THE FRÖHLICH KINETIC EQUATION WITH ADDITIONAL TERMS

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The Fröhlich kinetic equation (FKE) describes the coherent excitation in a band of polarization waves consisting of normal modes. The FKE involves the one and two quanta terms representing energy supply, energy losses and energy channeling between the modes with the help of the heat bath. The energy channeling between the vibration systems located at different positions and the channeling connected with multiple quanta processes without the help of the heat bath are analyzed. The additional terms of the FKE are derived. The multiple quanta processes may channel the energy from the coherently excited mode (or modes) to higher frequency ones.

1. INTRODUCTION

The excitation of coherent states by energy supply to a band of polarization waves consisting of normal modes is described by a kinetic equation derived by Fröhlich [1–5]. Energy condensation occurs in the lowest frequency mode. Under convenient conditions even higher frequency modes may store the energy of the vibration system [6].

The Fröhlich kinetic equation (FKE) includes the basic principle of the coherent states excitation and contains the fundamental terms representing the one and two quanta processes. The processes are the following: energy supply, energy losses to the heat bath, and energy channeling between the modes with the participation of the heat bath (S, ϕ and X terms, respectively). The X term is responsible for the energy condensation in the lowest frequency mode. Additional two quanta terms were derived by Livshitz and Yushina [7–9] with the conclusion that the additional terms compensate the Fröhlich X term and, therefore, no coherent state occurs. This conclusion results from conveniently chosen values of the transition probabilities, which is rather an artificial condition in a normal state [10–13]. Nevertheless, under extraordinary conditions the additional terms might quench the coherent state.

Coherent vibration systems are very likely located in the membranes carrying the "static" electric potential, especially in the cellular membranes [14]. The value of the electric field intensity in the membrane is of the order of 10^5 V/cm and the system is very likely in the nonlinear region. The cellular membrane has a heterogeneous character. The properties of the vibration systems located in the membrane may depend on the local membrane composition and structure. In order to assess the biological role of coherent states we have to analyze the interaction between the vibration systems located in different places of the membrane.

When the energy supply to the system in question is near the critical value, the energy stored in the lowest frequency mode steeply increases as follows from computer

simulation [15]. There occurs transition from the original nonlinear state to a highly nonlinear one. Besides the original terms of the FKE even the terms representing the multiple quanta processes may be significant. There may be multiple quanta processes with the help of the heat bath and those without the heat bath participation. We analyze the processes without the help of the heat bath.

2. CLASSICAL NONLINEAR OSCILLATOR

The changes of the potential energy with respect to time are given by the product of force and velocity ($\mathrm{d}W/\mathrm{d}t = P = fv$). We express the position, the velocity and the force in the Fourier expansion form

$$(1) \quad x = \sum_{m,n} X'_{m,n} \exp\left[\mathrm{j}(m\omega_1 + n\omega_2)\, t\right], \quad v = \sum_{m,n} V_{m,n} \exp\left[\mathrm{j}(m\omega_1 + n\omega_2)\, t\right],$$

$$f = \sum_{m,n} F_{m,n} \exp\left[\mathrm{j}(m\omega_1 + n\omega_2)\, t\right],$$

respectively. In eq. (1) ω_1 and ω_2 are the frequencies, t is the time, and m and n are integers. We make use of the relation for the spectral density

$$(2) \qquad F_{m,n} = \frac{1}{(2\pi)^2} \int_0^{2\pi} \mathrm{d}\eta \int_0^{2\pi} \mathrm{d}\xi \exp\left[-\mathrm{j}(m\xi + n\eta)\right] f,$$

where $\xi = \omega_1 t$ and $\eta = \omega_2 t$. From eqs. (1) and (2) after some manipulations and arrangements similar to those in [16] we get

$$(3) \qquad \sum_{n=-\infty}^{+\infty} \sum_{m=0}^{+\infty} \frac{mP_{m,n}}{m\omega_1 + n\omega_2} = 0, \quad \sum_{m=-\infty}^{+\infty} \sum_{n=0}^{+\infty} \frac{nP_{m,n}}{m\omega_1 + n\omega_2} = 0.$$

In eq. (3) the $P_{m,n}$ is related to the circular frequency $\omega_q = |m\omega_1 + n\omega_2|$. We assume the frequencies ω_q to be combinations of two basic ones, i.e. of ω_1 and ω_2. Generalisation of eq. (3) for more basic frequencies may be easily done.

The relations in eq. (3) were originally derived for nonlinear electrical elements [16] and determine the energy transfer between the modes with convenient frequency relations by a nonlinear mechanism.

3. QUANTUM NONLINEAR OSCILLATOR

We assume the total energy of the whole vibration system consisting of normal modes to be independent of time. The energy supply compensates the energy losses. The Hamiltonian of the system

$$(4) \qquad H = \sum_q H_q$$

(where the index q denotes the particular mode) is, therefore, independent of time too. Assuming the Heisenberg picture we get for the expectation value

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|H|\psi\rangle = \sum_q \frac{\mathrm{d}}{\mathrm{d}t}\langle\psi|H_q|\psi\rangle = \sum_q \frac{\mathrm{d}}{\mathrm{d}t}E_q = \sum_q P_q = 0\,, \tag{5}$$

where E_q contains all the energy components of the mode ω_q.

If the concept of two basic frequencies is adopted we get

$$\frac{\mathrm{d}}{\mathrm{d}t}E_q = P_q = \frac{1}{2\pi}(\omega_1 m W_{m,n} + \omega_2 n W_{m,n})\,. \tag{6}$$

$W_{m,n}$ in eq. (6) denotes the expectation value of the energy stored in the vibration mode within one period. Eq. (6) represents the terms without the heat bath involvement. After summation we get from eqs. (5) and (6)

$$\sum_q P_q = \frac{1}{2\pi}(\omega_1 \sum_m \sum_n m W_{m,n} + \omega_2 \sum_m \sum_n n W_{m,n})\,. \tag{7}$$

Eq. (7) has to equal zero for arbitrary values of ω_1 and ω_2 and, therefore, the right-hand side may be split into two parts. Both the integer multipliers may be positive or negative. After substitution of $W_{m,n} = P_{m,n}/\omega_q$ and arrangement of the summation we get from eq. (7) relations identical with those in eq. (3). In this case the summation should be limited to finite values of m and n.

Eq. (6) implies the assumption that the energy of all the modes is constant. The energy changes caused by the nonlinear mechanism given by eq. (3) have to be compensated by the energy supply or the energy losses to keep the mode energy level unchanged.

4. INTERACTION BETWEEN SYSTEMS WITH DIFFERENT SPACE LOCATIONS

We assume two systems of polarization waves consisting of normal modes in different space locations. The properties of the systems, i.e. the transition probabilities, the mode frequencies and the energy supplies, may differ. Both the systems interact with each other. The Hamiltonian of the systems may be expressed in the form

$$H = H_0 + H_1 + H_2\,, \tag{8}$$

where H_0 and H_1 satisfy the relations similar to those in [13, 17, 18]

$$H_0 = \sum_i \hbar\omega_i a_i^+ a_i + \sum_j \hbar\bar{\omega}_j b_j^+ b_j + \sum_k \hbar\Omega_k c_k^+ c_k + \sum_g \hbar\bar{\Omega}_g P_g^+ P_g\,, \tag{9}$$

$$H_1 = \sum_{i,k}(\varphi_a a_i c_k^+ + \varphi_a^* a_i^+ c_k) + \sum_{j,k}(\varphi_b b_j c_k^+ + \varphi_b^* b_j^+ c_k) + \tag{10}$$

$$+\sum_{g,i}(\xi_a P_g a_i^+ + \xi_a^* P_g^+ a_i) + \sum_{g,j}(\xi_b P_g b_j^+ + \xi_b^* P_g^+ b_j) +$$
$$+\sum_{i,l,k}(\chi_a a_i^+ a_l c_k^+ + \chi_a^* a_i a_l^+ c_k) + \sum_{j,s,k}(\chi_b b_j^+ b_s c_k^+ + \chi_b^* b_j b_s^+ c_k)\,.$$

The term H_2 representing the mutual interaction between the systems of polarization waves is given by

$$H_2 = \sum_{i,j,k}(\lambda a_i b_j^+ c_k^+ + \lambda^* a_i^+ b_j c_k + \lambda a_i^+ b_j c_k^+ + \lambda^* a_i b_j^+ c_k)\,. \tag{11}$$

Here ω_i, $\bar{\omega}_j$, Ω_k, $\bar{\Omega}_g$ are the circular frequencies; a_i^+, b_j^+, c_k^+, P_g^+ are the creation operators and a_i, b_j, c_k, P_g are the annihilation operators, respectively. The i, j, k and g indices are related to one system of polarization waves, to the other system, to the environmental medium and to the source of energy, respectively. In eqs. (9), (10) and (11) the φ_a, φ_b, ξ_a, ξ_b, χ_a, χ_b, and λ are the coupling constants in both the systems. In eq. (9) the environmental medium (the heat bath) is represented only by the terms which are oscillatory in nature. This apparently does not represent the real conditions in the biological systems.

The H_0 and H_1 terms given by eqs. (9) and (10) give rise to ordinary terms of the FKE as was derived in [17, 18] using the time dependent perturbation theory. Making use of the same method the mutual interaction term may be evaluated. On the basis of commutation relations we determine for the qth mode

$$\dot{N}_q = -\frac{\mathrm{j}}{\hbar}[N_q, H]\,, \tag{12}$$

where $N_q = a_q^+ a_q$. We determine the perturbed state vector $|\psi(t)\rangle$ and using eq. (12) we evaluate the expectation value

$$\langle \dot{N}_q \rangle = \langle \psi(t)| \dot{N}_q |\psi(t)\rangle\,. \tag{13}$$

The expectation value $\langle \dot{N}_q \rangle''$ representing the mutual interaction between the systems is given by

$$\langle \dot{N}_q \rangle'' = -\sum_j \Lambda\{\langle N_q \rangle (\langle M_j \rangle + 1) \exp[\beta(\omega_q - \bar{\omega}_j)] - \langle M_j \rangle (\langle N_q \rangle + 1)\}\,, \tag{14}$$

where $\beta = \hbar/(kT)$, $M_j = b_j^+ b_j$,

$$\Lambda = \left(\frac{2\pi}{\hbar}\right)|\lambda|^2 \exp[\beta(\bar{\omega}_j - \omega_q)] \begin{Bmatrix} Q \\ Q+1 \end{Bmatrix}, \quad \text{for} \quad \begin{Bmatrix} \bar{\omega}_j > \omega_q \\ \bar{\omega}_j < \omega_q \end{Bmatrix} \tag{15}$$

and Q is the number of excitation with energy $|\bar{\omega}_j - \omega_q|\,\hbar$ in the heat bath. Eq. (14) and (15) are valid for both the systems, but the positions of $\langle M_j \rangle$ and $\langle N_i \rangle$ are interchanged.

5. THE MULTIPLE QUANTA TERMS

The coherent excitation may shift the system of polarization waves into the highly nonlinear region where multiple quanta processes take place. The time dependent perturbation theory may also be used to analyze the highly nonlinear interaction without the heat bath help [19]. Besides the H_0, H_1, and H_2 terms determined by eqs. (9), (10), and (11) the Hamiltonian of the biological systems contains in this case the multiple quanta term which may be given by

$$H_3 = \sum_{i,j,l} \sum_{m,n} [\varkappa a_l^+ (a_i)^m (a_j)^n + \varkappa^* a_l (a_i^+)^m (a_j^+)^n + \sigma a_l^+ (a_i^+)^m (a_j)^n + \sigma^* a_l (a_i)^m (a_j^+)^n + \mu a_l^+ (a_i)^m (a_j^+)^n + \mu^* a_l (a_i^+)^m (a_j)^n] , \tag{16}$$

where $\varkappa$, σ, and μ are the coupling constants and $(a_i)^m$ stands for $a_i a_i a_i \ldots a_i$ (m times). We determine the expectation values $\langle \dot{N}_q \rangle'''$ $(q \neq i,\ q \neq j)$, $\langle \dot{N}_i \rangle'''$, and $\langle \dot{N}_j \rangle'''$ corresponding to the H_3 term given by eq. (16). The results depend on the relations giving rise to the combination frequencies. The particular cases are given below.

a) For $\omega_q = m\omega_i + n\omega_j$

$$\langle \dot{N}_q \rangle''' = B\,, \quad \langle \dot{N}_i \rangle''' = -\sum_{m=0}^{+\infty} \sum_{n=0}^{+\infty} mB\,, \quad \langle \dot{N}_j \rangle''' = -\sum_{m=0}^{+\infty} \sum_{n=0}^{+\infty} nB\,, \tag{17}$$

where

$$B = \left(\frac{2\pi}{\hbar}\right) |\varkappa|^2 [(\langle N_q \rangle + 1)\, \alpha_i(m)\, \alpha_j(n) - \langle N_q \rangle\, \beta_i(m)\, \beta_j(n)] . \tag{18}$$

Here $\alpha_i(m)$, $\beta_j(n)$ are given by

$$\alpha_i(m) = \langle N_i \rangle (\langle N_i \rangle - 1) \ldots (\langle N_i \rangle - m + 1)\,,$$
$$\beta_j(n) = (\langle N_j \rangle + n)(\langle N_j \rangle + n - 1) \ldots (\langle N_j \rangle + 1)\,, \tag{19}$$

respectively.

b) For $\omega_q = -m\omega_i + n\omega_j$:

$$\langle \dot{N}_q \rangle''' = C\,, \quad \langle \dot{N}_i \rangle''' = \sum_{n=0}^{+\infty} \sum_{m=0}^{m_0} mC\,, \quad \langle \dot{N}_j \rangle''' = -\sum_{m=0}^{+\infty} \sum_{n=n_0}^{+\infty} nC\,, \tag{20}$$

where $m_0 \leqq n\omega_j/\omega_i$, $n_0 \geqq m\omega_i/\omega_j$, and

$$C = \left(\frac{2\pi}{\hbar}\right) |\sigma|^2 [(\langle N_q \rangle + 1)\, \beta_i(m)\, \alpha_j(n) - \langle N_q \rangle\, \alpha_i(m)\, \beta_j(n)] . \tag{21}$$

c) For $\omega_q = m\omega_i - n\omega_j$:

$$\langle \dot{N}_q \rangle''' = D\,, \quad \langle \dot{N}_i \rangle''' = -\sum_{n=0}^{+\infty} \sum_{m=m_0}^{+\infty} mD\,, \quad \langle \dot{N}_j \rangle''' = \sum_{m=0}^{+\infty} \sum_{n=0}^{n_0} nD\,, \tag{22}$$

where $m_0 \geqq n\omega_j/\omega_i$, $n_0 = m\omega_i/\omega_j$, and

$$D = \left(\frac{2\pi}{\hbar}\right) |\mu|^2 \left[(\langle N_q\rangle + 1)\,\alpha_i(m)\,\beta_j(n) - \langle N_q\rangle\,\beta_i(m)\,\alpha_j(n)\right]. \tag{23}$$

The energy transfer between particular modes the frequencies of which are in convenient relationships is described by eqs. (17)–(23). The frequency relations determine how many nonlinear interaction terms increase or decrease the energy in the particular mode. The direction of the energy flow (downwards or upwards) depends on the energy stored in the modes in question. For the energy transfer to the qth mode the B, C, and D values (in eqs. (17), (20), and (22), respectively) have to be positive. These values may be determined from eqs. (18), (21), and (23) making use of eq. (19). All these equations represent only the first order perturbation terms. The results concerning the direction of the energy flow (determination of the point where the flow is reversed) are, therefore, highly approximative. Besides the approximative nature of the results the multiple quanta energy channeling may be modified by the changes of the mode frequencies in the nonlinear region.

From eqs. (17), (20), and (22) we may derive the relations given by eq. (3) where $P_{m,n} = P_q = \langle \dot{N}_q\rangle''' \omega_q \hbar$.

6. THE FRÖHLICH KINETIC EQUATION WITH ADDITIONAL TERMS

The FKE including terms representing the interaction between systems located at different positions and multiple quanta terms (without the heat bath participation) may be written in the form

$$\langle \dot{N}_q\rangle = \langle \dot{N}_q\rangle' + \langle \dot{N}_q\rangle'' + A_q\,, \tag{24}$$

where $\langle \dot{N}_q\rangle$ is the original Fröhlich term given by

$$\langle \dot{N}_q\rangle' = S_q - \phi[\langle N_q\rangle \exp(\beta\omega_q) - (\langle N_q\rangle + 1)] - \\ - \sum_i X\{\langle N_q\rangle (\langle N_i\rangle + 1) \exp[\beta(\omega_q - \omega_i)] - \langle N_i\rangle (\langle N_q\rangle + 1)\}\,, \tag{25}$$

$\langle \dot{N}_q\rangle''$ is given by eq. (14), and A_q stands for the multiple quanta term which may be determined from eqs. (17), (20), and (22).

The energy channeling caused by the nonlinear mechanism may be assessed from eq. (3). We assume a simple case: the direct interaction without the heat bath help between three modes with the frequencies ω_1; ω_2; and ω_3 the m and n values of which are 1, 0; 0, 1; and m_3, n_3, respectively. The corresponding A_q values in eq. (24) are, therefore, given by

$$A_1 = \langle \dot{N}_1\rangle'''\,, \quad A_2 = \frac{n_3}{m_3}\langle \dot{N}_1\rangle'''\,, \quad A_3 = -\frac{1}{m_3}\langle \dot{N}_1\rangle'''\,, \tag{26}$$

respectively. We assume the energy stored in the coherently excited mode to be

sufficiently high. For $m_3 > 0$, $n_3 < 0$ the energy may be channeled from the ω_1 mode to the remaining two modes. In the case $m_3 > 0$, $n_3 > 0$ the energy may be channeled from the ω_1 mode and the ω_2 one to the ω_3 mode.

The multiple quanta interaction processes without the heat bath participation may channel the energy upwards – to higher frequency modes [6, 19]. The total result of the Fröhlich X process is stransfer of the energy downwards – from the higher frequency modes to the lowest frequency one. Energy circulation is connected with losses: the downward step transports the energy with the help of the heat bath. The interaction processes without the heat bath help lead to the energy saturation in the coherently excited mode, contribute to the coherent excitation of higher frequency modes [6] and cause the increase of energy losses. The changes of the mode frequencies may disturb the multiple quanta energy transfer without the heat bath participation. If the energy supply to the system in question decreases, the multiple quanta processes lose their significance as the transition from the highly nonlinear region into a region with weaker nonlinearity takes place.

The interaction between the vibration system located at different positions is represented by the Λ term given by eq. (14). This space interaction term is responsible for the energy channeling between the systems: we may expect that the energy is transferred from a system with a higher energy storage to that with a lower one. That expresses the tendency to a uniform energy distribution. Nevertheless, the energy transfer depends on the lowest mode frequencies of the systems, too.

7. CONCLUSION

We assume that coherent vibration systems are located in the cellular membranes. The systems consist very likely of clusters of electrical dipoles excited by the energy supply. The systems located at different positions may have different properties and different energy supply. The interaction term representing the energy transition between the systems is derived.

Owing to the multiple quanta processes the energy in a system may be transferred from the lowest frequency mode, which is coherently excited, to higher frequency modes. The general relations describing the process are derived. These relations are identical with the famous classical Manley-Rowe equations.

The additional terms in the Fröhlich kinetic equation cover the space dependent energy channeling and those caused by the nonlinear mechanism, which may be very important in the biological systems. The kinetic equation derived is convenient for computer simulation of the coherent excitation processes.

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