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Bose–Einstein distribution temperature features of quasiparticles around magnetopolaron in Gaussian quantum wells of alkali halogen ions

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We have applied strong coupling unitary transformation method combined with Bose–Einstein statistical law to investigate magnetopolaron energy level temperature effects in halogen ion crystal quantum wells. The obtained results showed that under magnetic field effect, magnetopolaron quasiparticle was formed through the interaction of electrons and surrounding phonons. At the same time, magnetopolaron was influenced by phonon temperature statistical law and important energy level shifts down and binding energy increases. This revealed that lattice temperature and magnetic field could easily affect magnetopolaron and the above results could play key roles in exploring thermoelectric conversion and conductivity of crystal materials.

Keywords: temperature effect, quantum well, asymmetric Gaussian potential, magnetopolaron

PACS: 71.38.–k, 73.21.Fg, 63.20.kd, 63.22.–m **DOI:** 10.1088/1674-1056/ad5c3c

1. Introduction

Polaron[1,2] is defined as a quasiparticle that describes the interactions of free electrons and polarization induced by electron–phonon coupling in materials. These entities might be large[3] or small,[4,5] depending on how large their lattice distortion is in comparison with lattice constant.[6] The development of polaron concept was a gradual process. From the discussion of Landau[7] in 1933, through continuous theoretical[8,9] and experimental[10,11] evolutions, it has become gradually clear in people's vision. Mainly, there are two approaches for describing polaron concept, namely, idealized mathematical models such as that introduced by Fröhlich[12] in 1950, and numerical methods based on density functional theory.

Polarized fruit bodies are characterized by their characteristic responses to external magnetic and electric fields as well as effective masses, binding energies (or self-energies). Regarding electrical characteristics, they have various types, including piezoelectric polaron, acoustic polaron, magnetopolaron,[13,14] and polaron[15] in organic materials. They are applied for studying the properties of conjugated polymers,[16,17] fullerenes, high T_c superconductors, giant magnetic perovskite, quasi-one-dimensional conductors,[18] and semiconductor nanostructures.[19,20] Among them, magnetopolarons are quasiparticles[21–23] formed by electron–phonon interactions under external magnetic fields. Because of its unique polaron effect[24–26] and has inevitably attracted much attention of many researchers. For example, Donfack *et al.*[27] studied the combined influences of magnetic field, spin–orbit interaction, and temperature on RbCl quantum well magnetopolaron properties. Combination operation method and Lee low pine unitary transformation were applied to study RbCl quantum well magnetopolaron ground state binding energy. Yang *et al.*[28] explored deformation potential effects on magnetopolarons in monolayer graphene via carrier-acoustic phonon coupling-based simple unitary transformation and linear-combination operators. Wang *et al.*[29] studied the influences of magnetopolarons on semiconductor shallow-impurity states when simultaneously subjected to magnetic fields and intense terahertz laser fields within Faraday configuration and applied a time-dependent nonperturbative theory for describing interactions among electrons. Tiotsop *et al.*[30] explored Rashba effects on bound magnetopolarons in delta quantum dots. Pekar type-variational and unitary transformation methods have been employed for deriving the energies of ground and first excited states However, the ground state energy, binding energy, and surrounding phonon distribution in alkali metal halide quantum wells under the action of external magnetic field and temperature still need further investigation.

In this research, such as shown in Fig. 1, magnetopolaron energy level temperature effects in halogen ion crystal quantum wells were evaluated using Bose–Einstein statistical law and strong coupling unitary transformation method, which contributed to the investigation of thermoelectric conversion

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and conductivity of crystal materials.

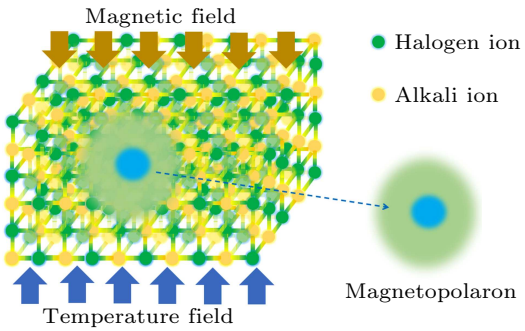


Fig. 1. Magnetopolaron temperature effects schematic diagram in halogen ion crystal quantum wells.

2. Theory model

An electron with asymmetrical Gaussian potential is assumed to be enclosed in a quantum well. The electron moved in a polar crystal and interacted with longitudinal optical phonons in decaying magnetic fields along z direction. The Hamiltonian of the electron–phonon system is stated based on effective mass approximation as

$$\begin{aligned} H &= \frac{1}{2m}\left(p_x-\frac{\bar{\beta}^2}{4}y\right)^2+\frac{1}{2m}\left(p_y+\frac{\bar{\beta}^2}{4}x\right)^2 \\ &+\frac{p_z^2}{2m}+\sum_q \hbar\omega_{\mathrm{LO}}a_q^+a_q \\ &+\sum_q\left[V_q a_q\exp\left(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}\right)+\mathrm{h.c.}\right]+V\left(z\right), \end{aligned} \tag{1}$$

where asymmetrical Gaussian potential is defined as

$$V\left(z\right)=\begin{cases} -V_0\exp\left(-\dfrac{z^2}{2R^2}\right), & z\geq 0, \\ \infty, & z<0. \end{cases} \tag{2}$$

In case of electron–phonon interaction, the coupling matrix is expressed as

$$V_q=\mathrm{i}\left(\frac{\hbar\omega_{\mathrm{LO}}}{q}\right)\left(\frac{\hbar}{2m\omega_{\mathrm{LO}}}\right)^{1/4}\left(\frac{4\pi\alpha}{AL_W}\right)^{1/2}. \tag{3}$$

Their coupling strength is described as

$$\alpha=\left(\frac{e^2}{2\hbar\omega_{\mathrm{LO}}}\right)\left(\frac{2m\omega_{\mathrm{LO}}}{\hbar}\right)^{1/2}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_0}\right). \tag{4}$$

The electron–phonon system Hamiltonian is employed by unitary transformation as

$$U=\exp\left[\sum_q\left(a_q^+f_q-a_qf_q^*\right)\right], \tag{5}$$

with f_q $\left(f_q^*\right)$ being variational function.

We employed the combined approach of linear combination operator of electron as[22]

$$p_j=\left[\frac{m\hbar\lambda}{2}\right]^{1/2}\left(b_j+b_j^+\right), \tag{6}$$

$$r_j=\mathrm{i}\left[\frac{\hbar}{2m\lambda}\right]^{1/2}\left(b_j-b_j^+\right) \tag{7}$$

with λ being variational parameter, which is equivalent to quadratic quantization.

The system Hamiltonian us unitary transformed and then replaced by linear combination operator; therefore, Hamiltonian metric is rewritten as

$$H'=U^{-1}HU. \tag{8}$$

We choose the ground state wave function $|\psi_0\rangle=|\phi\left(z\right)\rangle\left|0_q\right\rangle\left|0_j\right\rangle$ of strong-coupling magnetopolaron system to the Hamiltonian H'. Also, $|\phi\left(z\right)\rangle$ is z-direction wave function, satisfying $\langle\phi\left(z\right)|\,\phi\left(z\right)\rangle=1$, $\left|0_q\right\rangle$ is a non-perturbative phonon state, and $\left|0_j\right\rangle$ is polaron ground state energy.

The duration value of equation $|\psi\rangle$ is

$$\begin{aligned} F\left(\lambda,f_q\right) &= {}_b\langle 0|_a\langle 0|H'|0\rangle_a|0\rangle_b \\ &= \frac{3}{4}\hbar\lambda+\sum_q\hbar\omega_{\mathrm{LO}}\left|f_q\right|^2-V_0+\frac{\hbar U_0}{4m\lambda R^2} \\ &+\sum_q\left[V_q\left(a_q+f_q\right)\exp\left(-\frac{\hbar q^2}{4m\lambda}\right)+\mathrm{h.c.}\right] \\ &+\frac{\hbar e^2B_0^2\exp\left(2\mathrm{i}\omega t\right)}{16m^2\lambda C^2}. \end{aligned} \tag{9}$$

Equation (9) is rearranged as

$$\frac{\partial F\left(\lambda,f_q\right)}{\partial f_q}=0 \tag{10}$$

giving

$$f_q=-\frac{V_q\exp\left(-\dfrac{\hbar q^2}{4m\lambda}\right)}{\hbar\omega_{\mathrm{LO}}}. \tag{11}$$

In this case, the average phonon number around the magnetopolaron is obtained as

$$\begin{aligned} N &= \langle\psi_0|U^{-1}\sum_q a_q^\dagger a_qU\,|\psi_0\rangle \\ &= \langle\psi_0|\sum_q\left(a_q^\dagger+f_q^*\right)\left(a_q+f_q\right)|\psi_0\rangle \\ &= \sum_q\left|f_q\right|^2. \end{aligned} \tag{12}$$

When phonon formation is calculated from lattice vibration, equation (11) is substituted into formula (12) to give the average phonon number

$$N=\sum_q\frac{\left|V_q\right|^2}{\left(\hbar\omega_{\mathrm{LO}}\right)^2}\cdot\exp\left(-\frac{\hbar q^2}{2m\lambda}\right)=\alpha\sqrt{\frac{\lambda}{\pi\omega_{\mathrm{LO}}}}. \tag{13}$$

We established the relationship of average phonon number and lattice vibration frequency as

$$\lambda=\frac{N^2}{\alpha^2}\pi\omega_{\mathrm{LO}}. \tag{14}$$

Similarly, we calculated strong coupling magnetopolaron ground state energy as

$$E_0 = \frac{3}{4}\hbar\lambda - \frac{1}{\sqrt{\pi}}\alpha\hbar\omega_{\rm LO}\left(\frac{\lambda}{\omega_{\rm LO}}\right)^{1/2} - V_0 + \frac{\hbar V_0}{4m\lambda R^2} + \frac{\hbar e^2 B_0^2 \exp(2{\rm i}\omega t)}{16m^2\lambda C^2}, \quad (15)$$

where $\omega_{\rm c} = eB/mc$ is magnetic field cyclotron frequency. $E_{\rm b}$ of polaron in the Gaussian quantum wells of alkali halogen ions is derived variationally

$$E_{\rm b} = E_{\rm e} + E_{\rm p} - E_0 = \frac{2}{\sqrt{\pi}}\alpha\hbar\omega_{\rm LO}\left(\frac{\lambda}{\omega_{\rm LO}}\right)^{1/2} + V_0 - \frac{\hbar V_0}{4m\lambda R^2} - \frac{\hbar e^2 B_0^2 \exp(2{\rm i}\omega t)}{16m^2\lambda C^2}. \quad (16)$$

Based on quantum statistical theory, phonon around the electron satisfies Bose–Einstein distribution; therefore, the statistical average value of phonon is

$$\overline{N} = \left[\exp\left(\frac{\hbar\omega_{\rm LO}}{k_{\rm B}T}\right) - 1\right]^{-1}. \quad (17)$$

The above equation shows a self-consistent relationship between average phonon number around the electrons of core particles forming polaron and the statistical average of phonons; therefore, the internal relationship of polaron vibration frequency and temperature is established. Hence, the problem the temperature effect on polaron ground state and ground state binding energies is well solved.

3. Numerical calculations and discussion

Asymmetrical Gaussian potential quantum well strong coupling polaron energy is found to rely on both barrier height and range and effective confinement strength. For the verification of the influences of electron Landau and polaron energy levels, we considered strong electron–phonon interactions and adopted model parameter values. Matter physical parameters[23] reported in the literature are used in this research. The obtained results are summarized in Table 1.

Table 1. Parameter values used in calculations.

Material	Coupling constants α	m/m^*	LO phonon frequency $\omega_{\rm LO}$ (10^{13} Hz)
KBr	3.05	0.369	3.074
KCl	3.44	0.325	3.955
RbCl	3.81	0.432	3.282

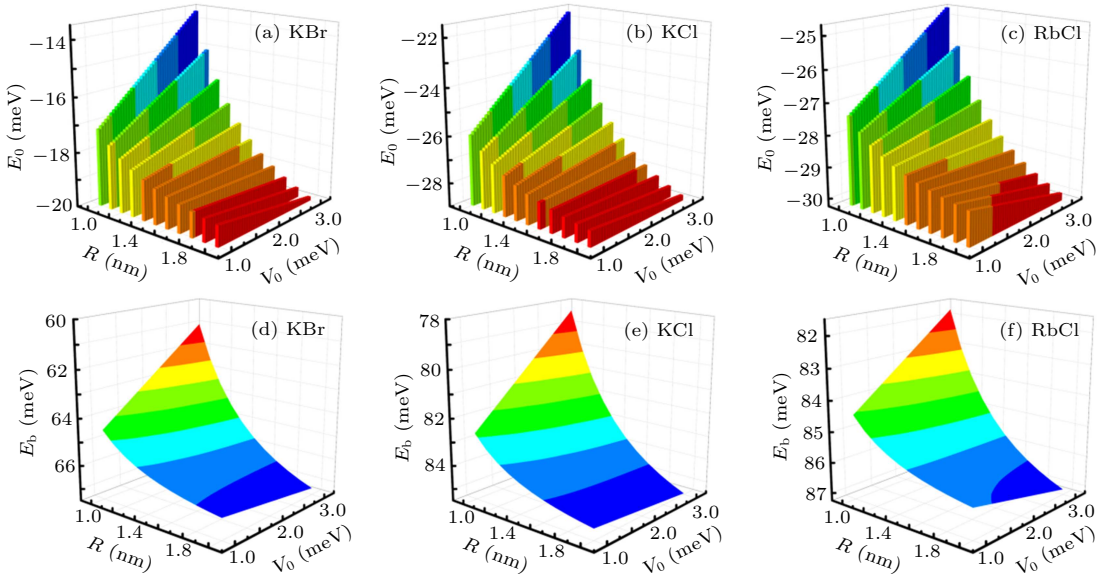


Fig. 2. Relationships of ground state (a)–(c) and ground state binding energies (d)–(f) as well as confined depth and range in three different metal halides KBr, KCl, and RbCl. $B_0 = 5$ T, $\omega = 0.5$ Hz, $t = 0.5$ s, $C = 0.1$, $\lambda = 2.83 \times 10^{13}$ Hz.

From Fig. 2, we found that polaron ground state energy varied with Gaussian potential confinement width and potential well height. Figures 2(a)–2(c) show polaron ground state energy variation in various alkali halide crystals. According to these diagrams, it is found that limited Gaussian potential width and potential well height affected polaron ground state energy level. The smaller potential well widths and deeper potential wells mean greater polaron–polaron binding, increasing ground state energy level, which is equivalent energy injection into the system and energy level increase in the crystal. Furthermore, crystal coupling constant has significant effect on polaron energy level, which is because of different atoms making up the crystal. When electrons passed through the crystal, the structure of the crystal composed of various components causes different coupling modes among electrons and lattice phonons, leading to polaron ground state energy level varia-

tions. When phonons and electrons are coupled, the binding energies of stable polarons in the three crystals are not the same. This phenomenon is also experimentally and theoretically analyzed.[24–27] The coupling strength of this type of alkali halide crystals is very high; therefore, it is practical to adopt these crystals for calculations. Figures 2(d)–2(f) show that potential well height and Gaussian confinement potential width in the crystal have obvious influences on electron–phonon coupling. High width and height of potential wells increase polaron binding energy. This is because wider and taller potential wells promote strong coupling between electrons and the lattice.

Figure 3 illustrates relationships among ground state and ground state binding energies as well as initial magnetic induction intensity and decay time. in Figs. 2(a)–2(c), polaron ground state energies in KBr, KCl, and RbCl quantum wells are increased by increasing magnetic induction intensity, but decreased with time, which reveal that polaron energy level is affected and regulated by magnetic induction intensity. This conclusion is verified by Eq. (15). Figures 3(d)–3(f) show that the ground state binding energy is decreased by increasing magnetic induction intensity, and the magnetic field changes the coupling between electrons and phonons, decreasing polaron binding energy. Higher coupling constants in KBr, KCl, and RbCl quantum wells mean easier formation of polaron and wider binding energy range.

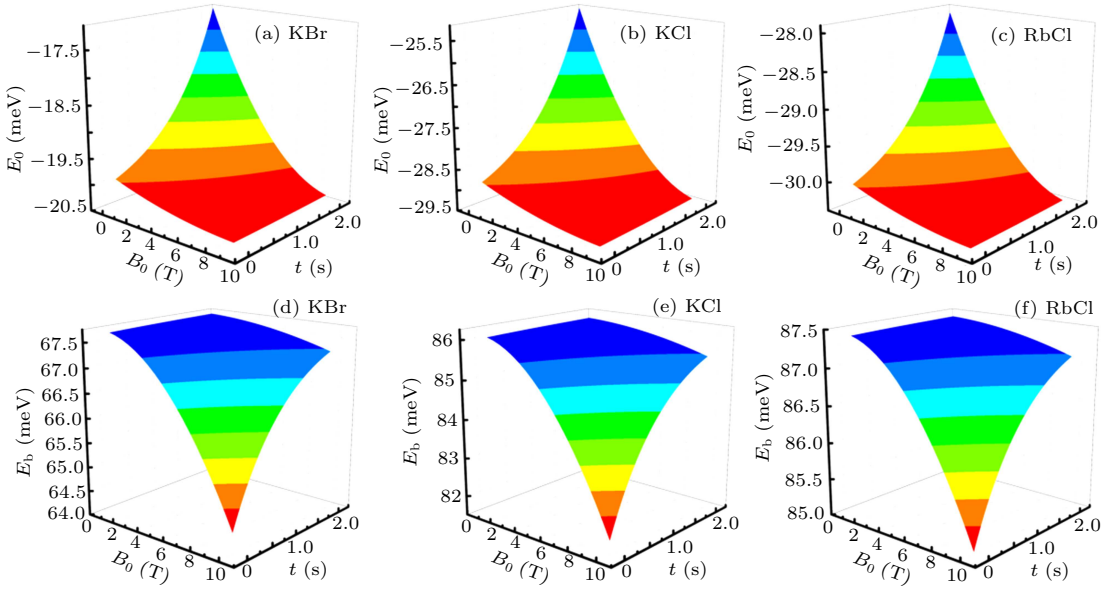


Fig. 3. Relationships among ground state (a)–(c) and ground state binding energies (d)–(f) as well as initial magnetic induction intensity and decay time in three different metal halides KBr, KCl, and RbCl. $\omega = 0.5$ Hz, $R = 2$ nm, $V_0 = 3$ meV, $C = 0.1$, $\lambda = 2.83 \times 10^{13}$ Hz.

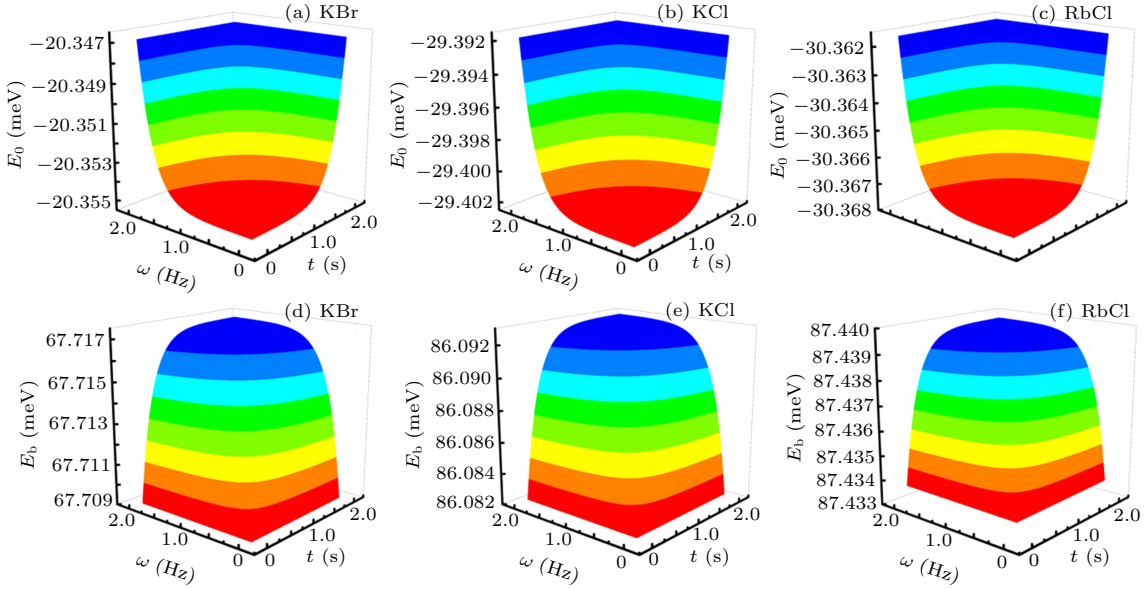


Fig. 4. Relationships among ground state (a)–(c) and ground state binding energies (d)–(f) as well as decay frequency and decay time in three different metal halides KBr, KCl, and RbCl. $B_0 = 0.5$ T, $R = 2$ nm, $V_0 = 3$ meV, $C = 0.1$, $\lambda = 2.83 \times 10^{13}$ Hz.

Figure 4 illustrates relationships among ground state and binding energies as well as decay frequency and decay time. The figure shows that the decay frequency effect on polaron ground state and binding energies are not obvious and the change is only in the range of 0.1 meV–0.2 meV. Because decay frequency and time affect magnetic field variations as well as ground state and binding energies, but magnetic field variations are not obvious due to the existence of the e index in the equation. Finally, polaron ground state and ground state binding energies are not obviously changed. However, in this energy range, we also observed that the ground state energy is obviously increased and the ground state binding energy is obviously decreased by decay time and decay frequency.

Figure 5 illustrates the relationships among vibrational frequency, average number of LO phonons, ground state and ground states binding energies, and temperature. The figure shows that the polaron vibration frequencies formed by the electron in three different metal halides KBr, KCl, and RbCl are different, but the law of change with temperature is consistent, indicating that the thermal vibration of atom in the crystal is increased by increasing temperature, leading to strong electron–phonon interactions in the lattice and polaron vibration frequency. Figure 5(b) shows that average phonon number around the polaron is linearly increased with temperature in the three crystals, indicating that temperature changes phonon cloud distribution around the polaron and increases average phonon number. Figure 5(c) reveals that the increase of temperature increases coupling strength and decreases polaron ground state energy level due to intense thermal vibrations of the crystal, which is consistent with the effect of magnetopolaron on shallow-impurity state in the presence of magnetic and intense terahertz laser fields in Faraday configuration experiment.[29,30] In addition, the polaron subsystem will also exhibit Gaussian potential quantum state characteristics.[31] Figure 5(d) shows that the polaron binding energy is increased by increasing temperature, showing that it is difficult for the electron to couple with phonons due to temperature increase; therefore, more energy is required for coupling. To sum up, four basic physical quantities of the polaron reflect the physical state of the electron coupled with phonon to form polarons in various lattices and some theoretical explanations are provided for further polaron regulation.

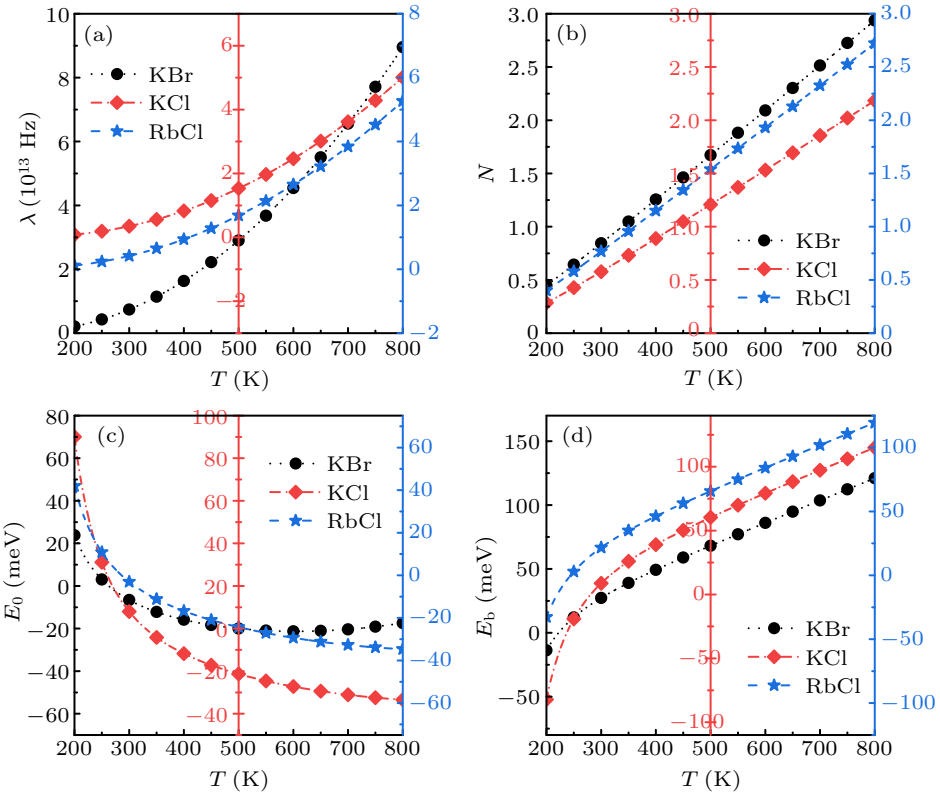


Fig. 5. Temperature dependence of vibrational frequency (a), ground state energy (b), ground state binding energy (c), and average number of LO phonons (d) in three different metal halides KBr, KCl, and RbCl. $B_0 = 0.5$ T, $\omega = 0.5$ Hz, $t = 0.5$ s, $C = 0.1$, $R = 2$ nm, $V = 3$ meV.

4. Conclusions

In this research, using strong coupling unitary transformation method combined with Bose–Einstein statistical law in quantum system, magnetopolaron temperature effects in metal halide crystal quantum wells are theoretically analyzed. It is concluded that under magnetic field effect, magnetopolaron quasiparticle is formed through the interactions of electrons and surrounding phonons. At the same time, magnetopolaron is affected by phonon temperature statistical law, important energy level shifted down, and binding energy increased. This

shows that magnetopolaron is easily affected by lattice temperature and magnetic field and these results can play key roles in investigating thermoelectric conversion and conductivity of crystal materials.

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