Many-body effects in the normal-state polaron system

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Dielectric response function of small polarons (SP's) is studied. The Debye radius is small, which reduces a short-range Coulomb repulsion to the magnitude of the order of the small-polaron (SP) bandwidth. Polaron-polaron attraction is enhanced by screening. A critical temperature of the bipolaron formation is found. The dielectric response becomes dynamic in a very low-frequency region. A multiphonon diagram technique is developed to obtain vibration excitations, that are a mixture of phonons with polaronic plasmons. A microscopic model of the anomalous extra modes, observed in neutron-scattering experiments in La_2CuO_4, is proposed.

Holstein,[1] and some other workers (for review, see the books in Ref. 1) showed in the framework of the one-electron problem that at some critical value of the coupling with phonons

$$\lambda > \lambda_c \ , \tag{1}$$

the electron prefers tunneling in a very narrow polaronic band, having a half bandwidth

$$W = D\exp(-g^2) \ , \tag{2}$$

which lies well below the bare one, with the half bandwidth D. Here

$$g^2 = \lambda \frac{D}{\omega_0} \ , \tag{3}$$

with ω_0 being the characteristic phonon frequency. It has now become clear,[2] that the traditional theory of a many-electron system[3] rules out the possibility of the local deformation of the lattice, thus preventing the system from relaxing into the lowest-energy state.

From a more general viewpoint, the instability of a boson vacuum develops in a system of interacting bosons and electrons under the critical value of λ, resulting in a polaron collapse of the electron band. A simple estimation with the perturbation theory in $1/\lambda$ shows[4] a jump-like transition from wide-band electrons with the power-law enhanced effective mass[3] to narrow-band small polarons with an exponentially large effective mass, Eq. (2), at

$$\lambda_c = \frac{1}{(2z)^{1/2}} < 1 \ , \tag{4}$$

which agrees well with some variational[5,6] and Monte Carlo[7] calculations, z being the coordination lattice number.

This condition demonstrates the necessity of the development of a theory for a many-electron system, strongly coupled to phonons, taking into account the nonadiabatic character of the carrier motion with the renormalized Fermi energy:

$$\varepsilon_F = E_F\exp(-g^2) < W < \omega_0 \ . \tag{5}$$

Low-temperature properties of a many-polaron system were first studied in Ref. 8. The ground state of electrons strongly coupled to phonons occurs as a charged Bose liquid, consisting of singlet or triplet pairs [small bipolarons (SB's)] with the charge $2e$ and moving in their narrow band with a heavy effective mass $m^{**} > m^*$.

However, not so much was done for the understanding of many-body effects in the normal state of SP's at temperatures well above the temperature of SB formation. In our recent paper[9] we developed a multiphonon diagram technique to obtain renormalized phonons, using the inverse coupling constant λ^{-1} as a small parameter.

In this paper, the dielectric response of a many-polaron system and the influence of the polaron-polaron interaction on the phonon frequencies are studied. In the first section, using the familiar Holstein-Lang-Firsov transformation[1] I determine a zero-order SP Green function (GF), which contains the main part of the electron-phonon interaction in a diagonal form leaving aside the rest in the form of the polaron-polaron interaction and of the residual SP-phonon interaction. For those interactions I adopt the ordinary random-phase approximation (RPA) and the perturbation theory in the inverse coupling λ^{-1}, correspondingly. With RPA the static and the dynamic response of SP's are calculated. Because of the exponentially large mass renormalization, Eq. (2), the Debye radius and the plasma frequency are much smaller than those for a weakly coupled electron-phonon system, and temperature dependent at $T > W$. SP's screen effectively the on-site Coulomb repulsion, reducing it to the value of the order of W. On the contrary the on-site attraction, if it exists, is enhanced by the many-body effects. In Sec. II I generalize our expression for the phonon self-energy,[9] taking into account the polaron-polaron interaction. The SP polarization loop is obtained in a site representation. The spectrum of vibrational excitations is found. One of the most interesting results is that phonons are coupled with polaronic plasmons forming a type of vibration excitations, which are a mixture of the ordinary phonon and the low-frequency plasmon. These vibrations are used to explain the extra modes, observed in neutron-scattering experiments[10] in high-T_c metal oxides.

I. GREEN FUNCTION AND DIELECTRIC RESPONSE OF SP's

After the familiar Holstein-Lang-Firsov transformation[1] and averaging with the phonon density matrix one obtains the free-polaron GF in the form (see for details Ref. 9)

$$G_{\mathbf{k}}(\omega_n)=(i\omega_n-\varepsilon_{\mathbf{k}}+\varepsilon_F)^{-1} \tag{6}$$

with $\omega_n=\pi T(2n+1)$, which corresponds in the site representation to

$$G_{ij}(\omega_n)=\frac{1}{N}\sum_{\mathbf{k}}\exp[-i\mathbf{k}\cdot(\mathbf{m}-\mathbf{n})](i\omega_n-\varepsilon_{\mathbf{k}}+\varepsilon_F)^{-1} . \tag{7}$$

Here

$$\epsilon(\mathbf{k})=\sum_{\mathbf{m}}\sigma(\mathbf{m})\exp(i\mathbf{k}\cdot\mathbf{m}) \tag{8}$$

is the SP energy dispersion in a narrow polaronic band,

$$\sigma(\mathbf{m}-\mathbf{n})=t(\mathbf{m}-\mathbf{n})\exp[-g^2(\mathbf{m}-\mathbf{n})] \tag{9}$$

is the SP hopping integral, averaged with the density matrix, $\sigma=\langle\hat{\sigma}_{ij}\rangle$,

$$g^2(\mathbf{m})=\frac{1}{2N}\sum_{\mathbf{q}}\gamma^2(\mathbf{q})\coth\left[\frac{\omega(\mathbf{q})}{2T}\right][1-\cos(\mathbf{q}\cdot\mathbf{m})] , \tag{10}$$

with T being the lattice temperature, $t(\mathbf{m})$ is a bare hopping integral in a rigid lattice, and N is the number of lattice sites. The normalization of electron energies is chosen in such a way that the atomic level with the polaronic shift,

$$E_p=\frac{1}{2N}\sum_{\mathbf{q}}\gamma^2(\mathbf{q})\omega(\mathbf{q}) , \tag{11}$$

corresponds to zero energy with $\gamma(\mathbf{q})$ and $\omega(\mathbf{q})$ being the matrix element of the electron- phonon Fröhlich interaction and phonon frequencies respectively.

The residual interaction, which remains after this procedure, is a polaron-phonon one:[9]

$$H_{p\text{-ph}}=\sum_{i,j}[\hat{\sigma}_{ij}-\sigma(\mathbf{m}-\mathbf{n})]c_i^\dagger c_j , \tag{12}$$

with

$$\hat{\sigma}_{ij}=t(\mathbf{m}-\mathbf{n})\exp\left[\sum_{\mathbf{q}}d_{\mathbf{q}}[u_i(\mathbf{q})-u_j(\mathbf{q})]-\text{h.c.}\right] ,$$

$$u_i(\mathbf{q})=(1/\sqrt{2N})\gamma(\mathbf{q})\exp(i\mathbf{q}\cdot\mathbf{m}) ,$$

and the direct (density-density) polaron-polaron interaction (see, for example, Ref. 8),

$$H_{p\text{-}p}=\frac{1}{2}\sum_{i,j}v(\mathbf{m}-\mathbf{n})c_i^\dagger c_j^\dagger c_j c_i , \tag{13}$$

where $i=(\mathbf{m},s)$, $j=(\mathbf{n},s)$, $c_i^\dagger(c_i)$ and $d_{\mathbf{q}}^\dagger(d_{\mathbf{q}})$ are electron and phonon operators, and $\mathbf{m}$ and s are a lattice vector and spin, respectively.

As opposed to the usual Fröhlich interaction the polaron-phonon one, Eq. (12), contains multiphonon vertices which are dominant. We further show, that this interaction may be treated as perturbation at $\lambda>1$ both for phonon and polaron GF's (see, also Ref. 11). At large distances the polaron-polaron interaction, Eq. (13), is an effective Coulomb repulsion, $e^2/|\mathbf{m}-\mathbf{n}|\epsilon$, with ϵ being a dielectric constant. This fact makes it possible to treat $H_{p\text{-}p}$ with the usual RPA at least for long-wave excitations. At short distances the polaron-polaron interaction may be attractive, which leads to instability versus SB formation at a low enough temperature.[8]

We consider the polaron-polaron and the polaron-phonon correlations only in the normal state, assuming that the temperature is above the critical temperature of SB's formation (see below), which, in turn, is higher than the critical temperature of the superconducting (superfluid) transition.

Taking into account the exponential smallness of the polaron bandwidth one can obtain the "total localization approximation" (TLA) for the polaron GF:

$$G_{ij}(\omega_n)=\delta_{ij}(i\omega_n+\varepsilon_F)^{-1} , \tag{14}$$

which is useful in calculations in the temperature range $T\gg W$. In TLA:

$$\varepsilon_F=T\ln\left[\frac{\nu}{2-\nu}\right] , \tag{15}$$

where ν is the atomic concentration of carriers, and the SP distribution function:

$$n_{\mathbf{k}}=\left[\exp\left[\frac{\varepsilon_{\mathbf{k}}-\varepsilon_F}{T}\right]+1\right]^{-1}\simeq\frac{\nu}{2}\left[1-\frac{\varepsilon_{\mathbf{k}}(2-\nu)}{2T}\right] . \tag{16}$$

If one takes into account the finite polaronic bandwidth $\varepsilon_k\sim W$ one obtains corrections of the order of $\lambda^{-1}\exp(-g^2)$. They are exponentially small compared to the main power-law contribution from $H_{p\text{-ph}}$ proportional to λ^{-2}.

This contribution of the second and highest orders k in $H_{p\text{-ph}}$ to the polaron self-energy Σ_p^k comes from multiphonon virtual processes (for details see Refs. 4 and 11):

$$\left|\Sigma_p^k\right|\simeq\frac{D^k}{zE_p^{k-1}} . \tag{17}$$

The second-order contribution lowers the energy and increases the SP effective mass, while the third-order one diminishes it.

Comparing this contribution with the polaronic shift E_p, Eq. (11), one obtains the criterion of the SP's existence, Eq. (4), with $\lambda=E_p/D$. For a smoothly varying electron density of states (DOS) this definition of the electron-phonon coupling constant is identical to the usual one.[12] Thus I conclude once more (see Ref. 2) that, at least for the Fröhlich interaction the usual strong-coupling theory,[12] which does not take into account the polaron collapse of the electron band, is unacceptable.

In RPA the effect of the polaron-polaron interaction may be described by the dielectric "constant" $\epsilon(\omega,\mathbf{q})$, which gives the response of SP's to longitudinal electric fields of the arbitrary wave vector $\mathbf{q}$ and the frequency ω.

From this the screening behavior of the system and the plasmon frequency can be calculated:

$$\epsilon(\omega,\mathbf{q})=1-2v(\mathbf{q})\sum_{\mathbf{k}}(n_{\mathbf{k}+\mathbf{q}}-n_{\mathbf{k}})(\omega-\varepsilon_{\mathbf{k}}+\varepsilon_{\mathbf{k}+\mathbf{q}})^{-1}\ , \tag{18}$$

where $v(\mathbf{q})=N^{-1}\sum_{\mathbf{m}}v(\mathbf{m})\exp(-i\mathbf{q}\cdot\mathbf{m})$ is the Fourier component of the polaron-polaron interaction. First I consider the static dielectric constant. For $T=0$ in the long-wave limit, $q\to 0$, we obtain the usual Debye screening:

$$\epsilon(0,q)=1+(qr_d)^{-2} \tag{19}$$

with the Debye radius

$$r_d=\left[\frac{\epsilon}{4\pi e^2N_p(0)}\right]^{1/2}, \tag{20}$$

where $N_p(0)=N(0)\exp(g^2)$ is the DOS in the polaronic band on the Fermi level, which is exponentially enhanced compared to the bare DOS $N(0)$. One can see from Eq. (20) that the Debye radius of SP's is much smaller than that of bare electrons due to the strong enhancement of their effective mass.

Now I obtain the temperature behavior of the SP response and show that the correlation effect enhances the short-range attraction opposite to the short-range repulsion.

At temperatures $T\gg W$ one can use TLA, Eq. (16), with the following result:

$$\epsilon(0,\mathbf{q})=1+\frac{\nu(2-\nu)v(\mathbf{q})N}{2T}\ . \tag{21}$$

The screened short-range interaction is given by

$$\tilde{U}=\frac{UT}{T\pm T^*}\ , \tag{22}$$

where

$$T^*=\frac{|U|\nu(2-\nu)}{2} \tag{23}$$

is the characteristic temperature, the upper sign (+) corresponds to the repulsion and the lower one (−) to the attraction. One can see from Eq. (22) that in the temperature region $T<T^*$ the short-range Coulomb repulsion U is sufficiently suppressed by the screening. The two-body collisions reduce the intraatomic Coulomb self-energy to a magnitude of the order of the polaronic bandwidth for $T\lesssim W$ (see, also, Ref. 13). In the case of attraction the singularity in the two-particle correlator, Eq. (22), occurs at $T=T^*$. Thus T^* is the critical temperature of the SB's formation. The short-range attraction is enhanced near T^*.

One can estimate T^* at which SB's may be formed in metal oxides using the assumption that a large temperature-independent gap observed in $YBa_2Cu_3O_7$, $\Delta_{gap}=8k_BT_c$, is of the order of the attraction of two polarons $|U|$.[14] Thus one can estimate,

$$|U|\simeq 720\ \mathrm{K}\ ,$$

and using Eq. (23) obtain for $\nu=1$

$$T^*\simeq 360\ \mathrm{K}\ .$$

The SP response becomes dynamic for a rather low frequency $\omega>W$:

$$\epsilon(\omega,\mathbf{q})=1-\frac{\omega_p^2}{\omega^2} \tag{24}$$

with the temperature-dependent plasma frequency

$$\omega_p^2(\mathbf{q})=2v(\mathbf{q})\sum_{\mathbf{k}}n_{\mathbf{k}}(\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}})\ , \tag{25}$$

which is proportional to $1/T$ in the temperature range $T\gg W$. For low temperatures $T<W$ the long-wave plasmon has the frequency

$$\omega_p^2=\frac{4\pi Ne^2\nu}{m^*\epsilon}\ , \tag{26}$$

which is much lower than the usual one due to the mass enhancement:

$$m^*/m=\exp(g^2)\ . \tag{27}$$

The small concentration is assumed in Eq. (26), $\nu\ll 1$.

Thus compared with the bare electrons response the simple RPA shows a rather unusual response of SP's with a small temperature-dependent Debye radius and plasma frequency. In the case of repulsion the polaronic plasmon has a well-defined dispersion for the whole region of wave vectors with a zero damping, Eq. (25). If $v(q)<0$ for some q, the plasmon disappears in this region of q space.

II. PHONON SELF-ENERGY

Polaron-phonon and polaron-polaron interactions change the phonon propagation. The second order in $H_{p\text{-ph}}$ phonon self-energy Σ_{ph} is given by the sum of diagrams, Fig. 1, which can be expressed in terms of the multiphonon correlator:[9]

$$\Phi_{ij}^{i'j'}(\tau)=\langle T_\tau\hat{\sigma}_{ij}(\tau)\hat{\sigma}_{i'j'}(0)\rangle\ , \tag{28}$$

where

$$\hat{\sigma}_{ij}(\tau)=\exp(H_0\tau)\hat{\sigma}_{ij}\exp(-H_0\tau)\ , \tag{29}$$

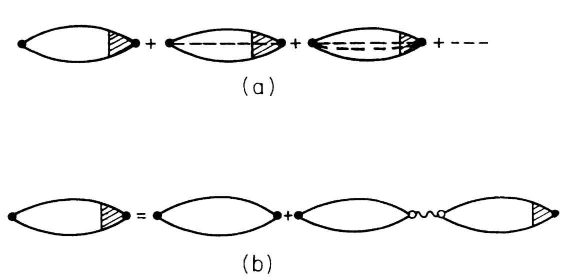

FIG. 1. Phonon self-energy (a) and SP polarization loop (b).

and $-1/T<\tau<1/T$. The first order in $H_{p\text{-ph}}$ diagrams as well as the second-order terms, containing two polarization loops, are exponentially small, proportional to $\exp(-g^2)$.[9]

For the real time t the correlator, Eq. (28), was calculated by Lang and Firsov.[15] To obtain $\Phi(\tau)$ one has to make the substitution $t\rightarrow -i|\tau|$ with the following result:

$$\Phi_{ij}^{i'j'}(\tau)=\sigma(\mathbf{a})\sigma(\mathbf{b})\exp\left\{\frac{1}{N}\sum_{\mathbf{q}}\frac{\gamma^2(\mathbf{q})}{\sinh[\omega(\mathbf{q})/2T]}f_{\mathbf{q}}\cosh\left[\omega(\mathbf{q})\left[\frac{1}{2T}-|\tau|\right]\right]\right\}, \tag{30}$$

where

$$f_{\mathbf{q}}=\tfrac{1}{2}\{\cos(\mathbf{q}\cdot[\mathbf{c}-\mathbf{a}])+\cos(\mathbf{q}\cdot[\mathbf{c}+\mathbf{b}])-\cos(\mathbf{q}\cdot\mathbf{c})-\cos(\mathbf{q}\cdot[\mathbf{c}-\mathbf{a}+\mathbf{b}])\} \tag{31}$$

with $\mathbf{a}=\mathbf{m}-\mathbf{n}$, $\mathbf{b}=\mathbf{m}'-\mathbf{n}'$, $\mathbf{c}=\mathbf{n}'-\mathbf{n}$. The sum of diagrams, Fig. 1(a) gives

$$\Sigma_{\rm ph}(q,\omega_n)=-T\sum_{\omega_{n'}}\sum_{iji'j'}(u_i^*-u_j^*)(u_{i'}-u_{j'})\Phi_{ij}^{i'j'}(\omega_{n'})\times\Pi_{iji'j'}(\omega_{n'}-\omega_n), \tag{32}$$

where

$$\Phi_{ij}^{i'j'}(\omega_n)=\tfrac{1}{2}\int d\tau\{\Phi_{ij}^{i'j'}(\tau)\exp(i\omega_n\tau)\}, \tag{33}$$

and $\omega_n=2\pi nT$, $\omega_{n'}=2\pi n'T$.

If one takes for the SP polarization Π a simple loop $\Pi^{(0)}$ (the product of two polaron GF's), one obtains our previous result.[9] Now I take into account polaron-polaron correlations to obtain in RPA, Fig. 1(b),

$$\Pi_{iji'j'}=\Pi_{iji'j'}^{(0)}+\sum_{l,p}\Pi_{ijll}^{(0)}v(1-\mathbf{p})\Pi_{ppi'j'}, \tag{34}$$

where the Matsubara frequency ω_n, which is the same in all terms, is omitted. To solve Eq. (34) one can take the Fourier transformation of Π:

$$\Pi_{iji'j'}=\frac{1}{N^3}\sum_{\mathbf{k},\mathbf{k}',\mathbf{g}}\Pi(\mathbf{k},\mathbf{k}',\mathbf{g})\exp[-i\mathbf{k}\cdot(\mathbf{m}'-\mathbf{n})+i\mathbf{k}'\cdot(\mathbf{n}'-\mathbf{m})+i\mathbf{g}\cdot(\mathbf{m}'-\mathbf{n}')] \tag{35}$$

with the Fourier component, which can be derived from the following equation:

$$\Pi(\mathbf{k},\mathbf{k}',\mathbf{g})=\Pi^{(0)}(\mathbf{k},\mathbf{k}')\left[N\delta_{\mathbf{g},0}+v(\mathbf{k}-\mathbf{k}')\sum_{\mathbf{g}'}\Pi(\mathbf{k}+\mathbf{g}'-\mathbf{g},\mathbf{k}'+\mathbf{g}'-\mathbf{g},\mathbf{g}')\right], \tag{36}$$

where

$$\Pi^{(0)}(\mathbf{k},\mathbf{k}')=2\frac{n_{\mathbf{k}}-n_{\mathbf{k}'}}{i\omega_n+\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'}}. \tag{37}$$

One can change in Eq. (36) $\mathbf{k},\mathbf{k}'$ in $\mathbf{k}+\mathbf{g},\mathbf{k}'+\mathbf{g}$, respectively, to obtain

$$\Pi(\mathbf{k}+\mathbf{g},\mathbf{k}'+\mathbf{g},\mathbf{g})=\Pi^{(0)}(\mathbf{k}+\mathbf{g},\mathbf{k}'+\mathbf{g})\times[N\delta_{\mathbf{g},0}+v(\mathbf{k}-\mathbf{k}')A(\mathbf{k},\mathbf{k}')] \tag{38}$$

with $A(\mathbf{k},\mathbf{k}')=\sum_{\mathbf{g}'}\Pi(\mathbf{k}+\mathbf{g},\mathbf{k}'+\mathbf{g}',\mathbf{g}')$. Taking the sum in Eq. (38) over $\mathbf{g}$ one finds

$$A(\mathbf{k},\mathbf{k}')=N\Pi^{(0)}(\mathbf{k},\mathbf{k}')\epsilon^{-1}(i\omega_n,\mathbf{k}-\mathbf{k}'). \tag{39}$$

Substituting Eq. (39) in Eq. (38), one obtains

$$\Pi(\mathbf{k},\mathbf{k}',\mathbf{g})=N\Pi^{(0)}(\mathbf{k},\mathbf{k}')\times[\delta_{\mathbf{g},0}+v(\mathbf{k}-\mathbf{k}')\Pi^{(0)}(\mathbf{k}-\mathbf{g},\mathbf{k}'-\mathbf{g})\times\epsilon^{-1}(i\omega_n,\mathbf{k}-\mathbf{k}')]. \tag{40}$$

To calculate the sum in Eq. (32) one can express $\Phi(\tau)$ in the form

$$\Phi(\tau)=\sigma(\mathbf{a})\sigma(\mathbf{b})+\tilde{\Phi}(\tau). \tag{41}$$

The function $\tilde{\Phi}(\tau)$, defined by Eq. (41), behaves like

$$\tilde{\Phi}(\tau)\sim\exp(2g^2e^{-\omega|\tau|})-1, \tag{42}$$

changing very quickly with the characteristic time $\tau<E_p^{-1}$. Thus its Fourier component $\tilde{\Phi}(\omega_n)$ weakly depends on the frequency for the entire range of ω_n under consideration. Substituting Eq. (42) in Eqs. (33,32) one obtains

$$\Sigma_{\rm ph}(\mathbf{q},\omega_n)=\Sigma_{\rm ph}^{\rm res}(\mathbf{q},\omega_n)-\tilde{\Delta}(\mathbf{q}), \tag{43}$$

where

$$\Sigma_{\rm ph}^{\rm res}(\mathbf{q},\omega_n)=-\sum_{i,j,i',j'}(u_i^*-u_j^*)(u_{i'}-u_{j'})\sigma(\mathbf{m}-\mathbf{n})\sigma(\mathbf{m}'-\mathbf{n}')\Pi_{iji'j'}(-\omega_n) \tag{44}$$

is a frequency-dependent resonance contribution and

$$\tilde{\Delta}(\mathbf{q})=T\sum_{i,j,i',j'}(u_i^*-u_j^*)(u_{i'}-u_{j'})\sum_{\omega_{n'}}\tilde{\Phi}_{ij}^{i'j'}(\omega_n+\omega_{n'})\Pi_{iji'j'}(\omega_{n'}) \tag{45}$$

is a softening. The Fourier transformation in Eqs. (44) and (45) gives

$$\Sigma_{\rm ph}^{\rm res}(\mathbf{q},\omega_n)=\frac{\gamma^2(\mathbf{q})}{2N^2}\sum_{\mathbf{k},\mathbf{g}}(\varepsilon_{\mathbf{k}}\varepsilon_{\mathbf{k}-\mathbf{q}-\mathbf{g}}+\varepsilon_{\mathbf{k}-\mathbf{q}}\varepsilon_{\mathbf{k}-\mathbf{g}}-\varepsilon_{\mathbf{k}-\mathbf{g}}\varepsilon_{\mathbf{k}-\mathbf{q}-\mathbf{g}}-\varepsilon_{\mathbf{k}}\varepsilon_{\mathbf{k}-\mathbf{g}})\Pi(\mathbf{k},\mathbf{k}-\mathbf{q},\mathbf{g};\omega_n)\ , \tag{46}$$

$$\tilde{\Delta}(\mathbf{q})=\frac{\gamma^2(\mathbf{q})}{2N^2}\sum_{\mathbf{k},\mathbf{g},\mathbf{k}'}\sum_{\omega_{n'}}\tilde{\Phi}(\mathbf{k},\mathbf{k}'+\mathbf{q},-\mathbf{g})[\Pi(\mathbf{k},\mathbf{k}',-\mathbf{g}-\mathbf{q};\omega_{n'})-\Pi(\mathbf{k}\mathbf{k}',-\mathbf{g};\omega_{n'})]$$
$$+\tilde{\Phi}(\mathbf{k}-\mathbf{q},\mathbf{k}',-g)[\Pi(\mathbf{k},\mathbf{k}',-\mathbf{g}+\mathbf{q};\omega_{n'})-\Pi(\mathbf{k},\mathbf{k}',-\mathbf{g};\omega_{n'})]\ , \tag{47}$$

with

$$\tilde{\Phi}_{ij}^{i'j'}=\frac{1}{N^3}\sum_{\mathbf{k},\mathbf{k}',\mathbf{g}}\tilde{\Phi}(\mathbf{k},\mathbf{k}',\mathbf{g})\exp[-i\mathbf{k}\cdot(\mathbf{m}'-\mathbf{n})+i\mathbf{k}'\cdot(\mathbf{n}'-\mathbf{m})+i\mathbf{g}\cdot(\mathbf{m}'-\mathbf{n}')] \tag{48}$$

To calculate the frequency-dependent contribution $\Sigma_{\rm ph}^{\rm res}$ one can expand the simple polarization loop, using W/ω as a small parameter:

$$\Pi^{(0)}(\mathbf{k},\mathbf{k}')=2\left\{\frac{n_{\mathbf{k}}-n_{\mathbf{k}'}}{i\omega_n}-\frac{(n_{\mathbf{k}'}-n_{\mathbf{k}})(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'})}{\omega_n^2}+\cdots\right\}. \tag{49}$$

Substitution of Eq. (49) in Eq. (40) and in Eq. (46) gives

$$\Sigma_{\rm ph}^{\rm res}(\mathbf{q},\omega_n)=-\frac{\beta(\mathbf{q})\omega_p^4(\mathbf{q})}{\omega(\mathbf{q})[\omega_n^2+\omega_p^2(\mathbf{q})]}\ , \tag{50}$$

where

$$\beta(\mathbf{q})=\frac{\omega(\mathbf{q})\gamma^2(\mathbf{q})}{v(\mathbf{q})} \tag{51}$$

is a dimensionless plasmon-phonon coupling constant.

To obtain the full expression for $\Delta(\mathbf{q})$ one should use TLA, which gives for the polarization

$$\Pi(\mathbf{k},\mathbf{k}',\mathbf{g};\omega_n)\simeq-N\delta_{\omega_n,0}\frac{\nu(2-\nu)}{2T}\left\{\delta_{\mathbf{g},0}-\frac{v(\mathbf{k}-\mathbf{k}')\nu(2-\nu)}{2T\epsilon(0,\mathbf{k}-\mathbf{k}')}\right\}, \tag{52}$$

and also takes into account the diagrams with two external phonon lines attached to the same vertex of $\Sigma_{\rm ph}$. The second term in Eq. (52) does not depend on $\mathbf{g}$. Thus one can see that a direct polaron-polaron interaction does not contribute to the softening of phonons:

$$\Delta(\mathbf{q})=\frac{\nu(2-\nu)\gamma^2(\mathbf{q})}{2}\sum_a[\tilde{\Phi}_{\mathbf{a}}(\omega_n)-\tilde{\Phi}_{\mathbf{a}}(0)][1-\cos(\mathbf{q}\cdot\mathbf{a})]\ , \tag{53}$$

where

$$\tilde{\Phi}_{\mathbf{a}}=\tilde{\Phi}_{ij}^{ji}\ . \tag{54}$$

Expanding the exponent in Eq. (30) we find according to the definitions, Eqs. (33), (41), and (54) for dispersionless phonons, $\omega(\mathbf{q})=\omega_0$:

$$\tilde{\Phi}_{\mathbf{a}}(\omega_n)=\frac{2\sigma^2(\mathbf{a})}{\omega_0}\sum_{k=1}^{\infty}\sum_{p=0}^{k}\begin{Bmatrix}k\\p\end{Bmatrix}\frac{\sinh[(k-2p)\omega_0/2T]}{2^k k!\sinh^k(\omega_0/2T)}\left\{N^{-1}\sum_{\mathbf{q}'}\gamma^2(\mathbf{q}')[1-\cos(\mathbf{q}'\cdot\mathbf{a})]\right\}^k\frac{(k-2p)\omega_0^2}{(k-2p)^2\omega_0^2+\omega_n^2}\ . \tag{55}$$

For the temperature range $T\ll\omega_0$ the terms with $p=0$ and $p=k$ dominate. As a result one finds

$$\tilde{\Phi}_{\mathbf{a}}(\omega_n)-\tilde{\Phi}_{\mathbf{a}}(0)\simeq\frac{t^2(\mathbf{a})}{\omega_0 g^6(\mathbf{a})}\ , \tag{56}$$

and (in Ref. 9 Δ contained g^2 instead of the correct g^6)

$$\Delta(\mathbf{q})=\frac{\nu(2-\nu)\gamma^2(\mathbf{q})}{2\omega_0}\sum_{\mathbf{a}}\frac{t^2(\mathbf{a})[1-\cos(\mathbf{q}\cdot\mathbf{a})]}{g^6(\mathbf{a})}\ . \tag{57}$$

The estimation of the softening, Eq. (57), shows that it is small compared with the bare frequency ω_0 as $1/\lambda^2$. At high concentrations of carriers the screening due to the exchange polaron-polaron interaction $\tilde{v}(\mathbf{m})$ diminishes the value of $\Delta(\mathbf{q})$ (for details see the Appendix):

$$\Delta(\mathbf{q})=\frac{\nu(2-\nu)\gamma^2(\mathbf{q})}{2\omega_0}\sum_{\mathbf{a}}\frac{t^2(\mathbf{a})[1-\cos(\mathbf{q}\cdot\mathbf{a})]}{g^6(\mathbf{a})[1+\tilde{v}(\mathbf{a})\nu(2-\nu)/2T]}\ . \tag{58}$$

Thus the strong electron-phonon interaction, $\lambda>\lambda_c$, results in a rather small plasma frequency, comparable with the phonon one, Eq. (25), and also in the coupling of bare phonons with polaronic plasmons, Eq. (51). The real vibration excitations are a mixture of phonons and plasmons. To obtain the dispersion relation for the phonon-plasmon mixture one has to carry out the analytic continuation of $\Sigma_{\text{ph}}(\mathbf{q},\omega_n)$ to real frequencies Ω. Taking into account that $\Sigma_{\text{ph}}^{\text{res}}$ has only simple poles $\omega_n=\pm i\omega_p$, Eq. (50), one can obtain this continuation by a simple substitution in Eq. (50):

$$i\omega_n \rightarrow \Omega \; , \tag{59}$$

which gives the following equation for the frequency Ω of the plasmon-phonon mixture:

$$\Omega=\omega(\mathbf{q})+\Sigma_{\text{ph}}(\mathbf{q},\Omega) \; , \tag{60}$$

or

$$\Omega-\omega(\mathbf{q})+\Delta(\mathbf{q})-\frac{\beta(\mathbf{q})\omega_p^4(\mathbf{q})}{\omega(\mathbf{q})[\Omega^2-\omega_p^2(\mathbf{q})]}=0 \; . \tag{61}$$

There are three solutions of Eq. (61):

$$\Omega_1=\frac{\tilde{\omega}}{3}+\frac{2}{3}\cos\left[\frac{\alpha}{3}\right]\sqrt{\tilde{\omega}^2+\omega_p^2} \; , \tag{62}$$

$$\Omega_2=\frac{\tilde{\omega}}{3}-\frac{2}{3}\cos\left[\frac{\alpha+\pi}{3}\right]\sqrt{\tilde{\omega}^2+\omega_p^2} \; , \tag{63}$$

$$\Omega_3=\frac{\tilde{\omega}}{3}-\frac{2}{3}\cos\left[\frac{\alpha-\pi}{3}\right]\sqrt{\tilde{\omega}^2+\omega_p^2} \; , \tag{64}$$

$$\cos(\alpha)=\frac{\tilde{\omega}^3-9\tilde{\omega}\omega_p^2+27\beta\omega_p^4/2\omega}{\sqrt{(\tilde{\omega}^2+3\omega_p^2)^3}} \; , \tag{65}$$

and $\tilde{\omega}=\omega-\Delta$. The dependence on $\mathbf{q}$ of all parameters is assumed in Eqs. (62)–(65).

Only two solutions, Ω_1 and Ω_2, are real and positive. The last one, Ω_3 (or Ω_2, depending on the choice of α) is negative and has no physical meaning.

Thus I conclude that instead of the bare phonon the vibration spectrum of the lattice, strongly coupled to carriers, consists of two branches of excitations, which describe the propagation of the coupled phonon and plasmon. In the case of weak plasmon-phonon coupling $\beta \ll 1$ the dispersions have the form

$$\Omega_{1,2}=\frac{1}{2}\{\tilde{\omega}+\omega_p\pm[(\tilde{\omega}-\omega_p)^2+2\beta\omega_p^3/\omega]^{1/2}\} \; . \tag{66}$$

In the limit $\beta\rightarrow 0$ $\Omega_1(+)$ and $\Omega_2(-)$ describe the phonon with the renormalized frequency $\tilde{\omega}$ and the plasmon, respectively. The ratio of weights of two contributions of the phonon-plasmon mixture to the phonon GF,

$$D(\mathbf{q},\Omega)=\sum_{i=1}^{3}\frac{P_i(\mathbf{q})}{\Omega-\Omega_i(\mathbf{q})} \; , \tag{67}$$

is given by

$$\frac{P_2}{P_1}=\frac{(\Omega_2^2-\omega_p^2)(\Omega_3-\Omega_1)}{(\Omega_1^2-\omega_p^2)(\Omega_3-\Omega_2)} \; . \tag{68}$$

Even for a weak coupling this ratio may be of the order of unity:

$$\frac{P_2}{P_1}\simeq\frac{\Delta-\Delta_0}{\Delta+\Delta_0} \tag{69}$$

if the plasmon and phonon frequencies are close enough to each other. Here $\Delta_0=\tilde{\omega}-\omega_p$ and $\Delta=[(\tilde{\omega}-\omega_p)^2+2\beta\omega_p^3/\omega]^{1/2}$ are the bare and the renormalized gaps between two branches of excitations.

The anomalous extra branch of high-frequency vibrations, observed in neutron-scattering experiments in La_2CuO_4 and probably in $YBa_2Cu_3O_7$,[10] was connected with the strong electron-phonon interaction.

Capellmann[16] proposed a phenomenological model of this phenomenon, in which phonons are coupled to a collective carrier mode with the frequency well below the one-particle continuous spectrum (see also Ref. 17). I explain the two high-frequency modes as bound states of polaronic plasmons with phonons. This assumption allows an estimation of the parameters $\omega_p,\tilde{\omega},\beta$ using the experimental values[10] of frequencies Ω_1 and Ω_2 and also their weight ratio, which is about unity in a certain region of q space:

$$\frac{\Omega_1}{2\pi}=22\text{ (THz)},\quad \frac{\Omega_2}{2\pi}=14\text{ (THz)},\quad \frac{P_2}{P_1}\simeq 1 \; . \tag{70}$$

Substituting these figures in Eqs. (66) and (69) one obtains

$$\frac{\omega_p}{2\pi}\simeq\frac{\tilde{\omega}}{2\pi}=18\text{ (THz)},\quad \frac{\beta\omega_p^3}{4\pi^2\omega}=34\text{ (THz)}^2 \; . \tag{71}$$

If one takes the bare phonon frequency of the order of the renormalized one, $\omega\simeq\tilde{\omega}$, one finds for the coupling

$$\beta\simeq 0.1 \; , \tag{72}$$

which is a lower estimation because in general $\omega>\tilde{\omega}$.

The extra mode disappears in the long-wave limit, $\mathbf{q}\rightarrow 0$.[10] This is the case for intramolecular and acoustic phonons with $\beta(\mathbf{q}\rightarrow 0)=0$, Eq. (51), but is not the case for long-wave optical phonons, for which $\beta\neq 0$ in this limit. The mode also disappears in the short-wave limit. This fact may be connected with the short-range polaron-polaron attraction, $v(\mathbf{q})<0$, resulting in the disappearance of the short-wave polaronic plasmon according to Eq. (25). The estimation of the plasmon frequency, Eq. (26), with experimental values of $\epsilon\simeq 50$,[18] $\nu=1$ (half-filled band), and $m^*=25m_e$ (Ref. 19) gives for La_2CuO_4 $\omega_p\simeq 110$ (THz), which is surprisingly close to the value, extracted from the neutron scattering, and supporting the phonon–polaronic-plasmon nature of the extra mode. The existence of the extra mode strongly depends on the parameters Δ_0 and β, small changes of which can lead to its disappearance.

To conclude I have shown that the Debye radius and the plasma frequency of SP's are small and temperature dependent, SP's screen effectively the short-range Coulomb repulsion, and enhance the short-range polaron-polaron attraction, the critical temperature of the SB's formation exists, Eq. (23), vibration excitations of a strongly coupled many-electron-phonon system exist, which are a mixture of polaronic plasmons and phonons. The anomalous extra mode, observed in the neutron-scattering experiments in La_2CuO_4 is explained. Two high-frequency branches of the vibrational spectrum are two of these mixtures.

I would also like to remark that the many-body polaronic effects, discussed above, are a result of the polaron collapse of the bare band, Eq. (2), which is a characteristic feature of the small-polaron theory of metal oxides.[2] The renormalized band structure, including the mass renormalization, can be detected with low-energy experiments. High-energy experiments with the characteristic energy of excitations $\delta\epsilon > \Delta_{\text{gap}} \sim 0.1$ eV can only detect the bare band structure with the bare mass $m \simeq m_e$, and with the bare plasma frequency $\omega_p^{(0)} > 1$ eV.

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APPENDIX

The exchange interaction in the form

$$H_{p\text{-}p}^{\text{ex}} = \frac{1}{2} \sum_{m \neq n, s, s'} \tilde{v}(\mathbf{m}-\mathbf{n}) c_{\mathbf{n},s}^{\dagger} c_{\mathbf{m},s'}^{\dagger} c_{\mathbf{n},s'} c_{\mathbf{m},s} \quad \text{(A1)}$$

diminishes $\Delta(\mathbf{q})$. The equation for the polarization is now

$$\Pi(\mathbf{k},\mathbf{k}',\mathbf{g}) = \Pi^{(0)}(\mathbf{k},\mathbf{k}') \left[N\delta_{g,0} + \sum_{\mathbf{g}'} [v(\mathbf{k}-\mathbf{k}') + \tilde{v}(\mathbf{g}-\mathbf{g}')] \Pi(\mathbf{k}+\mathbf{g}'-\mathbf{g}, \mathbf{k}'+\mathbf{g}'-\mathbf{g}, \mathbf{g}') \right] , \quad \text{(A2)}$$

with $\tilde{v}(\mathbf{g})$ being the Fourier component of $\tilde{v}(\mathbf{m})$. In TLA $\Pi^{(0)}(\mathbf{k},\mathbf{k}') = \pi_0$ is momentum independent, and $\Pi(\mathbf{k},\mathbf{k}',\mathbf{g}) = \Pi(\mathbf{k}-\mathbf{k}',\mathbf{g})$. For the Fourier component $\Pi(\mathbf{k}-\mathbf{k}',\mathbf{m})$ defined by

$$\Pi(\mathbf{k}-\mathbf{k}',\mathbf{g}) = \sum_{\mathbf{m}} \Pi(\mathbf{k}-\mathbf{k}',\mathbf{m}) \exp(i\mathbf{g}\cdot\mathbf{m}) , \quad \text{(A3)}$$

one obtains from Eq. (A2),

$$\Pi(\mathbf{k}-\mathbf{k}',\mathbf{m}) = \frac{\pi_0}{1-\pi_0[v(\mathbf{k}-k')\delta_{\mathbf{m},0} + \tilde{v}(\mathbf{m})]} . \quad \text{(A4)}$$

Thus

$$\Pi(\mathbf{k},\mathbf{k}',\mathbf{g}) = \frac{\pi_0}{1-\pi_0 v(\mathbf{k}-\mathbf{k}')} + \sum_{\mathbf{m}\neq 0} \frac{\pi_0 \exp(i\mathbf{g}\cdot\mathbf{m})}{1-\tilde{v}(\mathbf{m})\pi_0} . \quad \text{(A5)}$$

Substituting the last equation in Eq. (47) one obtains Eq. (58).

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