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## A HAWKING PROCESS IN SOLIDS: RELAXATION OF A STRONGLY EXCITED MODE

Vladimir HIZHNYAKOV and Dmitri NEVEDROV

Tartu Ülikooli teoreetilise füüsika instituut (Institute of Theoretical Physics, University of Tartu), Tähe 4, EE-2400 Tartu, Eesti (Estonia)

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HAWKINGI PROTSESS TAHKISTES: TUGEVASTI ERGASTATUD VONKUMISE RELAKSEERUMINE. Vladimir HIZHNIAKOV, Dmitri NEVEDROV

ХОКИНГОВСКИЙ ПРОЦЕСС В ТВЕРДОМ ТЕЛЕ: РЕЛАКСАЦИЯ СИЛЬНО ВОЗБУЖДЕННОГО КОЛЕБАНИЯ. Владимир ХИЖНЯКОВ, Дмитрий НЕВЕДРОВ

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In this communication we consider the anharmonic (two-phonon) relaxation (decay) of a strongly excited local mode. The mechanism of the relaxation is analogous to that of the Black Hole emission proposed by Hawking [1]. The basic equation which is used below was recently derived in [2]. The goal of this communication is to present the results of numerical calculations of the relaxation which show a strongly nonexponential decay law of the mode. Besides we demonstrate here that the relaxation rate is strongly enhanced (diverges) at some critical amplitudes. According to our knowledge such a critical behaviour of the relaxation rate of a single mode was not known earlier.

An essential peculiarity of the problem under consideration is large initial excitation of the local mode once all other modes are not excited initially. This allows us to consider the local mode classically and all other modes quantum-mechanically. In this approximation the cubic anharmonic interaction of the local mode with the crystalline is the sum of terms  $\sim \hat{x}_i \hat{x}_{i'} Q(t)$ , where  $\hat{x}_i$  and  $\hat{x}_{i'}$  are operators of normal coordinates of crystalline phonons,  $Q(t)$  is the time-dependent classical amplitude of the local mode. This interaction leads to the following time-dependent Hamiltonian of the phonon system:

$$\hat{H}_{\text{ph}}(t) = \frac{1}{2} \sum_i (\dot{x}_i^2 + \omega_i^2 \hat{x}_i^2) + \frac{1}{2} Q(t) \sum_{ii'} (e_i w e_{i'}) \hat{x}_i \hat{x}_{i'}. \quad (1)$$

Here  $\omega_i$  is the frequency of the mode  $i$ ,  $(e_i w e_{i'}) = \sum_n e_i e_{i'} e_n w_{nn'}$ ,  $n=1, 2, \dots, n_0$ ,  $\sum_i e_i e_{i'} e_{i'} = \delta_{nn'}$ ,  $n_0$  is the number of configurational coordinates contributing to anharmonic interaction. Below we consider the simplest case  $n_0=1$ .

The coordinate operators can be presented in the form  $\hat{x}_i = \hat{x}_i(t) = \left(\frac{\hbar}{2\omega_i}\right)^{1/2} g_i \hat{a}_i + C_c$ , where  $\hat{a}_i$  are initial (at  $t < 0$ ) destruction operators (it is supposed that the local mode is excited at  $t=0$ :  $Q(t)=0$ ,  $t < 0$ ),  $g_i(t)$  are  $c$ -functions satisfying the set of classical equations of motion with the initial conditions  $g_i(t) = \exp(-i\omega_i t + i\varphi_i)$ ,  $t \leq 0$ ,  $\varphi_i$  are random phases. These functions equal ([<sup>2</sup>]):

$$g_i(t) = e^{-i\omega_i t + i\varphi_i} + w \bar{e}_i \int_0^t dt \sin(\omega_i(t-\tau)) \sum_{i'} D_{i'}(\tau) \bar{e}_{i'} e^{i\varphi_{i'}}, \quad (2)$$

where  $D_i(t)$  satisfies the following Volterra-type equation ([<sup>2</sup>]):

$$D_i(t) = w Q(\tau) \left[ e^{-i\omega_i \tau} + \int_0^\tau d\tau' G(\tau - \tau') D_i(\tau') \right], \quad (3)$$

$G(\tau) = \sum_i \bar{e}_i^2 \sin(\omega_i \tau)$  being the Green's function of lattice dynamics ([<sup>3</sup>]).

Hamiltonian (1) can be diagonalized as follows ([<sup>2</sup>]):

$$\hat{H}_{ph}(t) = \sum_j \hbar \Omega_j(t) \left( \hat{b}_j^+(t) \hat{b}_j(t) + \frac{1}{2} \right), \quad (4)$$

where  $\Omega_j(t)$  are time-dependent phonon frequencies,

$$\hat{b}_j(t) = \sum_i (\mu_{ij}(t) \hat{a}_i + v_{ij}(t) \hat{a}_i^+) \quad (5)$$

are time-dependent destruction operators; expressions for  $\Omega_j$ ,  $\mu_{ij}$ , and  $v_{ij}$  are given in [<sup>2</sup>].

The anharmonic interaction considered causes not only time dependence of phonon frequencies but also changes of phonon operators in time. Note that relation (5) is analogous to the relation of Hawking [<sup>1</sup>] between field operators in different times of a gravitationally collapsing star (Black Hole). Therefore the mechanism of a local mode relaxation is analogous to that of the Black Hole emission: phonons (photons) are generated because the initial zero-point state  $|0\rangle$  is not the zeroth state for the time-dependent destruction operators  $\hat{b}_j$ ; there are phonons with frequencies  $\Omega_j$  in  $|0\rangle$  at the time moment  $t$ ; the number of phonons equals  $\sum_j N_j(t)$ , where  $N_j(t) = \langle 0 | \hat{b}_j^+(t) \hat{b}_j(t) | 0 \rangle$ .

The energy, which is generated in a phonon system at the time moment  $t$ , equals ([<sup>2</sup>]):

$$(II) \quad E_{ph}(t) = \sum_j \hbar \Omega_j(t) \left( N_j(t) + \frac{1}{2} \right) - \sum_i \frac{\hbar \omega_i}{2} = \\ = \frac{\hbar}{4} \sum_{ii'} \omega_i^{-1} e_i^2 e_{i'}^2 \left| \int_0^t D_i(\tau) e^{-i\omega_i \tau} d\tau \right|^2 \quad (6)$$

(fast oscillating terms are neglected). The energy is generated at the expense of the local mode:  $E_{ph}(t) = E_l(0) - E_l(t)$ ;  $E_l(t) \approx \omega_l^2 Q_0^2(t)/2$ ,  $Q_0(t)$  is the mode amplitude,  $\omega_l$  is its frequency. This relation between the energies  $E_{ph}$  and  $E_l$  gives an equation for  $E_l(t)$ . To solve this equation one needs to find solution of integral equation (3). This solution is given in [<sup>2</sup>]:

$$D_i(\tau) \approx v \left[ e^{i(\omega_l - \omega_i)\tau} [1 - v^2 \tilde{G}(\omega_l - \omega_i)]^{-1} - \sum_k e^{i\omega_k \tau} [\tilde{G}'(\omega_k)(\omega_i + \omega_k - \omega_l)]^{-1} \right]. \quad (7)$$

Here  $v = wQ_0(t)/2$ ,  $\tilde{G}(\omega) = G(\omega)G(\omega - \omega_l)$ ,  $G(\omega) = \int_0^\infty d\tau G(\tau)e^{i\omega\tau - \varepsilon\tau}$ ,  $\varepsilon \rightarrow 0$ ,  $\tilde{G}'(\omega) = d\tilde{G}(\omega)/d\omega$ ,  $\omega_k = \bar{\omega}_k + i\Gamma_k$  are upper poles of the resolvent  $(1 - v^2 \tilde{G}(\omega))^{-1}$ ;  $\bar{\omega}_k = \text{Re } \omega_k$  (fast oscillating terms are neglected).

In [2] the influence of the poles  $\omega_k$  on the local mode relaxation was noted but not studied. To do this, we take into account that only poles with small  $\Gamma_k$  are important. Such poles can appear only in the vicinity of zeros of  $\text{Im } \tilde{G}(\omega)$ . The latter function is asymmetric (while  $\text{Re } G(\omega)$  is symmetric) with respect to  $\omega_l/2$ . Therefore there is always a pole at  $\bar{\omega}_k = \omega_l/2$ . Besides, there may be some additional poles with  $\omega_k < \omega_l/2$  and the same number (denoted as  $m$ ) of poles for  $\omega_k > \omega_l/2$ . To find  $\Gamma_k$  for the poles mentioned one can expand  $\tilde{G}(\omega)$  near  $\omega_k$ :  $\tilde{G}(\omega) \approx \text{Re } \tilde{G}(\omega_k) + (\omega - \omega_k)\tilde{G}'(\omega_k)$ . This gives

$$\Gamma_k = \frac{E_k - E_l}{E_l} \frac{\tilde{G}(\omega_k) \text{Im } \tilde{G}'(\omega_k)}{|\tilde{G}'(\omega_k)|^2}, \quad (8)$$

where  $E_l \equiv E_l(t)$ ,

$$E_k = \frac{2\omega_l^2}{w^2 \tilde{G}(\omega_k)} \quad (9)$$

is the critical energy of the local mode for which  $\Gamma_k = 0$ ;  $E_l \equiv E_l(t)$ . The pole  $\omega_k$  gives a remarkable contribution to  $D_i$  only if  $E_l(t)$  is close to  $E_k$  (here we take into account that  $\text{Im } \tilde{G}'(\omega_k) < 0$ ). Differentiating (6) and taking into account that  $dE_{ph} = -dE_l$ , one obtains  $\dot{E}_l(t) \approx \approx -\gamma(t)E_l(t)$ , where

$$\gamma(t) \approx \frac{\pi \hbar \omega^2}{4\omega_l} \sum_{k=1}^{m+1} \int_{\omega_{k-1}}^{\bar{\omega}_k} \frac{d\omega Q(\omega)Q(\omega_l - \omega)}{|1 - w^2 E_l(t) \tilde{G}(\omega - \omega_l)/2\omega_l^2|^2} \times \\ \times [1 - \Theta(E_k - E_l(t))e^{-2\Gamma_k t}] \quad (10)$$

stands for the relaxation rate at the time moment  $t$  ( $\bar{\omega}_0 = 0$ ,  $\bar{\omega}_{m+1} = \omega_l/2$ ),  $Q(\omega) = -\text{Im } G(\omega)$  is the phonon density of states (for  $\omega > 0$ ). The second term in the square brackets of (10) takes into account the poles mentioned. When deriving expression (10) we took into account that for  $E_l \approx E_k$

$$\gamma_k \sim \frac{1 - \Theta(E_k - E_l(t))e^{-2\Gamma_k t}}{E_k - E_l(t)}. \quad (11)$$

It follows from formulae (10) and (11) that the damping rate of the local mode  $\gamma$  is strongly enhanced (diverges in our approximation as  $\sim |t - t_k|^{-1/2}$ ) if the mode energy approaches (at  $t = t_k$ ) one of the critical energies  $E_k$ . This enhancement of the  $\gamma$  is associated with the generation of quasimonochromatic phonons. These phonons are emitted in pairs: one phonon with the frequency  $\omega_k$  and another with the frequency  $(\omega_l - \omega_k)$ . As a result the decay of the strongly excited local mode is highly nonexponential: it has stepwise jumps near critical energies.

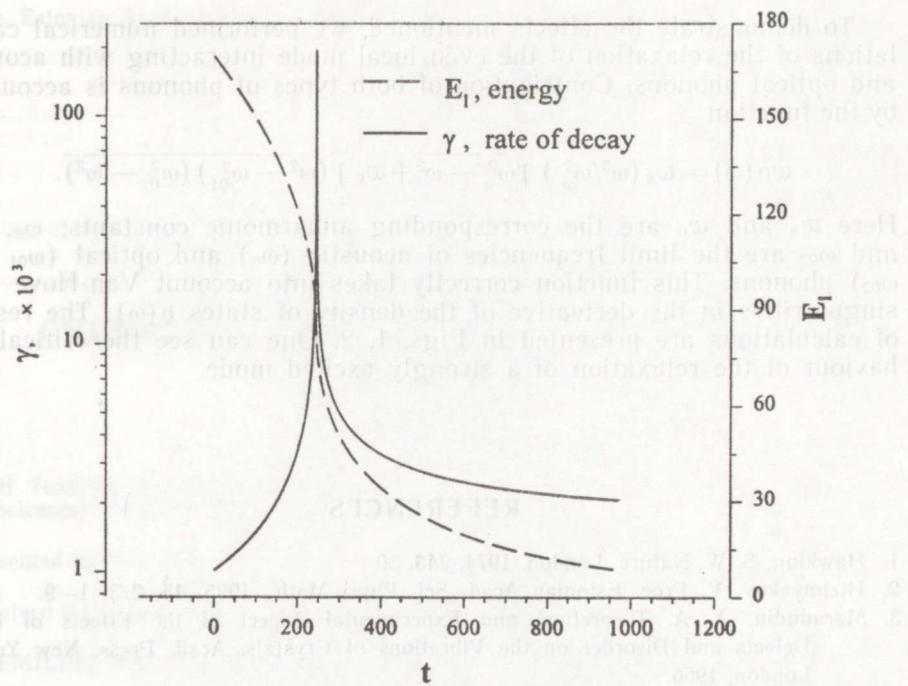


Fig. 1. Two-phonon relaxation of a strongly excited mode caused by anharmonic interaction with acoustic phonons;  $\tilde{\kappa}=1$ ,  $\omega_a=1$ ,  $\omega_l=1.5$ ,  $w_0=0$ ;  $w_a=0.5$ .

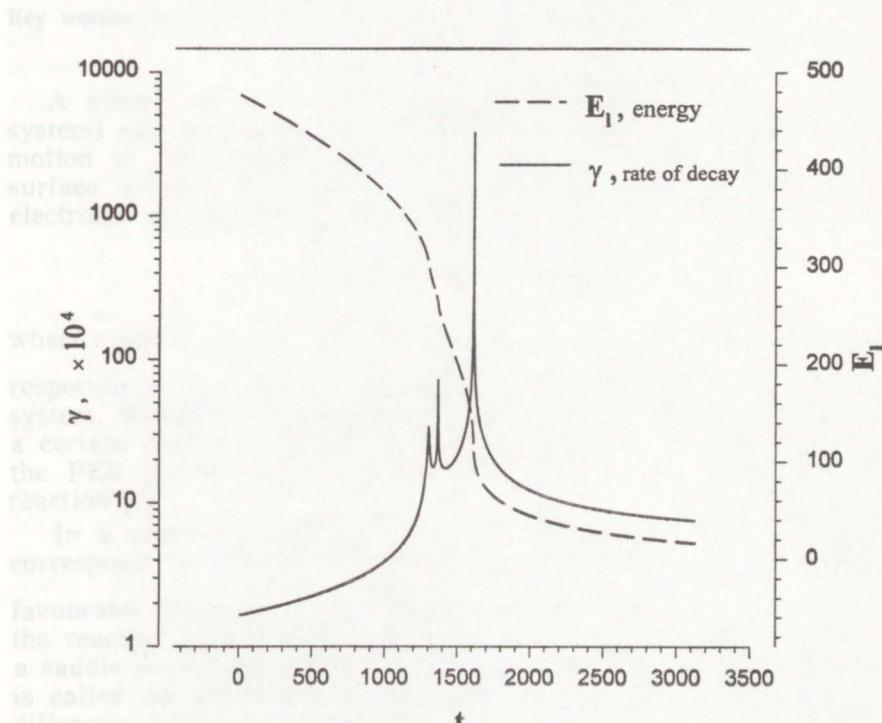


Fig. 2. Two-phonon relaxation of a strongly excited mode caused by anharmonic interaction with acoustic and optical phonons;  $\tilde{\kappa}=1$ ,  $\omega_a=1$ ,  $\omega_l=1.7$ ,  $\omega_{01}=1.2$ ,  $\omega_{02}=1.5$ ,  $w_a=0.3$ ,  $w_0=0.5$ .

To demonstrate the effects mentioned, we performed numerical calculations of the relaxation of the even local mode interacting with acoustic and optical phonons. Contribution of both types of phonons is accounted by the function

$$w\varrho(\omega) = w_a (\omega^3/\omega_a^2) \sqrt{\omega_a^2 - \omega^2} + w_o \sqrt{(\omega^2 - \omega_{01}^2)(\omega_{02}^2 - \omega^2)}. \quad (12)$$

Here  $w_a$  and  $w_o$  are the corresponding anharmonic constants;  $\omega_a$ ,  $\omega_{01}$ , and  $\omega_{02}$  are the limit frequencies of acoustic ( $\omega_a$ ) and optical ( $\omega_{01}$  and  $\omega_{02}$ ) phonons. This function correctly takes into account Van-Hove type singularities in the derivative of the density of states  $\varrho(\omega)$ . The results of calculations are presented in Figs. 1, 2. One can see the critical behaviour of the relaxation of a strongly excited mode.

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is the critical energy of the local mode for which  $\Gamma_c=0$ ;  $E_i=E_i(t)$ . The pole  $E_c$  gives a remarkable contribution to  $D_1$  only if  $E_c$  is close to  $E_s$  (here we take into account that  $\text{Im } C'(\omega_s) < 0$ ). Differentiating (6) and taking into account that  $dE_{ph} = dE_s$ , one obtains  $E_i(t) \approx \omega - \gamma(t) E_s$ , where

$$\gamma(t) = \frac{\text{Im } C'(\omega_s)}{4\pi \sum_{k=1}^n \frac{1}{(E_k - E_s)^2}} \times [1 - \eta(E_s - E_i(t)) e^{-i\omega t}] \quad (10)$$

$\gamma$  stands for the relaxation rate of the pole moment  $t$  ( $\omega=0$ ,  $\omega_s=2\omega_0/3$ ),  $\eta(\omega) = -\text{Im } C'(\omega)$  is the phonon density of states (for  $\omega>0$ ). The second term in the square brackets of (10) takes into account the poles mentioned. When deriving expression (10) we took into account that for  $E_i \approx E_s$

$$\eta(\omega) \approx \frac{1 - \eta(E_s - E_i(t)) e^{-i\omega t}}{E_s - E_i(t)} \quad (11)$$

It follows from formulas (10) and (11) that the damping rate of the local mode  $\gamma$  does not approach zero in our approximation as  $\sim |t-t_s|^{-1/2}$  if the mode energy approaches (at  $t=t_s$ ) one of the critical energies  $E_s$ . This enhancement of the  $\gamma$  is associated with the generation of quasi-monochromatic phonons. These phonons are emitted in pairs: one phonon with the frequency  $\omega_0$  and another with the frequency  $\omega_0$  below  $\omega_0$  to compensate energy loss due to the initial energy.