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# Existence of free and self-trapped positronium states in alkali halide crystals: Theoretical analysis and comparison with experiment

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A variational calculation is performed of the eigenstates of a positronium atom coupled with a field of longitudinal acoustic phonons in ionic crystals at finite temperatures. On the basis of this calculation a theoretical analysis is made of the possibility of self-localization (self-trapping) of positronium. The self-trapped states of positronium in NaF, NaCl, KCl, and KI crystals are found to be metastable with the energy higher by $\sim 0.01-0.1$ eV with respect to the stable delocalized (free) states. The self-trapped states of positronium in $MgF_2$ and $\alpha$-$SiO_2$ crystals are unstable at absolute zero temperature and become metastable with an increase in temperature for $T > \sim 300$ K. The difference in the energies of such ''high-temperature'' self-trapped states and the free states of positronium in $MgF_2$ and $\alpha$-$SiO_2$ is found to be at least one order of magnitude larger than that in the other alkali halides, explaining theoretically experimental evidence for the nonexistence of self-trapped positronium in these crystals. The basic characteristics (energy, effective mass, mean number of surrounding phonons, and localization radius) of the self-trapped and free states as well as the deformation potential constants are calculated for positronium in the crystals above. The results obtained are in good agreement with known experimental data. [S0163-1829(98)05641-0]

## I. INTRODUCTION

Positronium (Ps) formation in alkali halide crystals has presently been well established by means of a positron annihilation technique.[1–3] In crystals with low enough concentration of defects the Ps atom has been experimentally found to form in two types of states: the delocalized (Bloch-like, free) type and the localized type.[3,4] The formation of Bloch-type positronium is confirmed by observing very narrow peaks (the central peak and satellite peaks appearing at the momentum corresponding to the reciprocal lattice vectors of the sample crystal) in the momentum distribution of the photons resulting from the $2\gamma$-decay of Ps upon irradiating the crystals by low-energy positrons at sufficiently low temperatures (typically less than a few tens K).[5–10] Such a shape of the momentum distribution is possible only in the case in which the wave function of the annihilating positronium is a Bloch function.[2] The positronium atom in this case is delocalized throughout the volume of the entire crystal.

As the temperature increases it is observed[4,11–14] that the central Ps peak becomes drastically wider and the satellite peaks disappear, indicating the localization of positronium. The wave function of such localized positronium is a Gaussian, and the experimentally measured characteristic size of the localization region (the localization radius) is of the order of the lattice constant of the crystal. Since the localization is observed at quite low temperatures ($T < 150$ K), it is not possible to explain it in terms of the trapping of positronium by thermally created defects in the sample (see, however, Ref. 9). As a confirmation of this, note the absence of a localization effect in $MgF_2$ and $\alpha$-$SiO_2$, where positronium was observed delocalized up to temperatures $\sim 700$ K.[15–17] The localization observed with increase of temperature is explained by the self-trapping of positronium, specifically by the temperature activated transition of delocalized positronium to a metastable localized state arising as a result of its interaction with the short-range potential of a lattice vibration (acoustic phonons).[3,11–14] An analogous mechanism is well known for holes and excitons in crystal dielectrics.[18,19] For instance, it is known[18,19] that the ground stable state of an electron in alkali halide crystals is delocalized, whereas the ground states of the excitons and holes are localized. This is connected with the broad band of the electron (the band mass is $\sim m_0$, the free electron mass) and with the comparatively narrow bands [the band masses are $\sim(5-10)m_0$] of the excitons and holes in these crystals. For excitons, moreover, additional metastable states exist which are delocalized. The Ps atom can, to some extent, be regarded as an ''isotope'' of the exciton and, in this sense, for positronium in alkali halides an analogous situation takes place with the only difference being that, since the Ps band is less narrow than that of the exciton [the Ps band mass is $\sim(2.5-4)m_0$ (Ref. 14)], the ground stable state of Ps in alkali halides is delocalized and the metastable one is localized. In other words, since Ps is lighter, it is more difficult to be localized than an exciton in the same material.[18]

At present a significant amount of experimental material has been accumulated on the self-trapping of positronium in alkali halide crystals, while there have been hardly any theoretical papers analyzing this phenomenon. A numerical calculation of the energies and annihilation characteristics of the localized and delocalized Ps states in some alkali halides was performed in a recent paper.[20] However, as before, there is no theoretical analysis explaining the possibility itself of the temperature-activated transition of positronium from a stable delocalized state to a metastable localized state. The absence of the localization effect for Ps in $MgF_2$ and $\alpha$-$SiO_2$ still remains unexplained theoretically to this day too.

The purpose of the present paper is to investigate theoretically the possibility for initially delocalized Ps at low temperatures to be self-trapped with increase of temperature. The zero-temperature variational procedure first introduced by Toyozawa[21,22] for an electron interacting with the short-range potential of acoustic vibrations and then extended by Emin[23] to finite temperatures for the electron interacting with the short-range potential of nonpolar optical vibrations (Holstein's molecular crystal model[24]), is now applied to a compound system at finite temperatures such as a positronium atom coupled with a field of longitudinal acoustic phonons in ionic crystals and $\alpha$-quartz. The interaction of Ps with polar optical phonons is assumed to be negligibly small due to the electroneutrality of the Ps.[18,25] Contrary to Toyozawa and Emin, who directed their efforts toward determining the conditions for the existence of the self-trapped and free electron states, the present work is concerned with the theoretical analysis and the explanation of the results of miscellaneous experimental studies accumulated over nearly the last two decades.

In Sec. II a theory is developed of the self-trapping of the positronium atom in alkali halide crystals. Equations are derived for the energy of Ps as a function of its coupling constant with longitudinal acoustic phonons at finite temperatures. The self-trapping of Ps is shown to have a significant difference compared with the self-trapping of the electron.[21–23,26] The difference is caused by the fact that Ps is a compound system consisting of an electron and a positron. Specifically, one more small dimensionless parameter appears in the theory of the Ps self-trapping apart from $\gamma=\hbar u q_D/(\hbar^2 q_D^2/2m^*)\sim 0.01$ ($u$ is the sound velocity, $q_D$ the Debye cutoff phonon wave vector, $m^*$ the band mass of the electron), the nonadiabaticity parameter (the ratio of the maximum phonon energy to the band width), first introduced by Toyozawa in the theory of the self-trapping of the electron.[21] This additional parameter is $\alpha^2=(a_B\, q_D/4)^2\sim\gamma\sim 0.01$, where $a_B$ is the Bohr radius of Ps. It comes from the relative motion of the particles forming the Ps atom and leads to the dependence of the energy of the self-trapped state on the type of crystal that is absent for the case of the electron.

In Sec. III the basic characteristics (effective mass, mean number of surrounding phonons, and localization radius) of the delocalized and self-trapped states of Ps are analytically derived as functions of temperature. The expressions obtained, as well as those obtained in Sec. II for the energy, are then used in Sec. IV for the numerical calculations of the energy of Ps and its characteristics in crystals of NaF, NaCl, KCl, KI, $MgF_2$, and $\alpha$-$SiO_2$. In this section the deformation potential constants are also found for some of the crystals above by comparing the theoretical differences in the energies of the free and self-trapped states with those estimated experimentally. This section also discusses and concludes the results obtained in the previous two sections.

## II. THE ENERGY OF THE POSITRONIUM AS A FUNCTION OF ITS COUPLING CONSTANT WITH LONGITUDINAL ACOUSTIC PHONONS IN AN IONIC CRYSTAL

In this section the (zero-temperature) intermediate coupling formalism developed by Toyozawa[21,22] for an electron coupled with a field of longitudinal acoustic phonons and then extended by Emin[23] to finite temperatures for an electron coupled with a field of nonpolar optical phonons, will be applied to a compound system consisting of an electron and a positron, the positronium atom interacting with longitudinal acoustic phonons in an ionic crystal. The Ps interaction with polar optical phonons will be neglected due to the electroneutrality of Ps.[18,25] Making use of the tight-binding approximation for Ps in the crystal lattice with the overlap energies neglected other than that for nearest neighbors $(-W)$, one can write the the total secondly quantized Hamiltonian of the system as

$$H=H_{\mathrm{Ps}}+H_{\mathrm{ph}}+H_{\mathrm{int}}=-W\tilde{\sum_{\mathbf{n},\mathbf{m}}} a^{+}_{\mathbf{n}+\mathbf{m}}a_{\mathbf{n}}+\sum_{\mathbf{q}}\hbar u q b^{+}_{\mathbf{q}}b_{\mathbf{q}}+2\sum_{\mathbf{n},\mathbf{q}}F_a(\mathbf{q})\cos\left(\frac{\mathbf{q}\cdot\mathbf{r}}{2}\right)(b_{\mathbf{q}}-b^{+}_{-\mathbf{q}})a^{+}_{\mathbf{n}}a_{\mathbf{n}}e^{i\mathbf{q}\cdot\mathbf{n}}, \tag{1}$$

where the first term denotes the operator of the Ps band energy in the tight-binding approximation, the second term is the phonon Hamiltonian, and the third one is the energy operator of the Ps interaction with the longitudinal branch of acoustic vibrations in the crystal (longitudinal acoustic phonons). The operators $a^{+}_{\mathbf{n}}$ and $a_{\mathbf{n}}$ are those which create and annihilate, respectively, the Ps atom at the **n**th site of the lattice, $b^{+}_{\mathbf{q}}$ and $b_{\mathbf{q}}$ are those for a phonon with the wave vector **q**. The tilde over the double sum of the first term means that the summation is only to be carried out when **n** and **m** are the nearest neighbors to each other. The crystal is assumed to have a simple cubic lattice with the overlap integral $W$ between the nearest neighbors equal to $W=\hbar^2/(2M^*a^2)$ where $M^*$ and $a$ are the band mass of Ps, and the distance between the nearest atoms in the simple cubic lattice, respectively. Such an assumption looks quite natural for the Ps atom in an ionic crystal in view of the experimental fact that Ps in alkali halides hardly distinguishes the anion and cation and only ''sees'' the simple cubic lattice.[8,10] The factor $F_a(\mathbf{q})$ in the third term is equal for longitudinal acoustic phonons to

$$F_a(\mathbf{q})=-iE_d\sqrt{\frac{\hbar q}{2NMu}}=-F_a^*(\mathbf{q}), \tag{2}$$

where $N$, $M$, and $u$ are the total number of unit cells in the crystal, the mass of a unit cell, and the sound velocity, respectively. The parameter $E_d$ denotes the deformation potential constant. It is assumed to be the same for the electron and for the positron in the Ps atom since the deformation potential corresponds to the variation of the band structure of the particle with changing interionic distances, and the lowest positron band in alkali halides is not considerably different from the conduction band of the electron.[27] This approximation leads to an accounting of the compound nature of the Ps by a simple doubled cosine function in the third term of Eq. (1) with **r** being the relative position vector of the electron and positron.

The task of this section is to determine the energy of positronium as a function of its coupling constant with longitudinal acoustic phonons at finite temperatures. To do so one uses the variational approach in the spirit of the zero-temperature intermediate coupling formalism by Toyozawa.[21,22] The trial wave function of the total system is written as

$$|\Psi_{\mathbf{k},N_\mathbf{q}}\rangle=\frac{1}{\sqrt{N}}\sum_{\mathbf{n}} e^{i\mathbf{k}\cdot\mathbf{n}}S_\mathbf{k}(\mathbf{n})a_\mathbf{n}^{+}|N_\mathbf{q}\rangle|1S_{1/2}\rangle. \tag{3}$$

Here $|N_\mathbf{q}\rangle=|0\rangle_{Ps}|N_\mathbf{q}\rangle_{\mathrm{ph}}$ with $|N_\mathbf{q}\rangle_{\mathrm{ph}}$ representing the $N_\mathbf{q}$th excited state (with the phonon occupation number $N_\mathbf{q}$) of the $\mathbf{q}$th vibrational mode in an undisturbed lattice and $|0\rangle_{\mathrm{Ps}}$ is the vacuum state associated with the center-of-mass motion of the Ps atom; $|1S_{1/2}\rangle$ is the wave function of the internal ground state of Ps. The operator $S_\mathbf{k}(\mathbf{n})$ is defined as

$$S_\mathbf{k}(\mathbf{n})=\exp\left\{\sum_\mathbf{q}\beta_\mathbf{k}^{*}(\mathbf{q},\mathbf{n})b_\mathbf{q}-\mathrm{H.c.}\right\},$$

$$\beta_\mathbf{k}(\mathbf{q},\mathbf{n})=f_\mathbf{k}(\mathbf{q})e^{-i\mathbf{q}\cdot\mathbf{n}},\quad S_\mathbf{k}^{+}(\mathbf{n})=S_\mathbf{k}^{-1}(\mathbf{n}), \tag{4}$$

and has the following properties:

$$S_\mathbf{k}^{-1}(\mathbf{n})b_\mathbf{q}S_\mathbf{k}(\mathbf{n})=b_\mathbf{q}-\beta_\mathbf{k}(\mathbf{q},\mathbf{n}),$$

$$S_\mathbf{k}^{-1}(\mathbf{n})b_\mathbf{q}^{+}S_\mathbf{k}(\mathbf{n})=b_\mathbf{q}^{+}-\beta_\mathbf{k}^{*}(\mathbf{q},\mathbf{n}). \tag{5}$$

In other words, $S_\mathbf{k}(\mathbf{n})$ is the operator which [because of Eq. (5)] makes the lattice deform around the **n**th lattice site. The deformation is associated with the presence of Ps with the wave vector **k** at this point. The distribution of the Ps center-of-mass position around the point **n** is for the sake of simplicity supposed to be equal to $\delta_{\mathbf{n},0}$ which is appropriate in the case of the short-range (acoustic or nonpolar optical) modes of lattice vibrations.[21,23] Positronium located at the **n**th site of the lattice, distorts the lattice around itself. The magnitude and the **q** dependence of the distortion are, according to Eq. (4), characterized by the function $f_\mathbf{k}(\mathbf{q})$. For example, while $f_\mathbf{k}(\mathbf{q})=0$ refers to an undistorted lattice, a situation in which $f_\mathbf{k}(\mathbf{q})$ is only substantial for $|\mathbf{q}|$ less than some value $q_0<\pi/a$, is characterized by a local distortion of range $\sim 1/q_0$. The function $f_\mathbf{k}(\mathbf{q})$ is a trial function to be determined from the minimum condition of the total energy functional $J[f_\mathbf{k}(\mathbf{q})]$ obtained by averaging the Hamiltonian Eq. (1) over the wave function Eq. (3). Such an averaging yields

$$\begin{aligned}J[f_\mathbf{k}(\mathbf{q})]=\langle\Psi_{\mathbf{k},N_\mathbf{q}}|H|\Psi_{\mathbf{k},N_\mathbf{q}}\rangle={}&-W\tilde{\sum_\mathbf{m}}e^{i\mathbf{k}\cdot\mathbf{m}-\zeta_\mathbf{k}(\mathbf{m})}\\&+\sum_\mathbf{q}\hbar uq(N_\mathbf{q}+|f_\mathbf{k}(\mathbf{q})|^2)\\&-\sum_\mathbf{q}V_a(\mathbf{q})[f_\mathbf{k}(\mathbf{q})-f_\mathbf{k}^{*}(\mathbf{q})],\end{aligned} \tag{6}$$

where

$$\zeta_\mathbf{k}(\mathbf{m})=\sum_\mathbf{q}|f_\mathbf{k}(\mathbf{q})|^2\varphi(\mathbf{q},\mathbf{m})=\zeta_\mathbf{k}^{*}(-\mathbf{m}) \tag{7}$$

with $\varphi(\mathbf{q},\mathbf{m})=2N_\mathbf{q}+1-N_\mathbf{q}e^{i\mathbf{q}\cdot\mathbf{m}}-(N_\mathbf{q}+1)e^{-i\mathbf{q}\cdot\mathbf{m}}$ and

$$V_a(\mathbf{q})=2F_a(\mathbf{q})\langle 1S_{1/2}|\cos\left(\frac{\mathbf{q}\cdot\mathbf{r}}{2}\right)|1S_{1/2}\rangle=\frac{2F_a(\mathbf{q})}{[1+(qa_B/4)^2]^2} \tag{8}$$

is the form factor of the positronium as a compound particle, originating from the relative motion of the electron and positron in the positronium atom; $a_B$ is the Bohr radius of Ps. It is assumed in Eq. (8) that as Ps scatters on phonons, it all the time remains in the ground $|1S_{1/2}\rangle$-internal state since the typical energies of acoustic phonons ($\sim 0.01$ eV) are much smaller than the difference in the energies of the ground state and the first excited state of Ps ($\sim 5$ eV). The three terms in Eq. (6) [written in the same order as those in Eq. (1)] come from averaging the corresponding terms of the total Hamiltonian Eq. (1).

Minimizing Eq. (6) with respect to $f_\mathbf{k}(\mathbf{q})$, one has

$$f_\mathbf{k}(\mathbf{q})=-\frac{V_a(\mathbf{q})}{W\tilde{\sum_\mathbf{m}}e^{i\mathbf{k}\cdot\mathbf{m}-\zeta_\mathbf{k}(\mathbf{m})}\varphi(\mathbf{q},\mathbf{m})+\hbar uq}. \tag{9}$$

Inserting this into Eqs. (6) and (7), one obtains the total energy of the system in the form

$$\begin{aligned}E(\mathbf{k})={}&\sum_\mathbf{q}\hbar uqN_\mathbf{q}-W\tilde{\sum_\mathbf{m}}[1+\zeta_\mathbf{k}(\mathbf{m})]e^{i\mathbf{k}\cdot\mathbf{m}-\zeta_\mathbf{k}(\mathbf{m})}\\&-\sum_\mathbf{q}\frac{|V_a(\mathbf{q})|^2}{W\tilde{\sum_\mathbf{m}}e^{i\mathbf{k}\cdot\mathbf{m}-\zeta_\mathbf{k}(\mathbf{m})}\varphi(\mathbf{q},\mathbf{m})+\hbar uq}\end{aligned} \tag{10}$$

with

$$\zeta_\mathbf{k}(\mathbf{m})=\sum_\mathbf{q}\frac{|V_a(\mathbf{q})|^2\varphi(\mathbf{q},\mathbf{m})}{\left[W\tilde{\sum_\mathbf{m}}e^{i\mathbf{k}\cdot\mathbf{m}-\zeta_\mathbf{k}(\mathbf{m})}\varphi(\mathbf{q},\mathbf{m})+\hbar uq\right]^2}. \tag{11}$$

Equation (11) is a set of $\nu$ simultaneous transcendental equations for $\nu$ unknown $\zeta_\mathbf{k}(\mathbf{m})$, where $\nu$ is the number of the nearest neighbors in a crystal. The phonon occupation numbers $N_\mathbf{q}$ in Eqs. (10) and (11) are for the sake of simplicity assumed to be equal to

$$N_\mathbf{q}=\left[\exp\left(\frac{\hbar uq}{k_BT}\right)-1\right]^{-1}, \tag{12}$$

the mean number of acoustic phonons with wave vector **q** at temperature $T$ in an undisturbed lattice (the Bose-Einstein phonon distribution function). Such an assumption has been employed in prior polaron theories[24,23,28] and is, as a practical matter, expected to be justifiable in a wide variaty of circumstances. The equilibrium state of an excess particle in the deformable lattice must actually correspond to a minimum of the free energy of the total system. However, the procedure of minimizing the energy functional $J[f_\mathbf{k}(\mathbf{q})]$ of the system with respect to $f_\mathbf{k}(\mathbf{q})$ and then replacing the phonon occupation numbers $N_\mathbf{q}$ by the equilibrium values Eq. (12) they possess in the undistorted lattice, is proved in Ref. 23 to be equivalent (to the lowest order in the volume of the sample) to minimizing the free energy of the system with respect to $f_\mathbf{k}(\mathbf{q})$.

As is evident from Eq. (7), the function $\zeta_\mathbf{k}(\mathbf{m})$ represents the magnitude of the lattice distortion around the Ps. On the other hand, the mean number of phonons surrounding Ps in the crystal is given by

$$\langle n\rangle=\left\langle\Psi_{\mathbf{k},N_\mathbf{q}}\middle|\sum_\mathbf{q}b_\mathbf{q}^{+}b_\mathbf{q}\middle|\Psi_{\mathbf{k},N_\mathbf{q}}\right\rangle-\sum_\mathbf{q}N_\mathbf{q}=\sum_\mathbf{q}|f_\mathbf{k}(\mathbf{q})|^2, \tag{13}$$

which, at not too high temperatures, is of the same order of magnitude as $\zeta_\mathbf{k}(\mathbf{m})$. Thus, $\zeta_\mathbf{k}(\mathbf{m})$ can be considered as the quantity representing the strength of the Ps-phonon coupling:

a large number of the surrounding phonons (responsible for the strong coupling of positronium with the phonons) corresponds to large values of $\zeta_{\mathbf{k}}(\mathbf{m})$, and conversely. For fixed $\mathbf{k}$ in a simple cubic crystal all the $\zeta_{\mathbf{k}}(\mathbf{m})$ are identical, i.e., $\zeta_{\mathbf{k}}(\mathbf{m})=\zeta_{\mathbf{k}}$, and Eq. (11) reduces to one transcendental equation. If, moreover, one restricts oneself by the small $\mathbf{k}\sim 0$ near the bottom of the Ps band, then $\zeta_{\mathbf{k}\sim 0}\approx\zeta_0=\zeta$, the constant which upon going from summing over $\mathbf{q}$ to an integration in Eq. (11) and introducing the dimensionless variables, takes the form

$$\zeta=12\,g\,\gamma\,e^{2\zeta}\int_0^1 d\xi\,\frac{[2N(\xi)+1]\xi^3}{(1+\alpha^2\xi^2)^4\{[2N(\xi)+1]\xi+\gamma e^{\zeta}\}^2} \tag{14}$$

with

$$g=\frac{E_d^2}{12\,WMu^2}\quad\text{and}\quad\gamma=\frac{\hbar u q_D}{\hbar^2 q_D^2/2M^*} \tag{15}$$

being, respectively, the dimensionless coupling constant of the positronium atom with acoustic phonons, and the Ps nonadiabaticity parameter (the ratio of the maximum phonon energy to the band width of Ps) first introduced in Ref. 21 for the case of an electron; $q_D$ is the Debye cutoff phonon wave vector. The function $N(\xi)$ is the mean number of phonons Eq. (12) written in dimensionless variables

$$N(\xi)=\left[\exp\left(\frac{\hbar u q_D}{k_B T}\,\xi\right)-1\right]^{-1}. \tag{16}$$

The parameter $\alpha$ in Eq. (14) represents the contribution from the internal motion of the electron and positron forming the Ps atom:

$$\alpha=\frac{q_D a_B}{4}. \tag{17}$$

Note that the parameters $\gamma$ and $\alpha^2$ in typical ionic crystals are of the same order of magnitude: $\gamma\sim\alpha^2\sim 0.01$.

After some analogous transformations, the Ps total energy corresponding to Eq. (14) takes the form

$$-\frac{E(0)-E_{\text{vib}}}{6W}=(1+\zeta)e^{-\zeta}+12\,g\,\gamma\,e^{\zeta}\int_0^1 d\xi \times\frac{\xi^2}{(1+\alpha^2\xi^2)^4\{[2N(\xi)+1]\xi+\gamma e^{\zeta}\}}, \tag{18}$$

where $E_{\text{vib}}=\Sigma_{\mathbf{q}}\,\hbar u q N_{\mathbf{q}}$ is the vibrational energy of the crystal. The system of Eqs. (14) and (18) completely determines the energy of Ps near the band bottom as a function of its coupling constant $g$ with acoustic phonons at finite temperatures: the solution of Eq. (14) yields $\zeta$ as a function of the parameter $g$, whereupon the substitution of $\zeta$ obtained in Eq. (18) gives the energy of Ps as a function of the same parameter. The weak and strong phonon coupling approximations for the Ps energy are obtained from Eq. (18) for the small and large $\zeta$, respectively

$$\zeta\ll 1,\quad -\frac{E(0)-E_{\text{vib}}}{6W}\approx 1+6g\gamma\,[1-2F(T)], \tag{19}$$

$$\zeta\gg 1,\quad -\frac{E(0)-E_{\text{vib}}}{6W}\approx 4g\left(1-\frac{12}{5}\alpha^2\right), \tag{20}$$

where

$$F(T)=2\left(\frac{T}{T_D}\right)^2\int_0^{T_D/T} dx\,\frac{x}{e^x+1} \tag{21}$$

is the function that comes from the phonon distribution function Eq. (16) and determines the temperature dependence of the Ps energy, and $T_D$ is the Debye temperature of the crystal. In Eqs. (19) and (20) it is taken into account that the parameters $\gamma$ and $\alpha^2$ are of the order of 0.01 in typical ionic crystals, and consequently can be considered as small parameters in which one can expand functions that depend on them. Therefore, Eqs. (19) and (20) have been written out to terms linear in $\gamma$ and $\alpha^2$.

The difference in the energies of the Ps strongly coupled with the phonons and that weakly coupled with the phonons is given, according to Eqs. (19) and (20), by

$$\frac{\Delta E(0)}{6W}\approx 1-4g\left(1-\frac{3}{2}[1-2F(T)]\gamma-\frac{12}{5}\alpha^2\right). \tag{22}$$

Note that, as is seen from Eq. (19), the energy of the Ps weakly coupled with the phonons increases with the temperature due to the presence of the function $F(T)$ Eq. (21). The energy of Ps strongly coupled with the phonons does not, according to Eq. (20), depend on the temperature. In addition, the presence of $\alpha^2=(q_D\,a_B/4)^2\sim 0.01$, one more small parameter for positronium compared with an electron,[21,23] leads (through $q_D$) to the dependence of the energy of Ps strongly coupled with phonons on the type of crystal that is absent for the electron. The difference in the energies [Eq. (22)] of Ps strongly coupled with phonons and that weakly coupled with the phonons, depends on the type of crystal too. This dependence, although it also takes place for the electron (through $q_D$-dependence of $\gamma$), mainly comes from $\alpha^2$ rather than from $\gamma$ for Ps since $F(T)\sim 0$ at small temperatures ($T\ll T_D$) and $12\alpha^2/5>3\gamma/2$, and $F(T)\to 1/2$ at high temperatures ($T\gg T_D$) and the contribution of $\gamma$ vanishes.

## III. THE BASIC CHARACTERISTICS OF THE FREE AND SELF-TRAPPED POSITRONIUM STATES

### A. The effective mass

#### *1. Weak phonon coupling regime*

In calculating the effective mass of Ps for this regime the case of the absolute zero of temperature will only be considered since the influence of the Ps-phonon scattering at nonzero temperatures was already analyzed in Ref. 29. It was shown to lead to a very slow decrease of the effective mass of Ps with increase of temperature. The effective positronium mass renormalized by the virtual phonon field at $T=0$ K, can be obtained from an analysis of the positronium self-energy $\Sigma(p,\omega)$ with the use of the renormalization technique developed in Ref. 30. The positronium self-energy to the second order in the interaction with the virtual phonons, is written as[28]

$$\Sigma(p,\omega)=\sum_{\mathbf{q}} \frac{|V_a(\mathbf{q})|^2}{\omega-E(\mathbf{k}+\mathbf{q})-\hbar uq+i\delta}, \tag{23}$$

where $E(\mathbf{k}+\mathbf{q})=\hbar^2(\mathbf{k}+\mathbf{q})^2/(2M^*)$ and $p=\hbar k$ are the energy and momentum of ''bare'' positronium, respectively. The mass renormalization constants $\alpha_1$ and $\alpha_2$ are obtained by expanding the real part of the self-energy Eq. (23) to terms linear in $\omega$ and $p^2/2M^*$:[30]

$$\operatorname{Re}\Sigma(p,\omega)=\sum_{\mathbf{q}} \frac{|V_a(\mathbf{q})|^2}{\omega-E(\mathbf{k}+\mathbf{q})-\hbar uq}\approx\Delta_0+\alpha_1\omega+\alpha_2\frac{p^2}{2M^*} \tag{24}$$

with $\Delta_0$ being the polaron energy shift. The Ps effective mass $M^{**}$ renormalized by the virtual phonon field, is then given by

$$M^{**}=\left(\frac{1}{p}\frac{d\omega}{dp}\right)^{-1}=M^*\frac{1-\alpha_1}{1+\alpha_2}. \tag{25}$$

The calculation of $\alpha_1$ and $\alpha_2$ from Eq. (24) yields

$$\begin{aligned}\alpha_1&=-8\left(\frac{6}{\pi}\right)^{4/3} g\gamma\int_0^1 d\xi\frac{\xi}{(1+\alpha^2\xi^2)^4(\xi+\gamma)^2}\\&\approx-8\left(\frac{6}{\pi}\right)^{4/3} g\gamma\,[\ln(1+1/\gamma)-1],\\\alpha_2&=-\frac{8}{3}\left(\frac{6}{\pi}\right)^{4/3} g\gamma\int_0^1 d\xi\frac{\xi(\xi-3\gamma)}{(1+\alpha^2\xi^2)^4(\xi+\gamma)^3}\\&\approx-\frac{8}{3}\left(\frac{6}{\pi}\right)^{4/3} g\gamma\,[\ln(1+1/\gamma)-3].\end{aligned} \tag{26}$$

According to Eqs. (26), the positronium mass renormalization constants in the weak phonon coupling regime are of the order of the nonadiabaticity parameter $\gamma\sim0.01$. In this case it follows from Eq. (25) that the renormalized mass $M^{**}$ of the positronium only insignificantly exceeds its band mass $M^*$.

#### *2. Strong phonon coupling regime*

The Ps effective mass in this regime can be estimated directly from Eq. (10).[21] Taking into account that $\zeta_{\mathbf{k}}\gg1$ now, one obtains it to be weakly dependent on $\mathbf{k}$ from Eq. (11). Then Eq. (10) can approximately be rewritten in the form

$$E(\mathbf{k})-E(0)\approx-W\zeta e^{-\zeta}\tilde{\sum_{\mathbf{m}}}\,(e^{i\mathbf{k}\cdot\mathbf{m}}-1)\approx\frac{\hbar^2\mathbf{k}^2}{2M^{**}}, \tag{27}$$

from which it follows that

$$M^{**}\approx\zeta^{-1}e^{\zeta}M^* \tag{28}$$

and does not depend on temperature. As is seen from Eq. (28), the effective mass of Ps strongly coupled with the phonons greatly exceeds its band mass. This means that the Ps must practically be immobile (''self-trapped'') in this case.

### B. The mean number of surrounding phonons

The mean number of the phonons surrounding the Ps atom in the state Eq. (3) is given by Eq. (13). Inserting Eq. (9) in Eq. (13) and going from the summation over $\mathbf{q}$ to the integration, one obtains for $\mathbf{k}\sim0$

$$\langle n\rangle=12\,\lambda\,g\gamma e^{2\zeta}\int_0^1 d\xi\frac{\xi}{(1+\alpha^2\xi^2)^4\{[2N(\xi)+1]\xi+\gamma e^{\zeta}\}^2}, \tag{29}$$

where $\lambda=6/(q_D^2\,a^2)\sim1$ in typical ionic crystals, and $\zeta$ and $N(\xi)$ are given by Eqs. (14) and (16), respectively. Equation (29) is approximated for small and large $\zeta$ as

$$\zeta\ll1,\quad\langle n\rangle\approx12\,\lambda\,g\gamma\int_0^1 d\xi\frac{\xi}{\{[2N(\xi)+1]\xi+\gamma\}^2}, \tag{30}$$

$$\zeta\gg1,\quad\langle n\rangle\approx\frac{6\lambda g}{\gamma}. \tag{31}$$

Equations (30) and (31) give the weak and strong phonon coupling approximations for the mean number of the phonons surrounding the Ps atom in a crystal. In the cases of weak and strong coupling the nonadiabaticity parameter $\gamma$ stands in the numerator and in the denominator, respectively. Therefore, $\langle n\rangle$ is small for the weak coupling and large for the strong coupling of positronium with phonons. The mean number of the phonons surrounding Ps decreases with the increase of temperature in the weak phonon coupling regime, and does not depend on the temperature in the strong phonon coupling regime.

### C. The localization radius

To estimate the characteristic size of the center-of-mass motion of Ps (the localization radius) it is expedient to introduce the correlation function of the form

$$F(\mathbf{m})=\left\langle\Psi_{\mathbf{k},N_{\mathbf{q}}}\left|\sum_{\mathbf{n}}a^+_{\mathbf{n}+\mathbf{m}}a_{\mathbf{n}}\right|\Psi_{\mathbf{k},N_{\mathbf{q}}}\right\rangle. \tag{32}$$

Here $\mathbf{m}$ is a vector originating at the $\mathbf{n}$th lattice site, pointing in the direction of one of the other sites [not necessarily one of the closest, in contrast to Eq. (1)]. The function $F(\mathbf{m})$ characterizes the mean number of the simultaneously correlated lattice sites where this correlation is due to the presence of Ps. For small $\mathbf{k}\sim0$ in a simple cubic crystal the function $F(\mathbf{m})$, in view of Eq. (3), reduces to

$$F(\mathbf{m})\approx e^{-\zeta(\mathbf{m})} \tag{33}$$

with $\zeta(\mathbf{m})$ given by Eq. (11) for $\mathbf{k}=0$. This function, after the angular integration, transforms to

$$\begin{aligned}\zeta(m)=12\,\lambda\,g\gamma e^{2\zeta}\int_0^1 d\xi\\\times\frac{[2N(\xi)+1]\xi}{(1+\alpha^2\xi^2)^4\{[2N(\xi)+1]\xi+\gamma e^{\zeta}\}^2}\\\times\left(1-\frac{\sin(q_D\,m\,\xi)}{q_D\,m\,\xi}\right),\end{aligned} \tag{34}$$

where $m=|\mathbf{m}|=an$, $n=0,1,2,\ldots$, and $\zeta$ is given by Eq. (14). Next introducing the continuous coordinate $R=2m$, one can determine an effective localization radius of the Ps atom in a crystal in terms of the characteristic decay of the continuous analog $F(R)$ of the correlator Eq. (33) with increasing $R$.

The power Eq. (34) (expressed in terms of $R$) of the exponent in the correlator $F(R)$ reduces for the weak ($\zeta \ll 1$) and strong ($\zeta \gg 1$) Ps-phonon coupling to

$$\zeta \ll 1, \quad \zeta(R) \approx 12\lambda g \gamma \int_0^1 d\xi \frac{[2N(\xi)+1]\xi}{\{[2N(\xi)+1]\xi+\gamma\}^2} \times \left(1-\frac{\sin(q_D R \xi/2)}{q_D R \xi/2}\right), \tag{35}$$

$$\zeta \gg 1, \quad \zeta(R) \approx \frac{12\lambda g}{\gamma} \int_0^1 d\xi \, [2N(\xi)+1]\xi \times \left(1-\frac{\sin(q_D R \xi/2)}{q_D R \xi/2}\right). \tag{36}$$

The functions $\zeta(R)$ in Eqs. (35) and (36) are easily seen to have a similar behavior at small distances $R$: both of them tend to zero for $R\to 0$ at all temperatures. As a consequence, the correlator $F(R)\sim 1$ at small $R\sim 0$. At large $R$, in contrast, the behavior of $\zeta(R)$ in Eq. (35) is quite different from that in Eq. (36). Specifically, $\zeta(R)$ in Eq. (35) decreases with increase of the temperature as $R\to\infty$. Its maximal value is reached at $T=0$ K and is equal to $\langle n\rangle_{T=0}$ ($\ll 1$) given by Eq. (30). On the contrary, $\zeta(R)$ in Eq. (36) increases with temperature for $R\to\infty$. Its minimal value is reached at $T=0$ K and is equal to $\langle n\rangle$ ($\gg 1$) given by Eq. (31). The temperature dependence of $\zeta(R)$ in Eq. (36) at large $R$ is estimated as

$$T \gg T_D, \quad \zeta(R\to\infty) \approx \langle n\rangle \left(1+4\frac{T}{T_D}\right),$$

$$T \ll T_D, \quad \zeta(R\to\infty) \approx \langle n\rangle \left[1+\frac{2\pi^2}{3}\left(\frac{T}{T_D}\right)^2\right], \tag{37}$$

from which it follows that $\zeta(R)$ increases with temperature at large $R$. Thus, for weak phonon coupling the correlator $F(R)$ [or $F(\mathbf{m})$ Eq. (33)] hardly decays with increasing $R$ at all temperatures, while for the strong phonon coupling it decays very fast and the higher the temperature, the faster it decays. Correspondingly, in the weak coupling regime, by virtue of the nondecay of the correlation function, the localization radius of the positronium atom in a crystal $R_0$ is infinitely large: $R_0\sim\infty$, i.e., positronium is delocalized. In the strong coupling regime the localization radius of Ps is finite and the higher the temperature, the smaller the localization radius. It can be estimated from the condition

$$F(R_0)=\frac{1}{\langle n\rangle e} \tag{38}$$

with $F(R)$ given by Eq. (33) where $\zeta(R)$ is represented by Eq. (36), and $\langle n\rangle$ given by Eq. (31). The maximal value of $R_0$ (reached at $T=0$ K) is estimated from the simple transcendental equation obtained from Eq. (38) in view of Eq. (36):

$$\sin\left(\frac{q_D R_0}{4}\right)=\sqrt{1-\frac{1+\ln\langle n\rangle}{\langle n\rangle}\frac{q_D R_0}{4}}. \tag{39}$$

Since $\langle n\rangle$ for the strong coupling is large, one has from Eq. (39) that $q_D R_0/4\sim\pi/4$, from which noting that $q_D \sim\pi/(2a)$ in ionic crystals, one obtains $R_0\sim 2a$, i.e., the localization radius of a strongly coupled positronium atom is of the order of the lattice constant of the crystal, and the positronium is localized (‘‘self-trapped’’).

## IV. NUMERICAL RESULTS, DISCUSSION AND COMPARISON WITH EXPERIMENT

Figure 1 presents the zero-temperature graphs of the dependence of the energy of a positronium atom on the acoustic coupling constant $g$ for three alkali halides: NaF, NaCl, and KCl. The curves were obtained by the numerical tabulation of Eq. (18) with Eq. (14) taken into account. The calculations made use of numerical values of the constants of the ionic crystals, taken from Refs. 31,32, and numerical values of the Ps band masses calculated in Ref. 33. The two intersecting straight lines for each alkali halide correspond to the cases: gently sloping, to the weak coupling approximation described by Eq. (19) and steep, to the strong coupling approximation described by Eq. (20). The presence of $\alpha^2 \sim 0.01$ in Eqs. (18) and (14), the additional small parameter for positronium compared with an electron, leads to different slopes of the strong-coupling lines for different alkali halides, which is not the case for the electron.[21] The dependence of the Ps energy on $g$ for nonzero temperatures is shown in Fig. 2 for the crystal of KCl as a typical example. The weak coupling line is seen to change its slope in such a way that the energy [in accordance with Eq. (19)] increases with temperature, while the slope of the strong coupling curve [in accordance with Eq. (27)] does not at all depend on temperature. As a consequence, the difference $\Delta E(0)$ in the energies of Ps strongly coupled with the phonons and that weakly coupled with the phonons decreases somewhat with increase of temperature [in accordance with Eq. (22)]. For $g<\sim 0.25$ the simultaneous existence of two positronium states is possible at nonzero temperature, one of which (the weakly coupled state) is stable and the other of which (the strongly coupled state) is metastable. According to the formulas for the effective mass Eqs. (25)–(28), the mean number of phonons Eqs. (30) and (31), and the localization radius Eq. (39), the weakly coupled stable state should be delocalized and the metastable strongly coupled state should, on the contrary, be localized (self-trapped) in a region on the order of the lattice constant of the crystal.

As was noted in the Introduction, the situation just described has its experimental analog. Therefore, substituting the experimentally measured differences in the energies of the free and self-trapped Ps states $\mathcal{E}$ instead of $\Delta E(0)$ in Eq. (22), one can determine the deformation potential constants $E_d$ for those crystals in which Ps self-trapping is observed if the positronium band masses $M^*$ are known beforehand. In doing so the temperature dependence of $\Delta E(0)$ in Eq. (22)

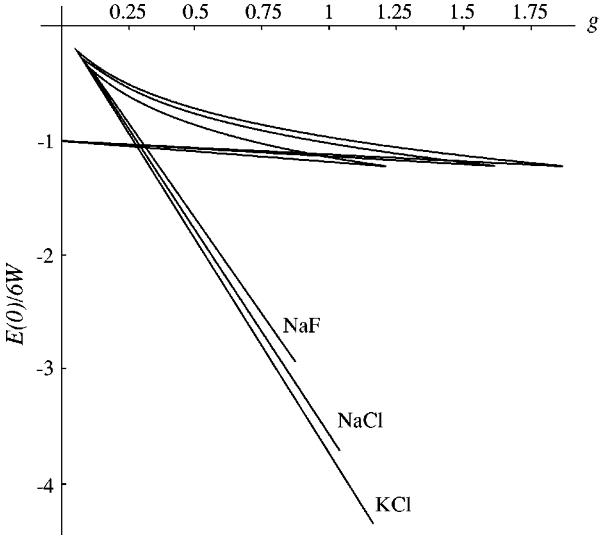

FIG. 1. The dependence of the Ps total energy on the dimensionless coupling constant $g$ with longitudinal acoustic phonons for crystals of NaF, NaCl, and KCl at absolute zero temperature.

can be neglected since the self-trapping, according to experiment,[14] mainly occurs at the temperatures $T< \sim T_D/4$. The function $F(T)$ in Eq. (22) can be approximated at such temperatures $(T \ll T_D)$ as $F(T) \approx (\pi^2/6)(T/T_D)^2 \sim 0$, and $\Delta E(0)$ can, therefore, be approximately considered as temperature independent. In this way the values of $E_d$ were estimated for NaF and KCl crystals since the values of $\mathcal{E}$ are available for these crystals from Refs. 12 and 13, respectively, and the Ps band masses have been numerically calculated in Ref. 33. [Note that the constants $E_d$ so obtained are, as a matter of fact, equal to those for an excess electron (or positron) in the same alkali halide crystals—see the explanation after Eq. (2) in Sec. II.] Then, with $E_d$ obtained, the coupling constant $g$ [Eq. (15)] of Ps with longitudinal acoustic phonons, the effective mass $M^{**}$ [Eq. (25)] of delocalized positronium, the mean numbers $\langle n \rangle_{T=0}$ [Eqs. (30) and (31)] of virtual phonons surrounding both types of positronium at absolute zero temperature, and the localization radius $R_0^{T=0}$ [Eq. (39)] of self-trapped positronium at absolute zero temperature, were calculated. For KI the experimental values of $\mathcal{E}$ and the effective mass $M^{**}$ are available,[3,14] but there are no published data for the band mass $M^*$ of positronium. Therefore, for KI the band mass was first estimated according to Eqs. (25) and (26) from the known value of the effective mass, and then the deformation potential constant $E_d$ was calculated by substituting the values of $\mathcal{E}$ and $M^*$ in Eq. (22). Then, the values of $M^*$ and $E_d$ so obtained were used to calculate the basic characteristics of Ps in KI. For NaCl, on the other hand, there are no experimental data on the difference $\mathcal{E}$ in the energies of the free and self-trapped Ps states, but the band mass of Ps has been calculated.[33] Therefore, the value of $E_d = 6.2$ eV, estimated using Eq. (22) from the condition $\Delta E(0) \approx 0.08$ eV, was used for the calculations of the Ps characteristics in this crystal. The results of all the enumerated calculations, and also the experimental data used in the calculations, are listed in Table I.

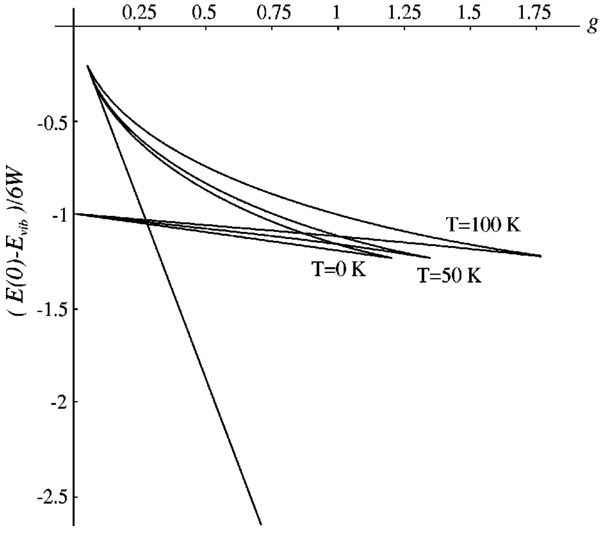

FIG. 2. The dependence of the total energy of the positronium on the coupling constant $g$ with acoustic phonons for the crystal of KCl at nonzero temperatures.

For the crystal of MgF$_2$ the computed dependence of the Ps energy on the acoustic coupling constant $g$ at the nonzero temperatures is shown in Fig. 3 as a typical example. Similar dependence has also been obtained for the crystal of $\alpha$-SiO$_2$. The curves have been obtained by the numerical tabulation of Eq. (18) with Eq. (14) taken into account. The calculations made use of the numerical values of the crystalline constants taken from Ref. 32. The band masses of Ps were estimated according to Eqs. (25) and (26) with the use of the values experimentally known of $M^{**}$ and $E_d$.[17] The self-trapped Ps state in MgF$_2$ (and in $\alpha$-SiO$_2$) is seen to be unstable at absolute zero temperature, while it becomes metastable at the nonzero temperatures higher than 300 K. These temperatures have been computed to be 306 K for MgF$_2$ and 334 K for $\alpha$-SiO$_2$. The corresponding differences $\Delta E(0)$ in the energies of self-trapped and delocalized Ps are, according to Eq. (22), equal to 2.32 and 1.37 eV for MgF$_2$ and $\alpha$-SiO$_2$, respectively. This is more than one order of magnitude larger than the same quantities in those alkali halides in which the self-trapping is observed experimentally (see Table I). The temperatures of the Ps self-trapping in MgF$_2$ and $\alpha$-SiO$_2$ (the temperature at which the half of all the Ps atoms decay from the self-trapped state) can be estimated from the temperature dependence of the fraction $f_{\mathrm{ST}}$ of the self-trapped Ps, given approximately by[12–14]

$$f_{\mathrm{ST}}(T) \approx \frac{1}{1+AT^{3/2}\exp[\Delta E(0)/k_B T]}, \tag{40}$$

where $A=(3u^3/4\pi T_D^3)(\pi M^{**}/2k_B)^{3/2} \sim 10^{-6}$ K$^{-3/2}$, and $\Delta E(0)$ is given by Eq. (22). The definition Eq. (40) is, in fact, the simplest allowing one to estimate the self-trapping temperature of the Ps. It takes into account neither the fact of the existence of the adiabatic potential barrier between the two Ps states nor the possibility of the quantum-mechanical tunneling of Ps through this barrier. Analysis accounting for these effects can be found elsewhere.[34,35] The self-trapping temperature $T_{\mathrm{ST}}$ is further given by the solution of the transcendental equation $f_{\mathrm{ST}}(T_{\mathrm{ST}})=1/2$. The self-trapping temperatures are estimated from this equation to be $T_{\mathrm{ST}} = 9621$ K for MgF$_2$ and $T_{\mathrm{ST}}=4041$ K for $\alpha$-SiO$_2$, explain-

TABLE I. The characteristics of the free and self-trapped Ps states in some alkali halide crystals.

| | NaF | NaCl | KCl | KI | $MgF_2$ | $\alpha$-$SiO_2$ |
|---|---|---|---|---|---|---|
| $\mathcal{E}$, eV | $0.10_7$ (Ref. 12) | | $0.04_3$ (Ref. 14) | $0.03_1$ (Ref. 14) | | |
| $\Delta E(0)$, eV | | 0.08 | | | 2.32 | 1.37 |
| $E_d$, eV | 8.51 | 6.2 | 6.04 | 5.28 | 3.80 (Ref. 17) | 1.80 (Ref. 17) |
| $g$ | 0.30 | 0.28 | 0.27 | 0.26 | 0.04 | 0.04 |
| $M^{**}_{\rm exp}/2m_0$ | $1.50\pm0.2$<br>(Ref. 14) | $1.37\pm0.2$<br>(Ref. 14) | $1.56\pm0.15$<br>(Ref. 14) | $1.98\pm0.1$<br>(Ref. 14) | $1.10\pm0.01$<br>(Ref. 17) | $1.54\pm0.08$<br>(Ref. 17) |
| $M^*/2m_0$ | 1.014 (Ref. 33) | 1.119 (Ref. 33) | 1.233 (Ref. 33) | 1.39 | 1.04 | 1.48 |
| $M^{**}/2m_0$ | 1.42 | 1.56 | 1.78 | | | |
| $\zeta \ll 1$: $\langle n\rangle_{T=0}$ | 0.35 | 0.35 | 0.41 | 0.38 | 0.06 | 0.04 |
| $\zeta \gg 1$: $\langle n\rangle$ | 112 | 99 | 74 | 78 | | |
| $R_0^{\rm exp}$, Å | 3.2 (Ref. 12) | | 3.5 (Ref. 13) | 4.3 (Ref. 14) | | |
| $R_0^{T=0}$, Å | 1.57 | 2.04 | 2.97 | 3.54 | | |

ing theoretically the experimental evidence for nonexistence of the self-trapped Ps states in these crystals. For those crystals in which the Ps self-trapping has been registered the self-trapping temperatures are estimated in the same way—from Eq. (40). The only difference now is that $\Delta E(0)$ is independent of temperature. In this case the experimental fact that the temperature region of the self-trapping transition scales well with the Debye temperature of the crystal becomes clear:[14] the reason is the $q_D$ (or $T_D$) dependence of $\Delta E(0)$—see the explanation following Eq. (22) in Sec. II.

As can be seen from Table I, the calculated values of the characteristics of positronium in alkali halide crystals are in good agreement with the available experimental data. One exception may be the localization radius $R_0^{T=0}$ of self-trapped positronium: the calculated values are somewhat underestimated compared with the experimental data. The reason for this, apparently, is the simplified form of the trial wave function Eq. (3): it does not take into account the distribution of positronium atoms in the vicinity of the lattice sites.[21] The temperature dependence of $R_0$ computed from Eqs. (33), (36), and (38) for KI crystal, is shown in Fig. 4 as an example. The localization radius decreases as the temperature is raised, indicating that Ps gets more localized with the temperature. Such a temperature behavior of the localization radius (although the calculated radii are in themselves underestimated compared with the experimental ones) appears to be plausible since it mainly originates from the phonon subsystem of a crystal. The dependence can be physically interpreted and understood as the reduction, with increase of temperature, of the number of lattice sites correlated by self-trapped Ps: because of the lattice vibrations the outer lattice sites located far from the ''Ps core'' and therefore less correlated by Ps, cannot follow the inner, strongly correlated, sites located near the Ps anymore, yielding the reduction of the Ps localization radius with increase of temperature. Such a reduction would, in the momentum space, imply the broadening of the spectrum of the momentum distribution of the self-trapped Ps with increasing temperature. It was such a broadening that was, in fact, experimentally observed for self-trapped positronium in a KI crystal in the temperature range 76–110 K.[14] At higher temperatures, according to Ref. 14, the Ps momentum spectrum in KI again narrows, which could be attributed to the beginning of the diffusion process of self-trapped Ps (motional narrowing). The temperature dependence of the mean number of the sur-

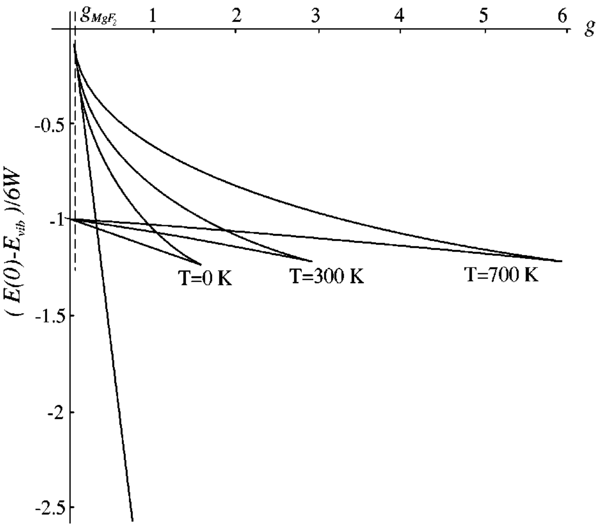

FIG. 3. The dependence of the Ps total energy on the coupling constant $g$ with acoustic phonons for the crystal of $MgF_2$ at nonzero temperatures. The vertical dashed line shows the value of $g$ for positronium in $MgF_2$.

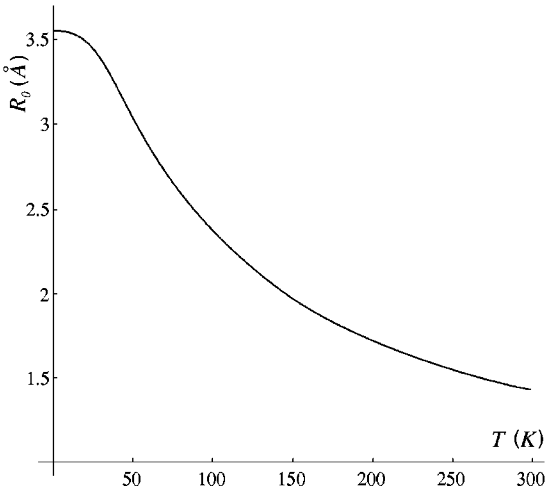

FIG. 4. The temperature dependence of the Ps localization radius in KI crystal.

rounding phonons Eqs. (30) and (31) can also be easily understood in terms of the polaron theory.[28] The decrease of $\langle n \rangle$ with increasing temperature in the weak phonon coupling regime [Eq. (30)] implies a reduction of the size of the virtual phonon cloud around Ps with an increase of its mobility. In the strong phonon coupling regime [Eq. (31)], on the other hand, self-trapped Ps is immobile and the virtual phonon cloud around it is so large from the very beginning that the real phonons appearing at nonzero temperature, practically do not influence it.

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