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Some properties of large polarons with squeezed states

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Abstract. The effective mass of the Fröhlich polaron is calculated with the two-mode squeezed states in the intermediate-coupling region and found to be in close agreement with the results of other models. Within the same approach, the induced charge density around an electron in polar solids is calculated. Our result for this charge density contains an additional term which shows a feature in the spatial dependence as a manifestation of the squeezing effect.

1. Introduction

An electron moving slowly in an ionic crystal distorts and displaces its surrounding ions, establishing a polarization field which acts back on the electron whose properties are then modified; in particular, the electron acquires a self-energy and an enhancement of its Bloch effective mass. The electron together with its polarization cloud is called a polaron and the model for such a system is investigated by the Fröhlich Hamiltonian (FH)

$$H = \frac{p^2}{2m} + \sum_q \hbar\omega_q b_q^\dagger b_q + \sum_q V_q (b_q^\dagger e^{-iq\cdot r} + \text{HC}) \tag{1}$$

where we have used the standard notation [1], and $V_q = -i(\hbar\omega_0/qu^{1/2})(4\pi\alpha/V)^{1/2}$. Here α is the coupling strength and $u = (2m\omega_0/\hbar)^{1/2}$, and the LO phonons are assumed to be dispersionless, i.e. $\omega_q = \omega_0$.

This Hamiltonian has not been exactly solved so far; however numerous mathematical techniques have been used to obtain its approximate solutions. These calculations can be classified in certain regimes according to the strength of the coupling α. The weak- and intermediate-coupling region, corresponding to the range $0 < \alpha < 6$, is dealt with by perturbation theories and variational techniques. In the case of $\alpha > 6$ we have a strong coupling region, where a completely different type of approximation is required [2]. Besides these approaches, the path integral method of Feynman is unique in a way to give results for all coupling strengths. An extensive review of the subject up to 1987 was given by Mitra *et al* [3].

No matter which approximation is made on the FH the ground state energy in zero temperature comes out to be in the following form:

$$E(P) = E_0 + \frac{P^2}{2m^*} + \cdots \tag{2}$$

where E_0 and m^* are respectively the self-energy and the effective mass of the polaron. Of the above mentioned regimes, the intermediate-coupling region is most interesting. This

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interest arises from the fact that variational techniques used in this region exhibit a critical behaviour in which a free polaron undergoes a formal phase transition from an itinerant state to a localized one. This, however, is now being accapted as an artifact of the approximation. In fact, as first pointed out by Peeters and Devreese [4], another type of variational approximation within the Feynman path integral approach does not exhibit this artifact.

Variational methods are based on two successive transformations, which are developed by Lee, Low and Pines (LLP) [5]. As an extension of this approach, it is possible to introduce a third transformation that includes a variational function so that the energy may be minimized further. Recently such a procedure has been carried out by a canonical transformation, which produced squeezed states of phonons. These have been used to calculate the ground state energy E_0, and the results showed a lowering of the energy [6].

In the present work, our aim is, on the basis of this approach, to calculate the effective mass and the reduced charge density of the large polarons. It is well known that there are several definitions for the polaron mass [7]. Our definition of the effective mass is such that

$$\frac{1}{m^*} = \frac{\partial^2}{\partial P^2} E(P)|_{P=0}. \tag{3}$$

This definition is due to the approach we have made, and is not necessarily the unique one to make contact with the experimentally measured mass, which is usually the cyclotron mass. Therefore in section 2, we calculate the ground state energy in the case of $P \neq 0$. In section 3, the dependence of the reduced charge density on the coupling strength is calculated by the same method.

2. The effective mass

The first canonical transformation of LLP is

$$U_1 = \exp\left[i\left(P - \sum_q \hbar q b_q^\dagger b_q \right) \cdot r \right]. \tag{4}$$

This eliminates the electron coordinate in the FH. The second transformation used by LLP is

$$U_2 = \exp\left[\sum_q (f_q b_q^\dagger - f_q^* b_q) \right] \tag{5}$$

where f_q is a variational function to be employed in minimizing the ground state energy. Furthermore, it should be pointed out that this latter transformation generates coherent states out of the phonon fields.

Under these transformations the new Hamiltonian contains terms that have combinations of b_q and $b_q^\dagger$, gradually changing from the zero degree up to the quartic one of their multiplication [8]. LLP used only H_0 of the new Hamiltonian to obtain the ground state energy and the effective mass in a variational method where the energy functional was minimized with respect to f_q. In order to diagonalize the part that contains quadratic terms, i.e. H_2, it is necessary to use a third canonical transformation. This is achieved through a type of Bogoliubov transformation [8] and a squeezed state transformation [6], both of

them consider only the case of $P = 0$. To obtain the effective mass we will follow the latter approach, which gives a lower ground state energy. We now introduce the third transformation, as discussed fully in [6], that is formed by two-mode squeezed states by which the correlation between phonons is involved in a natural way,

$$U_3 = \exp\left[\sum_{q \neq q'} \frac{\varphi_{qq'}}{N}(b_q^\dagger b_{q'}^\dagger - b_q b_{q'})\right] \tag{6}$$

where the squeezing angle $\varphi_{qq'}$ depends on two wave vectors q and q' of the LO phonons. The squeezed state vector for the ground state of the phonon subsystem is formed as follows:

$$|\Psi_{\rm ph}\rangle_{\rm s} = U_3|{\rm vac}\rangle \tag{7}$$

where the ket on the right is the zero phonon state. At this point we can either firstly transform H_0 and H_2 by U_3 and then calculate the expectation value in the zero phonon state or equivalently use (7) to calculate the expectation value H_0 and H_2.

Since two LO phonons are involved in the wave function it is essential to rewrite H_0 and H_2 in a convenient form as described in [6] and then the expectation value of the energy can be obtained as functions of f_q, $\varphi_{qq'}$ and P. The energy functional $E[f_q, \varphi_{qq'}]$ is to be minimized with respect to these functions, which gives rise to two coupled equations,

$$\left[\bar{\omega}_0(q) + 2\left(\frac{q}{u}\right)\cdot\sum_{q'}\frac{q'}{u}|f_{q'}|^2 - 2\left(\frac{q}{u}\right)\cdot\bar{P} + 2\left(\frac{q}{u}\right)^2\mathcal{G}(q)\right]f_q + \bar{V}_q^* + \sum_{q'}\frac{q}{u}\cdot\frac{q'}{u}f_{q'}^*\sinh\left(\frac{2\varphi_{qq'}}{N}\right) = 0 \tag{8}$$

$$\left[\bar{\omega}_0(q) + \bar{\omega}_0(q') - 2\left(\left(\frac{q}{u}\right) + \left(\frac{q'}{u}\right)\right)\cdot\bar{P} + 2\left(\left(\frac{q}{u}\right) + \left(\frac{q'}{u}\right)\right)\cdot\sum_k\frac{k}{u}|f_k|^2\right]\sinh\left(\frac{2\varphi_{qq'}}{N}\right) + 4\frac{q}{u}\cdot\frac{q'}{u}f_q f_{q'}\cosh\left(\frac{2\varphi_{qq'}}{N}\right) = 0 \tag{9}$$

where $\bar{\omega}_0(q) = 1 + (q/u)^2$, $\bar{P} = P/\hbar u$ and $\bar{E} = E/\hbar\omega_0$ are dimensionless quantities. Here $\mathcal{G}(q) = \sum_{q'}\sinh^2(\varphi_{qq'}/N)$ is a scalar function of q and proportional to α^2 due to the dependence on $\varphi_{qq'}$, therefore this term is to be neglected at a further stage. By rearranging the equations (8) and (9) we express the ground state energy in a simpler form

$$\bar{E}[f_q, \varphi_{qq'}, \bar{P}] = \bar{P}^2(1-\eta^2) + \frac{1}{4}\sum_q(\bar{V}_q f_q + {\rm HC}) + \frac{1}{4}\sum_{q'}(\bar{V}_{q'} f_{q'} + {\rm HC}) + \frac{1}{2}\sum_{q,q'}\left[\bar{\omega}_0(q) + 2\left(\frac{q}{u}\right)\cdot\bar{P}(\eta-1)\right]\sinh^2\left(\frac{\varphi_{qq'}}{N}\right) + \frac{1}{2}\sum_{q,q'}\left[\bar{\omega}_0(q') + 2\left(\frac{q'}{u}\right)\cdot\bar{P}(\eta-1)\right]\sinh^2\left(\frac{\varphi_{qq'}}{N}\right) \tag{10}$$

where η is defined by

$$\eta\bar{P} = \sum_q \frac{q}{u}|f_q|^2. \tag{11}$$

Calculation of the ground state energy (10) requires solutions of two coupled equations (8) and (9) for f_q and $\varphi_{qq'}$ as well as η. Since it is impossible to solve them exactly, we try to obtain the results to a first approximation. Keeping the first terms of the expansion of the hyperbolic function in powers of $\varphi_{qq'}/N$ that is very small, one can easily write

$$f_q = -\frac{\bar{V}_q^*}{\bar{\omega}_{02}(q)} - \frac{1}{\bar{\omega}_{02}(q)}\sum_{q'}\frac{q}{u}\frac{q'}{u}\cos\gamma f_{q'}^*\frac{2\varphi_{qq'}}{N} \tag{12}$$

$$\frac{\varphi_{qq'}}{N} = -\frac{2(q/u)(q'/u)\cos\gamma}{\bar{\omega}_{01}(q,q')}f_q f_{q'} \tag{13}$$

where $\bar{\omega}_{01}(q,q')$ and $\bar{\omega}_{02}(q)$ are given in the following form:

$$\bar{\omega}_{01}(q,q') = 2 + \left(\frac{q}{u}\right)^2 + \left(\frac{q'}{u}\right)^2 + 2\left(\left(\frac{q}{u}\right) + \left(\frac{q'}{u}\right)\right)\cdot\bar{P}(\eta-1) \tag{14}$$

$$\bar{\omega}_{02}(q) = 1 + \left(\frac{q}{u}\right)^2 + 2\left(\frac{q}{u}\right)\cdot\bar{P}(\eta-1) + 4\left(\frac{q}{u}\right)^2\mathcal{G}(q) \tag{15}$$

and γ is the angle between q and q'. In the first approximation, f_q can be chosen as $-\bar{V}_q^*/\bar{\omega}_{02}(q)$ which corresponds to the unsqueezed case and only terms up to the order of $\bar{P}^2$ in all expressions are considered. Under these assumptions we put the ground state energy (10) and the equation (11) for η in the following form

$$\bar{E} = \bar{P}^2(1-\eta^2) - \frac{\alpha}{2\pi^2}\int d\Omega\int dx\frac{1}{\bar{\omega}_{02}(x)} - \frac{\alpha^2}{\pi^4}\int d\Omega\int d\Omega'\int dx\int dy\frac{x^2y^2\cos^2\gamma}{\bar{\omega}_{02}^2(y)\bar{\omega}_{01}(x,y)\bar{\omega}_{02}^2(x)} \tag{16}$$

$$\eta\bar{P}^2 = \frac{1}{2\pi^2}\alpha\int d\Omega\int dx\frac{x\cdot\bar{P}}{\bar{\omega}_{02}^2(x)} + \frac{2}{\pi^4}\alpha^2\int d\Omega\int d\Omega'\int dx\int dy \times\frac{x^2y^2x\cdot\bar{P}\cos\gamma}{\bar{\omega}_{02}^2(y)\bar{\omega}_{01}(x,y)\bar{\omega}_{02}^3(x)} \tag{17}$$

where $x = q/u$ and $x' = q'/u$ are dimensionless variables. After expanding $\bar{\omega}_{01}(x,y)$ and $\bar{\omega}_{02}(x)$ as a power series in $\bar{P}$ and retaining terms up to $\bar{P}^2$ for small $\bar{P}$ and performing integrals we finally obtain

$$E = \frac{P^2}{2m}\left\{(1-\eta^2) - (1-\eta)^2\left[\frac{1}{6}\alpha + \frac{2400}{9\pi^2}10^{-3}\alpha^2\right]\right\} - \alpha\hbar\omega_0 - 0.0135\alpha^2\hbar\omega_0 \tag{18}$$

$$\frac{\eta}{1-\eta} = \frac{1}{6}\alpha + \frac{1984}{9\pi^2}10^{-3}\alpha^2. \tag{19}$$

Table 1. Various analytical results for the effective polaron mass in the intermediate-coupling region.

	m^*/m
LLP	$(1+\alpha/6)[1-0.01\alpha^2/(1+\alpha/6)]^{-1} \simeq 1+\alpha/6+0.01\alpha^2$
Haga [10]	$(12+\alpha)/(12-\alpha) \simeq 1+\alpha/6+0.01389\alpha^2$
Larsen [9] and Röseler [11]	$1+\alpha/6+0.02362\alpha^2$
Peeters and Devreese [12]	$1+\alpha/6+\frac{73}{2916}\alpha^2 = 1+\alpha/6+0.02503\alpha^2$

Inserting the expression (19) for η into the ground state energy (18) results in

$$E = \frac{P^2}{2m^*(\alpha)} - \alpha\hbar\omega_0 - 0.0135\alpha^2\hbar\omega_0 \tag{20}$$

where $m^*(\alpha)$ is the effective mass in the two-mode squeezed state approximation and is given by

$$\frac{m^*}{m} = \frac{(1+\frac{1}{6}\alpha+\frac{1984}{9\pi^2}10^{-3}\alpha^2)^2}{1+\frac{1}{6}\alpha+\frac{1568}{9\pi^2}10^{-3}\alpha^2}. \tag{21}$$

To make contact with the other works, (21) can be written, by expanding as a power series in α and keeping terms up to α^2, as follows:

$$\frac{m^*}{m} = 1+\tfrac{1}{6}\alpha+0.0270\alpha^2. \tag{22}$$

We summarize the results for the effective mass obtained by various authors in table 1 from which we see that our result is in good agreement with them. The LLP result was obtained, after the above mentioned two transformations and variational procedures, by calculating the lowest order correction to the energy resulting from that part of the Hamiltonian which was neglected, i.e. H_2. The method developed by Larsen [9] is notable as being a sophisticated calculation in which correlations between phonons are taken into account through the wave vectors of pairs of emitted virtual phonons, as well as giving the best available results for the energy and the effective mass of the polaron in the intermediate coupling region, for $\alpha < 4.5$.

Haga and Röseler's works are based on the variational techniques; while the former work is valid for the intermediate coupling, the latter one is calculated in the limiting case of weak coupling.

Table 2. Various numerical results for the effective polaron mass in the intermediate-coupling region.

m^*/m	α				
	1	2	3	4	5
Schultz [13]	1.196	1.472	1.889	2.579	3.887
Gerlach *et al* [14]	1.196	1.476	1.900	2.606	3.940
Alexandrou *et al* [15]	1.196	—	1.824	—	3.080
Lu *et al* [16]	1.194	1.465	1.868	2.526	3.763
SQZ	1.194	1.442	1.744	2.102	2.514

Various numerical results for the polaron effective mass are given in table 2 where (22) is listed numerically in the last row as SQZ. All of them are developed by path integral or functional integral techniques and use a different definition of the effective mass from (3), with the exception of Gerlach *et al* , who have derived the polaron mass by means of the ground state energy. The difference from our result is attributed to the fact that the definition of the effective mass is not well founded in the path integral approach, contrary to the ground state energy.

3. Induced polarization charge density

Since the squeezing transformation affects the ground state energy and the effective mass of the polaron, it would be of interest to investigate the polarization charge density induced by the electron within this approach. The induced polarization charge density at point r is defined by Poisson's equation

$$\langle \nabla^2 \Phi(r) \rangle = -4\pi\rho(r) \tag{23}$$

where the avarage is taken over the transformed phonon states under LLP and the two-mode squeezed state transformations successively. Since the electrostatic potential operator is represented by the interaction term in the FH, the induced polarization charge density around the electron becomes

$$\rho(r) = -\frac{1}{4\pi e}\, {}_s\langle \Psi | \sum_q \nabla^2 [V_q b_q e^{iq\cdot r} + \text{HC}] | \Psi \rangle_s \tag{24}$$

where we have taken $P = 0$ and $|\Psi\rangle_s = U_3 U_2 |0\rangle$, and r is measured from the position of the electron which is at rest. When the transformed forms of annihilation and creation operators are considered, the resulting polarization charge density can be written as a sum of two terms

$$\rho(r) = \rho_{\text{LLP}}(r) + \rho_{\text{SQZ}}(r) \tag{25}$$

and these are given by

$$\rho_{\text{LLP}}(r) = \frac{\hbar\omega_0}{er}\left(\frac{\alpha u}{\pi^2}\right)\int_0^\infty x\, \mathrm{d}x \frac{\sin(xur)}{1+x^2} \tag{26a}$$

$$\rho_{\text{SQZ}}(r) = -\frac{8}{3\pi^3 e}\hbar\omega_0(\alpha u)^2 \frac{1}{ur}\frac{\partial^2}{\partial(ur)^2}\int_0^\infty x \sin(xur)\mathrm{d}x \times \int_0^\infty y^2 \mathrm{d}y \frac{1}{(1+x^2)^2(1+y^2)^2(2+x^2+y^2)}. \tag{26b}$$

Performing the integrals in (26*a*) and (26*b*), the total induced charge density is found to be in the form

$$\rho(r) = \frac{\alpha\hbar\omega_0 u^2}{2\pi e}\frac{e^{-ur}}{ur} + \frac{\alpha^2\hbar\omega_0 u^2}{72\pi e}[12 - (ur)^2]e^{-ur} \tag{27}$$

where the first term is the LLP result and the second one is due to the two-mode squeezed state transformation. The total induced charge around the electron is obtained by integrating (27) over the whole space in spherical polar coordinates

$$Q = \int \mathrm{d}^3 r\, \rho(r) = \frac{e}{\bar{\epsilon}}. \tag{28}$$

This is exactly the total charge induced by the electron in a dielectric medium. In order to examine the spatial behaviour of (27), it is firstly rewritten as

$$\bar{\rho}(\bar{r}) = \frac{1}{2\pi}\left[\frac{1}{\bar{r}} + \frac{\sqrt{2}}{18}\alpha(6-\bar{r}^2)\right]\mathrm{e}^{-\sqrt{2}\bar{r}} \tag{29}$$

where $\bar{r} = r/(\hbar/m\omega_0)^{1/2}$ and $\bar{\rho}(\bar{r}) = \rho(r)/[Q/(\hbar/m\omega_0)^{3/2}]$ are the dimensionless variables. Finally (29) is represented by the sum of two terms

$$\bar{\rho}_{\mathrm{LLP}}(\bar{r}) = \frac{1}{2\pi}\frac{\mathrm{e}^{-\sqrt{2}\bar{r}}}{\bar{r}} \tag{30}$$

$$\bar{\rho}_{\mathrm{SQZ}}(\bar{r}) = \frac{1}{2\pi}\frac{\sqrt{2}}{18}\alpha(6-\bar{r}^2)\mathrm{e}^{-\sqrt{2}\bar{r}} \tag{31}$$

where $\bar{\rho}_{\mathrm{LLP}}(\bar{r})$ and $\bar{\rho}_{\mathrm{SQZ}}(\bar{r})$ are the dimensionless forms of (26*a*) and (26*b*), respectively. Their $\bar{r}$ dependences are separately shown in figure 1. The dependence on $\bar{r}$ of the total induced charge density given by (29) is plotted in figure 2 for $\alpha = 3$.

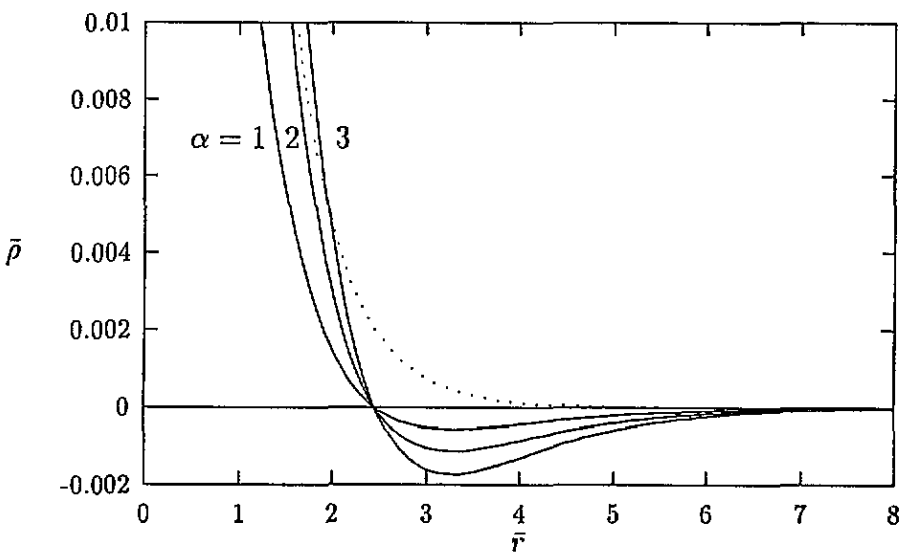

Figure 1. Induced charge densities as a function of $\bar{r}$. The dotted curve is for $\bar{\rho}_{\mathrm{LLP}}$; the solid curves are for $\bar{\rho}_{\mathrm{SQZ}}$ for $\alpha = 1, 2, 3$.

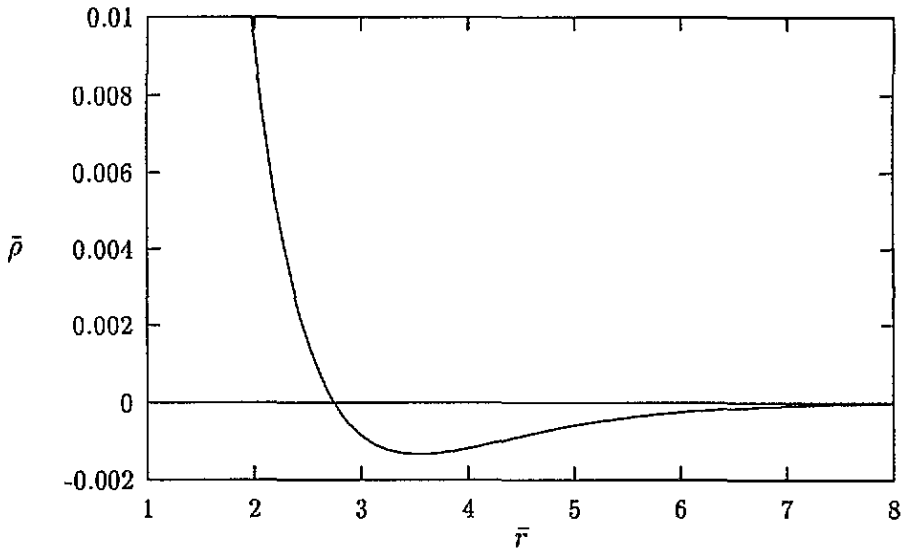

Figure 2. The total induced charge density for $\alpha = 3$ as a function of $\bar{r}$.

As seen in figure 1, there is a negative charge density region in the behaviour of $\bar{\rho}_{SQZ}(\bar{r})$ beyond $\bar{r} = \sqrt{6}$, in addition to the normal positive one in the range $0 < \bar{r} < \sqrt{6}$; furthermore both of them change with α by the same amount. This can be verified easily by calculating the total charge due to $\bar{\rho}_{SQZ}(\bar{r})$ for both regions, the result is $\mp 0.227\alpha Q$ respectively so they are summed up to zero. Accordingly, the overall charge due to polarization is the same as given in (28). It is normally expected that the charge density induced by the electron should be positive; however the appearance of such a negative region in the accompanying charge cloud is a manifestation of the squeezing effect. Such a feature is absent in the LLP result and in the expression for the polarization charge density derived by the path integral method [17]. As for the total density, this negative region is slightly suppressed as seen in figure 2.

It should be noted in figure 1 that $\bar{\rho}_{SQZ}(\bar{r})$ becomes zero and independent of α at the point $\bar{r} = \sqrt{6} = 2.4$, due to (31). However the point where the total charge density becomes zero is α dependent.

4. Discussion and conclusion

The polaron effective mass is an important quantity that can be a link between experimental results and theoretical studies where all the fundamental assumptions are made. In the present paper we have calculated the effective mass of the Fröhlich polaron by means of squeezed states, which are adapted from quantum optics [18]. The result has come out to be larger than those of the methods obtained in the intermediate-coupling region. This can be attributed to an excess number of virtual phonons accompanying the electron. Indeed, this is justified by calculating the average number of virtual phonons which is defined as

$$\langle N \rangle = \left\langle \sum_q b_q^\dagger b_q \right\rangle \tag{32}$$

where the average is taken through squeezed states with minimum uncertainties. It is easy to see that within the approximation used in section 2, this number becomes

$$\langle N\rangle = \sum_{q} |f_q|^2 + \sum_{q,q'} \sinh^2\left(\frac{\varphi_{qq'}}{N}\right) \tag{33}$$

where the first term gives $\alpha/2$, which is the well known LLP result, while the second term is from the squeezing effect. The final result is

$$\langle N\rangle = \frac{\alpha}{2} + 0.0253978\alpha^2. \tag{34}$$

In the weak-coupling limit, this number is $\alpha/2$ within the perturbative approach and $\frac{\alpha}{2} + 0.0318392\alpha^2$ on the basis of the diagram technique [19]. In the Feynman description of the polaron by Peeters and Devreese, this number of virtual phonons is plotted as a function of α in figure 2 of [20]. As clearly seen from this figure, it is proportional to $\alpha/2$ in the weak-coupling region, and appears to have corrections proportional to α^2 in the intermediate region.

In section 3 we calculated the polarization charge density induced by the electron in polar solids. The result found by LLP for this density decreases with Coulomb-like behaviour at small distances and becomes exponentially damped at large distances. This result is verified by the path integral method for small electron–phonon coupling [17]. Apart from the usual charge density of LLP, a term containing a negative region appearing in our result is entirely unique to the squeezing effect. The physical origin of the negative region is charge conservation. It is well known that the total induced charge around an electron in a dielectric medium is $e/\bar{\epsilon}$. In our approach the total charge density is given in (25), where the first term is equal to the LLP result and already gives a total charge of $e/\bar{\epsilon}$. Therefore $\bar{\rho}_{SQZ}(\bar{r})$ has to contain a negative region if there exists a positive one that will arise from an additional polarization of the medium. The squeezing effect is responsible for this polarization. This can be qualitatively seen from the phase space picture of quantum oscillators representing ionic motions. For simplicity let us have a single oscillator with position x and momentum p. After the squeezed transformation they will become $x\exp(-\varphi)$ and $p\exp(\varphi)$ respectively [18]. Since the displacement yields the induced polarization ($\mathcal{P}$) whose divergence ($-\nabla\cdot\mathcal{P}$) is the charge density, any change in them will provide an excess charge density and consequently this will give rise to a negative region, considering the conservation of the total charge.

It is thus to be concluded from the present study that squeezed states can play a prominent role in condensed matter physics. Here we have calculated the polaron effective mass and the induced charge density around an electron. While the result for the effective mass is very accurate, the latter calculation shows a characteristic feature which is absent from other works.

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