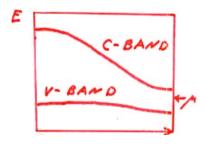


FIG. 4. The wave function of internal motion in real space: (a) Wannier $[E_c = E_v = 60]$; (b) intermediate $[E_c = E_v - 10]$; (c) near-Frenkel $[E_c = E_v = 0.4]$ regimes [21]. The solid line in the panel (a) is the Wannier model result while solid lines in other panels are to guide an eye only. Statistical errorbars are of order 10-4

0.0 -0.05 5 -0.1 5 10 Coordination sphere number FIG. 5. The wave function of internal motion in real space

for the optically forbidden monopolar $(W(2\mathbf{p}) = 0)$ exciton defined by the following model parameters: $\tilde{E}_c = 1.5$, $\tilde{E}_v = 0$, $E_c = -0.5, E_v = 0.05, \epsilon = 10, V_0 = 0.578$. Statistical errorbars are of order 10⁻⁴.



Diagrammatic expansion for charge transfer exciton: twolevel system.

Quasiparticle dispersion for two bands i = 1, 2:

$$H_{\epsilon} \,=\, \sum\limits_{i=1}^{2} \sum\limits_{\mathbf{k}} \,arepsilon_{i}(\mathbf{k}) \, a_{i,\mathbf{k}}^{\dagger} a_{i,\mathbf{k}} \;.$$

Boson dispersion:

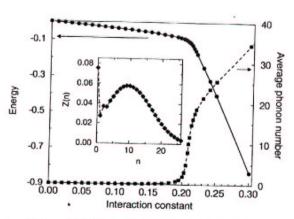
$$H_{\mbox{\tiny ph}}\,=\,\sum_{{f q}}\,\omega_{{f q}}\,b_{{f q}}^{\dagger}b_{{f q}}\,.$$

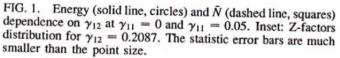
Quasiparticle-boson interaction:

$$H_{\text{\tiny s-ph}} \,=\, \sum_{i=1}^2 \sum_{j=1}^2 \sum_{\mathbf{k},\mathbf{q}} \, V_{ij}(\mathbf{q}) \, \left(b_{\mathbf{q}}^\dagger - b_{-\mathbf{q}} \right) \, a_{i,\mathbf{k}-\mathbf{q}}^\dagger a_{j\mathbf{k}} + h.c.$$

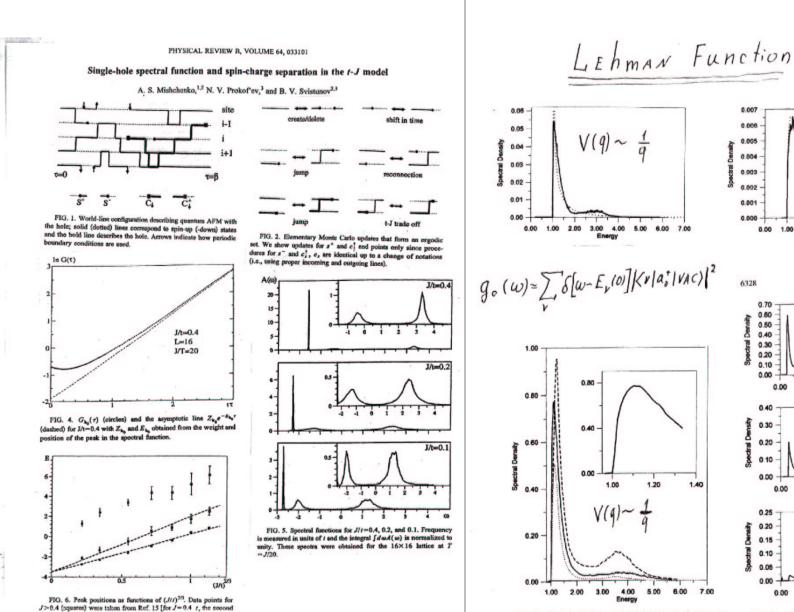
$$G_{11}(5) = \frac{1}{G_{11}^{(0)}(5)} \frac{1}{V_2} \frac{1}{V_2}$$

16 TOPOLOGICAL CLASSES. A.S. Mishchank, and N. NAGAOSA Phys. Rev. Lett. v. 86, p. 9624(2001) Charge transfer two-level exciton-polaron.





SElf-TRApping is possible in ID in spite of RASHBA-TOYOZAWA THEOREM!



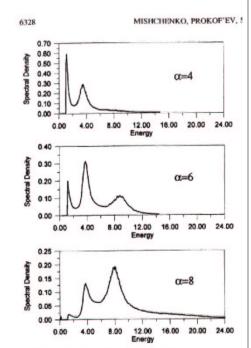
peak was not resolved in Ref. 15 because of large error bars in

 $G(\tau)$]. The two lines are fits $y(x) = a + b(J/t)^{2/3}$ with a

= -3.5 t, b=3.77 t for the ground state, and b=5.5 t for the

first peak in continuum.

FIG. 14. The spectral density of Fröhlich polaron for $\alpha = 0.5$ (dotted line), $\alpha = 1$ (solid line), and $\alpha = 2$ (dashed line), with energy counted from the position of the polaron. The initial fragment of the spectral density for $\alpha = 1$ is shown in the inset.



0.00 1.00 2.00 3.00 4.00 5.00 6.00 7.00

0.007

0.006

0.005

0.004 å

0.003

0.002

0.001

0 000

FIG. 15. Evolution of spectral density with α in the crossover region from intermediate to strong couplings. (The polaron groundstate peak is shown only for $\alpha = 8$. Note, that the spectral analysis still resolves it, despite its very small weight < 10⁻³.) The energy is counted from the position of the polaron.

$$\frac{RE lation to the REAL PART}{0+ optical conductivity.}} =$$

$$m = \hbar - e = 1; T = 0.$$

$$\left\{ \hat{\vec{p}}(\tau) \hat{\vec{p}}(o) \right\} = \int_{0}^{\infty} e^{-\omega T} \hat{\vec{Q}}^{(t)}(\omega) d\omega$$

$$\int_{0}^{\infty} \hat{\vec{p}}(\tau) \hat{\vec{p}}(o) \hat{\vec{p}}(\sigma) = \int_{0}^{\infty} \hat{\vec{Q}}^{(t)}(\omega) d\omega$$

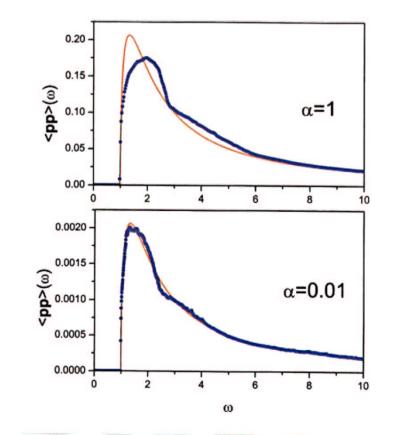
$$\int_{0}^{\infty} \hat{\vec{p}}(\tau) \hat{\vec{p}}(\sigma) \hat{\vec{p}}(\sigma) = \int_{0}^{\infty} \hat{\vec{Q}}^{(t)}(\omega) d\omega$$

$$\int_{0}^{\infty} \hat{\vec{p}}(\tau) \hat{\vec{p}}(\sigma) \hat{\vec{p}}(\sigma) = \int_{0}^{\infty} \hat{\vec{Q}}^{(t)}(\omega) d\omega$$

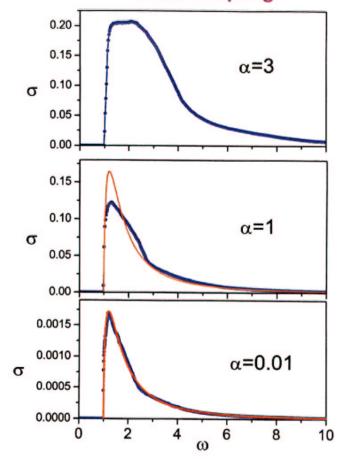
$$\int_{0}^{\infty} \hat{\vec{p}}(\tau) \hat{\vec{p}}(\sigma) \hat{\vec{p}}(\sigma) \hat{\vec{p}}(\sigma) = \int_{0}^{\infty} \hat{\vec{p}}^{(t)}(\omega) d\omega$$

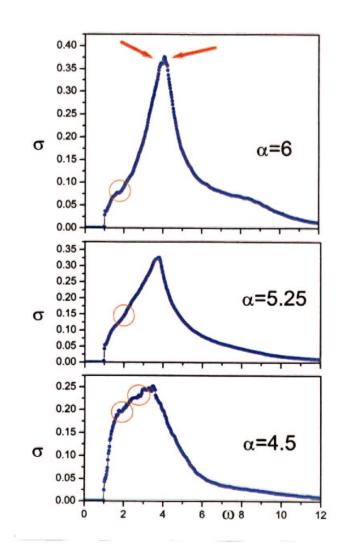
$$\left\langle \hat{\vec{p}}(\tau) p(o) \right\rangle =$$

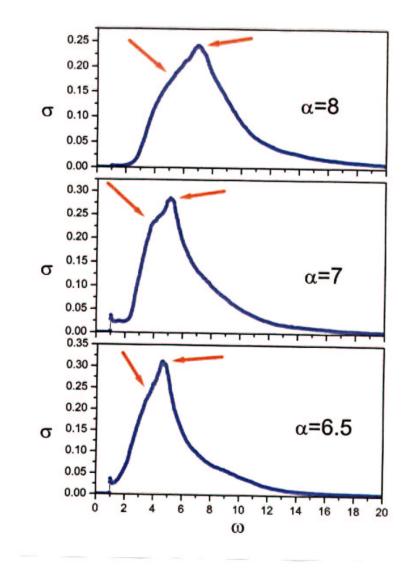
$$= \frac{4}{2} \frac{4}{9} \int_{0}^{9} dt \sum_{n=0}^{\infty} \int_{0}^{9} d\tau_{n} \int_{0}^{7} d\tau_{n-1} \dots \int_{0}^{7} d\tau_{n} \vec{K}(\tau + \tau) \vec{K}(\tau) \times \int_{0}^{7} d\vec{q}_{n} \prod (\vec{r}_{1} \vec{q}_{n}) |^{2} \dots \int_{0}^{7} d\vec{q}_{n} \prod (\vec{r}_{1} \vec{q}_{n}) |^{2} \vec{q}_{n}) |^{2} \vec{q}_{n} |^{2} \vec{q}_{n} |^{2} \vec{q}_{n} |^{2} \vec{q}_{n}) |^{2} \vec{q}_{n} |$$



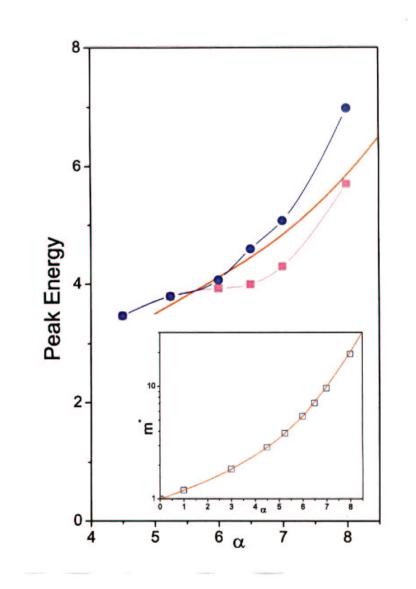








S.



$$egin{aligned} H_{t-J} &= -t\sum\limits_{i,j}^{nn}\sum\limits_{\sigma}\left(c_{i\sigma}^{\dagger}c_{j\sigma}+h.c.
ight) + J\sum\limits_{i,j}^{nn}\mathbf{S}_{i}\mathbf{S}_{i}\ H_{hole-ph} &= \omega\sum\limits_{i}b_{i}^{\dagger}b_{i}+\gamma\sum\limits_{i}\sum\limits_{\sigma}c_{i\sigma}^{\dagger}c_{i\sigma}\left(b_{i}^{\dagger}+b_{i}
ight) \end{aligned}$$

Spin-wave approximation

$$\begin{split} H_{t-J} &= \sum_{k} \epsilon_{k} h_{k}^{\dagger} h_{k} + \sum_{k} \kappa_{k} \alpha_{k}^{\dagger} \alpha_{k} + \sum_{k,q} M_{k,q} \left[\alpha_{q} h_{k}^{\dagger} h_{k-q} \alpha_{q}^{\dagger} h_{k-q}^{\dagger} h_{k} \right] \\ H_{hole-ph} &= \omega \sum_{i} b_{k}^{\dagger} b_{k} + \gamma \sum_{k,q} h_{k}^{\dagger} h_{k-q} \left(b_{q}^{\dagger} + b_{-q} \right) \\ \mathbf{Where} \end{split}$$

$$\kappa_k = 2J\sqrt{1-k^2}$$

$$\lambda_k = (\cos k_x + \cos k_y)/2$$

$$M_{k,q} = 4t(u_q\lambda_{k-q} + v_q\lambda_k)$$

$$u_k = \sqrt{\frac{1+\nu_k}{2\nu_k}}; v_k = -sign(\lambda_k)\sqrt{\frac{1-\nu_k}{2\nu_k}}$$

$$\nu_k = \sqrt{1-\lambda_k}$$

