ON THE MORE REALISTIC DESCRIPTION OF THE PARAMETRIC RESONANCE IN KDP FERROELECTRICS

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The dynamical pseudospin-phonon model is used for a more realistic description of the parametric resonance in KDP ferroelectrics

Several years ago we developed the theory of possible parametric resonance in KDP ferroelectrics on the basis of the kinetic Ising model[1]. In a subsequent paper we also took into account the influence of lattice /heavy-ion/vibrations on such resonance in the spirit of similar approaches in magnetoelastic systems[2]. More recently[3] we proposed a possible stimulation of tunneling excitations /directly through a modulated local field, i. e. via double-well potential vibrations due to residual proton - heavy-ion interaction/. However it is tempting to describe more realistically a complete parametric mechanism in the frames of the convenient dynamical pseudospin-phonon model[4], which is widely used in various studies of hydrogen bonded ferroelectrics. To do this, the strongly interacting system of protons /p/ and heavy-ions /phonons//f/ which is submitted both to external dc /E_0/ and rf /$e_0 \cos\omega t$/ is described by the following Hamiltonian in the Fourier-transformed form

$$\mathcal{H} = \mathcal{H}_p + \mathcal{H}_f + \mathcal{H}_{pf} \, , \qquad /1/$$

where

$$\mathcal{H}_p = -\sqrt{N}\,H\,S_o^{\zeta} - \sum_k J_k\left[\cos\varphi\,S_k^{\zeta} - \tfrac{1}{2}\sin\varphi\,(S_k^- + S_k^+)\right]\left[\cos\varphi\,S_{-k}^{\zeta} - \tfrac{1}{2}\sin\varphi\,(S_{-k}^- + S_k^+)\right] - 2\sqrt{N}\mu e_o\cos\omega t\,\left[S_o^{\zeta}\cos\varphi - \tfrac{1}{2}\sin\varphi(S_o^- + S_o^+)\right];$$

$$\mathcal{H}_f = \sum_k \lambda_k(b_k^+ b_k + 1/2)\quad; \qquad /2/$$

$$\mathcal{H}_{pf} = \sum_k F_k\left[\cos\varphi\,S_{-k}^{\zeta} - \tfrac{1}{2}\sin\varphi\,(S_k^- + S_{-k}^+)\,(b_k^+ + b_{-k}^-)\right].$$

Here $H = \sqrt{H_x^2 + H_z^2}$, $tg\varphi = H_x/H_z$ - the transforming angle from the /x,z / to the temperature dependent /ξ,ζ /–axes in the pseudospin space, $H_x = 2\Omega$ - the tunneling energy of each proton inside a hydrogen bond; $H_z = 2\left[\langle S_z\rangle (J_o + |F_o|^2/\lambda_o) + \mu E_o\right]$, $\langle S_\alpha\rangle$ /$\alpha = x,z$ / being the mean values of pseudospin components; J_k and F_k correspond to the proton-proton and proton-phonon interactions, respectively; λ_k is the frequency of the optical mode / b_k - the normal phonon coordinate / strongly coupled to the proton mode[4] of the frequency[5] $\omega_k = \left[H^2 - 2H\Delta_k\right]^{1/2}$, $\Delta_k = J_k \langle S_\zeta\rangle \sin^2\varphi$ and μ is the dipole moment of the /K-PO_4/ complex.

Writing now the equations of motion

$$i\,\dot{S}_k^{\pm} = \left[\mathcal{H}, S_k^{\pm}\right]\quad;\quad i\,\dot{b}_k^{\pm} = \left[\mathcal{H}, b_k^{\pm}\right] \qquad /3/$$

after Bogolyubov's transformation / $\vec{S}_k \to \vec{\sigma}_k$ / and linearization one obtains

$$i\dot{\sigma}_k^+ = \left\{\left[H - h(t) - \Delta_k\right](u_{k1}^2 + |u_{k2}|^2) - 2\Delta_k u_{k1}u_{k2}^*\right\}\sigma_k^+ + \left\{2\left[H + h(t) - \Delta_k\right] u_{k1}u_{k2}^* - \Delta_k(u_{k1}^2 - |u_{k2}|^2)\right\}\sigma_{-k}^- + (u_{k1} + u_{k2}^*)\,F_{-k}\langle S_\zeta\rangle\sin\varphi \cdot (b_{-k}^+ + b_k) + (u_{k1} + u_{k2}^*)\sqrt{N}\mu\langle S_\zeta\rangle\sin\varphi\,\delta_{ko}\,h(t), \qquad /4/$$

$$i\dot{b}_k^- = \lambda_k b_k^- + \tfrac{1}{2}(u_{k1} + u_{k2}^*)F_{-k}\sin\varphi(\sigma_k^+ + \sigma_{-k}^-)\ ;$$

$$h(t) = 2e_o\cos\omega t\ ;\quad u_{k1,2} = \sqrt{H - \Delta_k \pm \omega_k / 2\omega_k}\,.$$

By the request for trial solutions to vary as $f(t)e^{i\omega t - \gamma t}$, from the above and their adjoint complex conjugated equations a standard procedure[6] / $\gamma \leq 0$, $b_k^{\pm}, \sigma_k^{\pm} \neq 0$, $\frac{\omega}{2} = w_k^{\mp}$ - the two hybridized proton-phonon frequencies, explicited hereafter/ leads to the expression for a treshold amplitude of the rf electric field

$$e_o^t = (\Delta_k \cos\varphi)^{-1} \Big[\Gamma_{k-}^2 - (\omega_k - \omega/2)^2 - |F_k|^2 \frac{H \langle S_\zeta \rangle \sin^2\varphi}{\omega_k} \cdot \\ \cdot \frac{\Gamma_{k-}\Gamma_{k+} - (\lambda_k - \omega/2)(\omega_k - \omega/2)}{\Gamma_{k+}^2 + (\lambda_k - \omega/2)^2} \Big]^{1/2} \frac{\omega_k}{\mu} \quad /5/$$

It is seen that e_o^t is a rather complicated function of the model energy parameters, temperatura and the wave vector k. The linewidths Γ_{k-} and Γ_{k+} /which should be estimated; see, e.g. ref.7 / correspond to proton-like / w_k^- / and phonon-like / w_k^+ / modes[4], respectively,

$$(w_k^{\mp})^2 = (\omega_k^2 + \lambda_k^2)/2 \pm \Big[(\omega_k^2 - \lambda_k^2)^2/4 - 2|F_k|^2 \lambda_k H \langle S_\zeta \rangle \sin^2\varphi \Big]^{1/2}. \quad /6/$$

For $\vec{k} = 0$, from the resonance condition / $\omega/2 = w_k^{\mp}$ / by a way of approximation one obtains characteristic dc electric field strengths in ferroelectric and paraelectric phases, respectively,

$$E_f^c \simeq \frac{1}{2\mu} \Big[(\omega/2)^2 + H_x^2 \big(J_o/2k_B T - |F_o|^2 \lambda_o / (\lambda_o^2 - \omega^2/4) \big) - 1 \Big]^{1/2}, \quad /7/$$

$$E_p^c \simeq \frac{1}{2\mu} \Big\{ \Big[(\omega/2)^3 + H_x^2 \Big(J_o - \frac{F_o{}^2 \lambda_o}{\lambda_o^2 - \omega^2/4} \Big) \Big]^{2/3} - H_x^2 \Big\}^{1/2} - J_o/2\mu \quad .$$

From the above equations /5-7/ it is easily seen that both hybridized modes can simultaneously be excited, but with different wawe vectors / $e_o > e_o^t|_{\omega = 2w_{k-}} = e_o^t|_{\omega = 2w_{q+}}$; $\vec{k} \neq \vec{q}$ / - on account of a nonlinear energy "pumping" by the external rf electric field, except for too small $\vec{k}$ or sufficiently large dc fields / $E_o \gg E^c_{p,f}$ / when the given plane-wave analysis does not hold /the wavelength of the unstable modes becomes comparable with the sample dimensions /[1,2]. Of course, if the condition $w_k^- = w_q^+ = \omega/2$ is not fulfilled in some parts of the $\vec{k}$-space, or at all /being dictated by mode dispersions /, then only one of two modes could be stimulated for a given rf frequency:

$$\omega = 2w_k^- \lessgtr 2\left(\lambda_k + \sqrt{\left||F_k|^2 H \langle S_\zeta\rangle \sin^2\varphi / \omega_k \Gamma_{k-} - \Gamma_{k+}\right| \Gamma_{k+}}\right)$$

or /8/

$$\omega = 2w_k^+ \lessgtr 2\left(\lambda_k + \sqrt{\left||F_k|^2 H \langle S_\zeta\rangle \sin^2\varphi / \omega_k \Gamma_{k-} - \Gamma_{k-}\right| \Gamma_{k-}}\right).$$

Concluding this paper it should be added that as for a possible direct stimulation, via residual proton-lattice interaction / $(1/2)\sum_k B_k S_k^x S_{-k}^x$ /[3], the obtained results and discussions hold completely under substitution $\cos\varphi \to \sin\varphi$, $\omega \to 2\omega$, $\mu \to (1/4)\, e_o (d^2B_o/dE^2) \langle S_x\rangle$ and $2\Omega \to 2\Omega + (B_o + d^2B_o/dE^2)\langle S_x\rangle e_o^2/2$; the regular parametric resonance via the two hybridized modes is accompanied by another one of a similar origin but with the doubled frequency. Mindfull of the zeroth wave number contribution /i.e. linear in $S_o^{\pm}$, in eq./2 // we note that it is just relevant for dissipative processes, being, otherwise, the subject of a particular treatment.

References

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