

Superradiant phase transition in nonlinear quantum field - matter system with translational symmetry

Maciej Kalinski

Center for Theoretical Physics, Polish Academy of Sciences
Al.Lotnikow 32/46, 02-668 Warsaw, Poland

We investigate a superradiant phase transition induced by a polariton instability in the system of nonlinear quantum oscillators. We assume for simplification that the system possesses a translational symmetry e.a. the oscillators are placed on a lattice. It enables us to introduce the soft polaritons concept similar to the soft phonons concept in models of ferroelectrics. We find the critical condition for the phase transition and see that it is quite similar to that which appears for the Dicke superradiance. We also suggest the physical realization of the model by the quantum well system and point out difficulties.

I. Introduction

It is clear for almost thirty years that the electromagnetic interactions can lead to the phase transition. It is proved for the Dicke model of superradiance [1], [2]. This model is however very restrictive assuming a system consisting of two level atoms coupled through the dipole interaction with the finite number of modes of the electromagnetic field. We deal with the case of the opposite type, when the number of interacting modes is the same as the number of atoms or other electromagnetically active centers. It happens in the solid state limit, when the matter excitations and electromagnetic excitations photons create a new type of excitations, polaritons. First, we use the translational symmetry of the system to simplify the linear part of the Hamiltonian and see that it is nothing, but the Hopfield Hamiltonian which is easy to diagonalize by the canonical transformation [3]. We need not to drop out quadratic terms of the electromagnetic field since we work within dipole approximation and can eliminate them by Zienau-Power transformation. We also need

not to drop interactions between centers. We find that for the coupling between the field and matter strong enough the linear system collapses. Nonlinear part of the Hamiltonian however can stabilize the system, but in this case the phase transition occurs. We want to underline the strong analogy between this model and the model of the displacive ferroelectric when, the situation is very similar to that. The other problem we discuss is the physical realization of the system. It is done by us for the Quantum Well system, when one can easily see, that the strong coupling requirement and the realization of the model are not independent.

II. Hamiltonian

We use the usual field-matter Hamiltonian in the dipole approximation

$$\begin{aligned}
H = & \sum_{A=1}^N \frac{1}{2m} [p_A - eA(r_A)]^2 + \frac{m\omega_0^2}{2} x_A^2 + V(x_A) \quad (2.1) \\
& + \frac{e^2}{\pi} \sum_{A,B=1, A \neq B}^N \frac{[x_A \cdot x_B - 3(n_{AB} \cdot x_A)(n_{AB} \cdot x_B)]}{r_{AB}^3} \\
& + \sum_{\lambda=1}^2 \int d^3k a_{\lambda}^+(k) a_{\lambda}(k) k,
\end{aligned}$$

which after Zienau-Power transformation $U = e^{ie \sum_A x_A \cdot A(r_A)}$ can be written as [4]

$$\begin{aligned}
H = & \sum_{A=1}^N p_A^2 + \frac{m\omega_0^2}{2} x_A^2 + V(x_A) - e x_A \cdot E(r_A) + \frac{e^2}{2} \sum_{A,B=1}^N W_{AB} x_A \cdot x_B \\
& + \sum_{\lambda=1}^2 \int d^3k a_{\lambda}^+(k) a_{\lambda}(k) k, \quad (2.2)
\end{aligned}$$

where

$$E(r_A) = -i \sum_{\lambda=1}^2 \int d^3k k g(k) [e_{\lambda}(k) a_{\lambda}(k) \exp(ikr_A) - H.C.],$$

$$g(k) = [2k(2\Pi)^3]^{\frac{1}{2}} \varrho(k),$$

$$W(r) = \frac{1}{(2\pi)^3} \int d^3k \varrho^2(k) \exp(ikr),$$

$$W_{AB} = \begin{cases} W(r_{AB}), & A \neq B; \\ \frac{2}{3}W(0), & A = B \end{cases}$$

and $\rho(k)$ is the spatial charge distribution. The $V(x_a)$ is the nonlinear part of the oscillator and is approximated by $\gamma x_A^4 = \gamma(x_A \cdot x_A)^2$. Within the validity of this model e.a when the distance between oscillators is much larger then the size of the oscillators we can assume W_{AB} proportional to δ_{AB} and then drop the fourth term in

Hamiltonian (2.2) but renormalize the oscillator frequency e.a now we have

$$H = \sum_{A=1}^N p_A^2 + \frac{m\tilde{\omega}_0^2}{2} x_A^2 + V(x_A) - ex_A \cdot E(r_A) \quad (2.3)$$

$$+ \sum_{\lambda=1}^2 \int d^3k a_{\lambda}^+(k) a_{\lambda}(k) k.$$

For the later purposes we will drop the tilde over the oscillator frequency understanding ω_0 as the full renormalize frequency. We drop for a moment the nonlinear part of the oscillator potential $V(x_a)$. When introducing usual creation and annihilation operators for oscillators $x_a = \frac{a_A + a_A^+}{\sqrt{2}\beta}$, $p_A = \frac{m\omega_0}{i} \frac{a_A - a_A^+}{\sqrt{2}\beta}$, $\beta^2 = \frac{m\omega_0}{\hbar}$ the Hamiltonian (2.3) changes to

$$H = \sum_{A=1}^N \sum_{i=1}^3 (a_A^+ \cdot a_A) w_0 - \frac{e}{\sqrt{2}\beta} (a_A + a_A^+) \cdot E(r_A) + \sum_{\lambda} \sum_k a_{\lambda k}^+ a_{\lambda k}. \quad (2.4)$$

We converted integrals to sums assuming that the system is in the limited volume $V = L^3$ and take usual Born-Karman (B-K) conditions, so $k = \frac{2\pi}{L}(n_x, n_y, n_z)$. As we mentioned before, we assume the translational symmetry of the system. In the simplest case $r_A = a(n_x, n_y, n_z)$ when oscillators are placed on a cubic lattice, where a is the lattice constant. Now we can introduce the polaronic transformation

$$B_k^+ = \frac{1}{\sqrt{N}} \exp(ikr_A) a_A^+,$$

$$B_k = \frac{1}{\sqrt{N}} \exp(-ikr_A) a_A \quad (2.5)$$

and define

$$B_{\lambda k}^+ = e_{\lambda}(k) \cdot B_k^+,$$

$$B_{\lambda k} = e_{\lambda}(k) \cdot B_k,$$

where $N = N_i^3$ is the total number of oscillators. We see that the B-K conditions for photons and polaritons are consistent since $L = N_i a$. For $N \rightarrow \infty$ we have $\sum_{r_A} e^{i(k-k')r_A} = N \delta_{kk'}$ so in this limit

$[B_k, B_{k'}^+] = \delta_{kk'}$ and also $[B_{\lambda k}, B_{\lambda k'}^+] = \delta_{\lambda\lambda'}\delta_{kk'}$ if only $[a_A, a_{A'}^+] = \delta_{AA'}$ holds as it does. After the transformation (2.5) and dropping all terms which do not appear in field-matter coupling we get for $V \rightarrow \infty, N \rightarrow \infty, \frac{N}{V} = \text{const}$

$$H = \sum_{\lambda} \sum_k (B_{\lambda k}^+ B_{\lambda k} + \frac{1}{2}) \omega_0 + k a_{\lambda}(k)^+ a_{\lambda}(k) \quad (2.6)$$

$$+ \frac{ie}{\sqrt{2m\omega_0}} \sqrt{\frac{N}{V}} \sqrt{k} [B_{\lambda k} a_{\lambda-k} + B_{\lambda k}^+ a_{\lambda k} - B_{\lambda k}^+ a_{\lambda-k}^+ - B_{\lambda k} a_{\lambda k}^+]$$

as the linear Hamiltonian. It has the same form that the well known Hopfield Hamiltonian for linear dielectric and can be easily diagonalized by the canonical transformation. We drop the cut off function, since now the more natural limitation in the sum appears after dropping not matter-field coupled operators. It is implied by the fact that no shorter polarization waves are coupled to photons than those with the length, which is equal to the smallest distance between oscillators. In the area of parameters for which the model is sensible, the oscillator size is much smaller than a so $\rho(k) = \frac{\beta^2}{\beta^2 + k^2}$ can be approximated by 1 since $\beta \gg \frac{1}{a}$ and the cut off can be ignored. The first term of the Hamiltonian (2.6) represents the collective polarization oscillators and the last their coupling to photons. In order to diagonalize (2.6) let us introduce

$$a_1 = B_{\lambda k}, \quad a_2 = a_{\lambda k}$$

$$a_3 = B_{\lambda-k}, \quad a_4 = a_{\lambda-k}$$

and now (2.6) is the sum of independent parts of the same form

$$H_{\lambda k} = \hbar\omega(a_1^+ a_1 + a_2^+ a_2) + \hbar\Omega(a_2^+ a_2 + a_4^+ a_4) + iV(a_1^+ + a_3)(a_2 + a_4^+) + H.C.. \quad (2.7)$$

Let us take

$$a_i = \sqrt{\frac{m_i \omega_0}{2\hbar}} (x_i + \frac{ip_i}{m_i \omega_0}),$$

$$a_i^+ = (a_i)^+,$$

$$m_i = \begin{cases} m & \text{for } i = 1, 2 \\ M & \text{for } i = 3, 4 \end{cases}, \quad \omega_i = \begin{cases} \omega & \text{for } i = 1, 2 \\ \Omega & \text{for } i = 3, 4 \end{cases}.$$

Then

$$H_{\lambda k} = \frac{p_1^2 + p_2^2}{2m} + \frac{m\omega^2}{2}(x_1^2 + x_3^2) + \frac{p_2^2 + p_4^2}{2M} + \frac{M\Omega^2}{2}(x_2^2 + x_4^2) - \frac{V}{\hbar} \sqrt{\frac{m\omega}{M\Omega}} [(p_2 + p_4)(x_1 + x_4) + (p_3 - p_1)(x_2 - x_1)] \quad (2.8)$$

and after the canonical transformation

$$\begin{aligned} X_1 &= \frac{1}{\sqrt{2}}(x_1 + x_3), \quad Y_1 = \frac{1}{\sqrt{2}}(x_2 - x_4), \\ X_2 &= \frac{1}{\sqrt{2}}(x_2 + x_4), \quad Y_2 = \frac{1}{\sqrt{2}}(x_3 - x_1), \\ P_1 &= \frac{1}{\sqrt{2}}(p_1 + p_3), \quad R_1 = \frac{1}{\sqrt{2}}(p_2 - p_4), \\ P_2 &= \frac{1}{\sqrt{2}}(p_2 + p_4), \quad R_2 = \frac{1}{\sqrt{2}}(p_2 - p_1), \end{aligned} \quad (2.9)$$

we have $H_{\lambda k} = H_1 + H_2$, where

$$\begin{aligned} H_1 &= \frac{1}{2m}P_1^2 + \frac{m\omega^2}{2}X_1^2 + \frac{1}{2M}P_2^2 + \frac{M\Omega^2}{2}X_2 - \chi_1 P_2 X_1 \\ H_2 &= \frac{1}{2M}R_1^2 + \frac{M\Omega^2}{2}Y_1^2 + \frac{1}{2m}R_2^2 + \frac{m\omega^2}{2}Y_2 - \chi_2 R_2 Y_1. \end{aligned} \quad (2.10)$$

So we get two pairs of two coupled oscillators. After the second canonical transformation for H_1

$$\begin{aligned} X_1 &= a\alpha_2\tilde{X}_1 + \alpha_2\tilde{P}_2, \\ P_2 &= \frac{\alpha_2}{c}\tilde{X}_1 + \frac{b}{c}\alpha_2\tilde{P}_2, \\ X_2 &= c\beta_2\tilde{P}_1 + \beta_2ac\tilde{X}_2, \\ P_1 &= b\beta_2 + \beta_2\tilde{X}_2, \end{aligned} \quad (2.11)$$

where

$$\begin{aligned} ab + mM\Omega^2a^2c^2 &= 0, \\ ab + M\omega^2ma^2c^2 - \chi Mac - \chi abac &= 0, \\ \alpha_2\beta_2(ab - 1) &= 1 \end{aligned}$$

and analogical for X_2 , H_1 (H_2) is

$$H_1 = a_1 \tilde{P}_2^2 + b_1 \tilde{X}_1^2 + a_2 \tilde{P}_2^2 + b_2 \tilde{X}^2,$$

with

$$\tilde{\omega}^2 = 4a_1b_1 = \frac{\omega_0^2 + \Omega^2 - \sqrt{(\omega_0^2 - \Omega^2)^2 + 16\tilde{V}^2\omega_0^2\Omega^2}}{2}, \quad (2.12)$$

$$\tilde{\Omega}^2 = 4a_2b_2 = \frac{\omega_0^2 + \Omega^2 + \sqrt{(\omega_0^2 - \Omega^2)^2 + 16\tilde{V}^2\omega_0^2\Omega^2}}{2}$$

and $\tilde{V}^2 = \frac{Ne^2}{Vm\epsilon_0\omega_0^2}$ is the effective dimensionless coupling constant. For $\tilde{\omega}^2, \tilde{\Omega}^2$ both positive we can introduce A_i, A_i^+ creation and annihilation operators for \tilde{P}_i, \tilde{X}_i and $H_1, (H_2)$ is now $H_1 = (A_1^+A_1 + \frac{1}{2})\tilde{\Omega}\hbar + (A_2^+A_2 + \frac{1}{2})\tilde{\omega}\hbar$. So we get two polaritonic branches with dispersion relations given by (2.12). For $\tilde{V}^2 > 0.25$ however $\tilde{\omega}^2 < 0$ for every k and the linear system collapses. When we take the nonlinear Hamiltonian with γx_a^4 potential correction for the oscillator ($\gamma > 0$) the system will not collapse because the nonlinearity will stabilize it, but now the phase transition can occur.

III. Soft polaritons and the phase transition

Now we will discuss the case when nonlinear term is added to the linear Hamiltonian. We use the polaritonic transformation (2.5) to express nonlinear γx^4 term by $B_{\lambda k}$, $B_{\lambda k}^+$ operators. We drop all terms which do not give the contribution to the first order energy corrections to the linear Hamiltonian energies. This yields

$$H_N = \frac{3\hbar^2}{2m^2\omega_0^2} \frac{\gamma}{N} \sum_{k,\lambda,k',\lambda'} 'B_{\lambda k}^+ B_{\lambda k} B_{\lambda' k'}^+ B_{\lambda' k'} [1 + [e_\lambda(k) e_{\lambda'}(k')]^2] \\ + \frac{\hbar^2}{4m\omega_0^2} [4\gamma + \frac{2\gamma}{N} [e_\lambda(k') e_{\lambda'}(k)]^2] B_{\lambda k}^+ B_{\lambda k}. \quad (3.1)$$

Now the full Hamiltonian becomes

$$H = H_L + H_N, \\ H_L = \sum_{\lambda k} 'H_{\lambda k}, \quad (3.2) \\ H_{3k} = (B_{3k}^+ B_{3k} + \frac{1}{2})\omega_0,$$

where $\sum_{\lambda k}'$, ($\lambda = 1, 2, 3$, $e_3(k) = \frac{k}{|k|}$) means the sum over longitudinal modes also and $\sum_{\lambda k}$ over tranvers modes only. In order to obtain the temperature dependent polaritonic branches we approximate the anharmonic Hamiltonian (3.2) by an effective quadratic Hamiltonian

$$H_{eff} = H_L \\ + \frac{3\hbar^2\gamma}{2m\omega_0^2} \sum_{k,k',\lambda,\lambda'} 'B_{\lambda k}^+ B_{\lambda k} < B_{\lambda' k'}^+ B_{\lambda' k'} > [1 + [e_\lambda(k) e_{\lambda'}(k')]^2] \\ + \frac{\hbar^2}{4m\omega_0^2} [4\gamma + \frac{2\gamma}{N} [e_\lambda(k') e_{\lambda'}(k)]^2] B_{\lambda k}^+ B_{\lambda k}, \quad (3.3)$$

where

$$< B_{\lambda k}^+ B_{\lambda k} > = \frac{Tr(B_{\lambda k}^+ B_{\lambda k} e^{-\beta H_{eff}})}{Tr e^{-\beta H_{eff}}}.$$

It is a sum of independent Hamiltonians $H_{\lambda k}$

$$H_{k\lambda} = (B_{\lambda k}^+ B_{\lambda k} + \frac{1}{2})\tilde{\omega}_{0k\lambda} + a_{\lambda k}^+ a_{\lambda k} k + H_{f-m}, \quad \lambda = 1, 2, \quad (3.4)$$

$$\begin{aligned}
H_{k3} &= (B_{3k}^+ B_{3k} + \frac{1}{2}) \tilde{\omega}_{0k3}, \\
\tilde{\omega}_{0k\lambda} &= \omega_0 + \frac{3\hbar^2 \gamma}{2m\omega_0^2 N} \sum_{k'\lambda'} < B_{\lambda'k'}^+ B_{\lambda'k'} > [1 + [e_\lambda(k) e_{\lambda'}(k')]^2] \\
&\quad + \frac{\hbar^2}{4m\omega_0^2} [4\gamma + \frac{2\gamma}{N} \sum_{k'} [e_\lambda(k') e_\lambda(k)]^2],
\end{aligned}$$

where H_{f-m} is defined by (2.6), which are now linear. The self consistent frequencies $\tilde{\omega}$, $\tilde{\Omega}$ can now be obtained from the solution of the system of equations

$$\begin{aligned}
< B_{k\lambda}^+ B_{k\lambda} > &= \frac{1}{4\omega_0} \left[\frac{(\tilde{\Omega}^2 + \tilde{\omega}_0^2)(\tilde{\Omega}^2 - \Omega^2)}{\tilde{\Omega}} \coth(\frac{1}{2}\beta\tilde{\Omega}) \right. \\
&\quad \left. - \frac{(\tilde{\omega}^2 + \tilde{\omega}_0^2)(\tilde{\omega}^2 - \Omega^2)}{\tilde{\omega}} \coth(\frac{1}{2}\beta\tilde{\omega}) \right] \frac{1}{\tilde{\Omega}^2 - \tilde{\omega}^2} - \frac{1}{2}, \quad (3.5) \\
< B_{k3}^+ B_{k3} > &= \frac{1}{\exp(\beta\tilde{\omega}_0) - 1},
\end{aligned}$$

where Ω is the photon frequency, and $\tilde{\omega}$, $\tilde{\Omega}$ are given by (2.12) with ω_0 and \tilde{V}^2 replaced by $\tilde{\omega}_0$ and $\tilde{V}^2 \frac{\omega_0}{\tilde{\omega}_0}$, $\tilde{\omega}_0 = \tilde{\omega}_{0k\lambda}$ since does not really depend on λ and k . It is quite similar to that which appears for the soft mode problem in the ferroelectric [5]. The system (3.5) can be simplified to the form

$$\tilde{\omega}_0 = \omega_0 + f(\tilde{\omega}_0, T), \quad (3.6)$$

where the function $f(\tilde{\omega}_0, T)$ is defined by the system. If we assume $\tilde{V}^2 > 0.25$ then for some $\tilde{\omega}_0 = \tilde{\omega}_0^* > \omega_0$, $\tilde{V}_{eff}^2 = \tilde{V}^2 \frac{\omega_0}{\tilde{\omega}_0^*} = 0.25$ and $\tilde{\omega} = 0$. For $\tilde{\omega}_0 \approx \tilde{\omega}_0^*$ and $\tilde{\omega}_0 > \tilde{\omega}_0^*$, $\tilde{\omega} \approx 0$, so we can approximate

$$< B_{k\lambda}^+ B_{k\lambda} > = \frac{1}{\beta(4\tilde{\omega}_0 - 16\tilde{V}^2\omega_0)}. \quad (3.7)$$

For temperatures low enough we can drop transvers contribution to $\tilde{\omega}_0$ corrections in (3.4) and the equation (3.6) is now

$$\tilde{\omega}_0 = \omega_0 + \frac{\hbar^2 \gamma}{m\omega_0^2} \left[\frac{7}{6} + \frac{kT}{8\hbar(\tilde{\omega}_0 - 4\tilde{V}^2)} \right] \quad (3.8)$$

and can be easily solved. Since $\tilde{\omega}_0(T)$ is the increasing function of the temperature, if only $V_{eff}^2 > 0.25$, then for $T < T_c$, T_c : $\tilde{V}_{eff}^2(T_c) = 0$, $\tilde{V}_{eff}^2 > 0.25$ and the smaller of frequencies $\tilde{\omega}$ becomes imaginary. It means that below some critical temperature the ‘paraelectric’ phase becomes unstable and we expect $\langle x_a \rangle \neq 0$ for $T < T_c$ to compensate the collapse, like in case of usual ferroelectric. For $T \rightarrow T_c$ from above $\tilde{\omega} \rightarrow 0$ and the soft polariton branch appears. In order to show the spontaneous polarization for ‘ferroelectric’ phase we try a different approximation. Let us return to the full Hamiltonian of the system and define some mean-field Hamiltonians

$$\begin{aligned} H_{\langle a \rangle} &= H_{L0} + H_N + H_{f-m}(a_{\lambda k} \rightarrow \langle a_{\lambda k} \rangle), \\ H_{\langle B \rangle} &= H_{L0} + H_N + H_{f-m}(B_{\lambda k} \rightarrow \langle B_{\lambda k} \rangle), \end{aligned} \quad (3.9)$$

where $H_{L0} = H_L - H_{f-m}$ and for selfconsistency

$$\begin{aligned} \langle a_{\lambda k} \rangle &= \frac{Tr e^{-\beta H_{\langle B \rangle}} a_{\lambda k}}{Tr e^{-\beta H_{\langle B \rangle}}}, \\ \langle B_{\lambda k} \rangle &= \frac{Tr e^{-\beta H_{\langle a \rangle}} B_{\lambda k}}{Tr e^{-\beta H_{\langle a \rangle}}}. \end{aligned} \quad (3.10)$$

One can check

$$\begin{aligned} \langle a_{\lambda k} \rangle &= \frac{i\chi}{\sqrt{k}}(\langle B_{\lambda k} \rangle + \langle B_{\lambda-k}^+ \rangle), \\ \langle a_{\lambda k}^+ \rangle &= -\frac{i\chi}{\sqrt{k}}(\langle B_{\lambda k}^+ \rangle + \langle B_{\lambda-k} \rangle). \end{aligned} \quad (3.11)$$

So, we have

$$\begin{aligned} H_{\langle a \rangle} &= H_{L0} - 2\chi^2 \sum_{\lambda k} [B_{\lambda k}(\langle B_{\lambda-k} \rangle + \langle B_{\lambda k}^+ \rangle) \\ &\quad + B_{\lambda k}^+(\langle B_{\lambda k} \rangle + \langle B_{\lambda-k}^+ \rangle)] + H_N. \end{aligned} \quad (3.12)$$

Since the averages $\langle B_{\lambda k} \rangle$ and $\langle B_{\lambda-k}^+ \rangle$ are taken with respect to the density operator with $H_{\langle a \rangle}$ our problem reduces to

$$\begin{aligned} H_{eff} &= H_{\langle a \rangle} - 2\chi^2 \sum_k B_{3k}(\langle B_{3-k} \rangle + \langle B_{3k}^+ \rangle) + \\ &\quad B_{3k}^+(\langle B_{3k} \rangle + \langle B_{3-k}^+ \rangle) \end{aligned} \quad (3.13)$$

$$\langle B_{\lambda k} \rangle = \frac{\text{Tr} e^{-\beta H_{eff}} B_{\lambda k}}{\text{Tr} e^{-\beta H_{eff}}}$$

where we sum over all polaritons, because the transverse mode is not coupled to its average and $B_{\lambda 3}$ can be approximate by 0, when the nonlinearity is small. Now we can use the inverse polaritonic transformation. One can easy check that it yields

$$\begin{aligned} H_{eff} &= \sum_A H_A^{eff} \\ H_A^{eff} &= \frac{p_A^2}{2m} + \frac{m\omega_0^2}{2} x_A^2 - \frac{2e^2 N}{\epsilon_0 V} x_A \cdot x_A + \gamma x_A^4 \\ \langle x_A \rangle &= \frac{\text{Tr}(e^{-\beta H_{eff}} x_A)}{\text{Tr} e^{-\beta H_{eff}}}. \end{aligned} \quad (3.14),$$

The interesting thing which happens is that after elimination of the field coordinates by the mean field method the system is equivalent to the noninteracting oscillators system, where every oscillator is described by the Hamiltonian H_A^{eff} . So, the effect of the translational symmetry is, that the every oscillator feels other oscillators and field only by its own coordinate average $\langle x_A \rangle$. The trivial solution of (3.14) is $\langle x_A \rangle = 0$. We will show that there is also nonzero solution for $\tilde{V}^2 > 0.25 + \Theta(\gamma)$. We use the minimum free energy principle [5] with the trial Hamiltonian

$$H_0 = \frac{p_A^2}{2m} + (x_A - \langle x_A \rangle)^2 \frac{m\omega_0^2}{2} \quad (3.15)$$

to calculate the free energy for the system characterized by the Hamiltonian (3.14). We know that the free energy $F \leq F_0 + \langle H_{eff}^A - H_0 \rangle_0$, where F_0 is the free energy of the system with the Hamiltonian H_0 , $F_0 = kT \ln[2 \sinh(\frac{\hbar\omega_0}{2kT})]$ and $\langle \rangle_0$ means the average taken with the density operator with H_0 . We have

$$\langle H_A^{eff} - H_0 \rangle_0 = \frac{m\omega_0^2}{2} \langle x_A \rangle_0^2 - \frac{2e^2 N}{\epsilon_0 V} \langle x_A \rangle_0^2 + \langle x_A^4 \rangle_0. \quad (3.16)$$

We have also

$$\langle x_{Ai}^4 \rangle = \langle x_{Ai} \rangle^4 + 6\sigma_{Ai} \langle x_{Ai} \rangle^2 + 3\sigma_{Ai}^2$$

$$\sigma_{Ai} = \langle (x_{Ai} - \langle x_{Ai} \rangle)^2 \rangle = \frac{\hbar}{2m\omega_0} \coth \frac{\hbar\omega_0}{2kT}. \quad (3.17)$$

Assuming $\langle x_{Ai} \rangle = 0$ for $i = 1, 2$ without the loss of generality and defining $x = \langle x_A \rangle$ we have

$$F \leq F_0 + \frac{m\omega_0^2}{2}x^2 - \frac{2e^2n}{\epsilon_0 V} + \frac{5\gamma\hbar}{m\omega_0}x^2 \coth\left(\frac{\hbar\omega_0}{2kT}\right) + \gamma x^4 \quad (3.18)$$

The best estimation for F is achieved by minimizing the right side of (3.18) with respect to x . For $\frac{m\omega_0}{2} - \frac{2e^2N}{m\omega_0} + \Theta(\gamma) > 0$, $\tilde{V}^2 < 0.25 + \Theta(\gamma)$ (small nonlinearity) the minimum is for $x = 0$ for all temperatures, so there is no phase transition in this case. Otherwise the situation depends on the temperature. Defining T_c by the condition

$$\frac{m\omega_0^2}{2} - \frac{2e^2n}{\epsilon_0 V} + \frac{5\gamma\hbar}{m\omega_0} \coth\left(\frac{\hbar\omega_0}{kT_c}\right) = 0 \quad (3.19)$$

We have $x = 0$ for $T > T_c$ for the ‘paraelectric’ phase and $x \neq 0$

$$x^2 = \frac{1}{2\gamma} \left[\left(\frac{2e^2N}{\epsilon_0 V} - \frac{m\omega_0^2}{2} - \frac{5\gamma\hbar}{m\omega_0} \coth\left(\frac{\hbar\omega_0}{2kT}\right) \right) \right]$$

for $T > T_c$ or for ‘ferroelectric’ phase. We see that for temperatures below some critical value spontaneous polarization appears. It is driven by polariton instability similiary to the case of the usuall ferroelectric [7], when the phonon instability leads to the spontaneous displacement of ions.

IV. Physical realization of the model

We see from the previous section that the necessary condition for the phase transition is that $\tilde{V}^2 > 0.25 + \Theta(\gamma)$. We try to answer now how it is possible to achieve such a region of parameters in the real physical system to keep the model applicable. First we find, how the critical condition is related to that which appears in the Dicke model of superradiance. In the later case it is

$$\frac{2|D_{12}|^2 N}{\epsilon \epsilon_0 V} > 1 \quad (4.1).$$

Where D_{12} is electric dipole matrix element and ϵ is energy difference between two levels of the system. The square of the matrix element D_{12} for the harmonic oscillator between its ground state and the first excited level is simply $|D_{12}|^2 = \frac{e^2 \hbar}{2m\omega_0}$. If we use it in the condition (4.1) and take $\epsilon = \hbar\omega_0$ we get $\tilde{V}^2 > 1$. So the critical parameter in our model is of the same order as the critical parameter in the case, when someone approximate the harmonic oscillator by its two levels and asks for the Dicke superradiance in such system. The first conclusion of the last note is that it is difficult to achieve the critical region in the real physical system. One can easily estimate $\tilde{V}^2 \approx (\frac{\omega_B}{\omega_0})^2 n_b$ where $\hbar\omega_b = 13.6 \text{ eV}$ and n_B is the number of oscillators per Bohr volume (Volume of the cube with the edge length equal to the Bohr radius), so for real dielectrics $\tilde{V}^2 \approx 10^{-4}$. First we will try to answer why it is difficult to get the critical value of \tilde{V}^2 without the loss of the applicability of our model for optical oscillator frequencies. Let us define the harmonic oscillator size as $d = \frac{1}{\beta}$, where $\beta^2 = \frac{m\omega_0}{\hbar}$, since the ground state wave function is $\varphi_0 \sim e^{\frac{-\beta^2 r^2}{2}}$. It somehow informs where the electron is mainly localized, so can be define as the size of the oscillator. One can easily estimate $d \approx (\frac{\omega_B}{\omega_0})^{\frac{1}{2}} a_0$. Otherwise knowing, that $\frac{N}{V} \sim \frac{1}{a^3}$ (a is the distance between nearest oscillators, a_0 the Bohr radius) one can ask now how large the a should be to keep \tilde{V}^2 critical. We can easily find $a \approx a_0 (\frac{\omega_B}{\omega_0})^{\frac{2}{3}}$. So, when we order \tilde{V}^2 to be critical, the distance between nearest oscillators and the oscillator size are not independent. We just have $\frac{\omega_B}{\omega_0} = (\frac{d}{a})^6$. So, if we want to apply our model we have to assume

$d \gg a$. It makes even for $\frac{d}{a} \sim 2$, $\omega_0 \approx 10^{-2}\omega_B$, so in the infrared region. Now we have clear requirements for the real physical system. The simplest one which seems to be proper is the periodic system of tree dimensional quantum wells (Q.W.). The energy levels for the 3-dim Q.W. are $E_n = \frac{\pi^2\hbar^2}{2md^2}(n_x^2 + n_y^2 + n_z^2)$. If we define $n'_i = n_i - 1$ then

$$E_{n'} = \frac{\pi^2\hbar^2}{md^2}(n'_x + n'_y + n'_z) + \frac{\pi^2\hbar^2}{2md^2}(n_x^2 + n_y^2 + n_z^2) + const \quad (4.2)$$

and we can treat the quantum well as the nonlinear quantum oscillator with $\omega_0 = \frac{\pi^2\hbar^2}{2md^2}$. Now the edge of the Q.W. is the oscillator dimension and all previous considerations about the applicability of the model holds on. Using the fact that the dipole matrix elements is significant only between two neighboring states (in the sense of energy levels) of the Q.W. $|D_{n',n'+1}|^2 \approx \frac{e^2\hbar}{2m\omega_0(n'+1)}$ and for low excited states we have $|D_{12}|^2 \approx \frac{e^2\hbar}{2m\omega_0}$, so approximately the same as for the oscillator. We have here a little different type of the nonlinearity then we discussed in the previous section which is γa^+aa^+a . For low excited states we have $(a^+ + a)^4 \approx 6a^+aa^+a + 6a^+a$. The Hamiltonian of the nonlinear oscillator which gives low excited energy levels of the quantum well is now

$$H = \frac{p^2}{2m} + \frac{m\omega_0^2}{2}x^2 + \frac{2m^2\omega_0^3}{3\hbar}(x_1^4 + x_2^4 + x_3^4) \quad (4.3)$$

The necessary condition for the phase transition is now $\tilde{V}^2 > \frac{9}{4}$, so a little stronger then for the small nonlinearity but of the same order. The critical temperature is now determined by the condition

$$\coth \frac{\hbar\omega_0}{kT_c} = \frac{e^2N}{2m\omega_0^2\epsilon_0V} - \frac{1}{8} \quad (4.4)$$

If we want the critical temperature measurable $T_c \approx 10^4 K$ and $\frac{\hbar\omega_0}{kT_c} \approx 10$ to keep \tilde{V}^2 a little below its critical value then $\hbar\omega_0 \approx 10^{-5} eV$, $(\frac{d}{a}) \approx 10$ as it should be and $d \approx 500 \text{\AA}$.