On the phase transition in A^4-phonon theory

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Abstract. For a A^4-quantum mechanical phonon Hamiltonian it is proven that the free energy is complex if the harmonic, dynamical matrix of the model has negative definite portion in the Brillouin zone. From this fact it follows that the free energy exhibits always an instability associated with the ground state.

(1) The partition function of a phonon system can be represented in a closed form containing functional derivatives. The study of this representation presents a definite interest by its simplicity.

The functional technique has been used by Martin and Schwinger [1] to describe many-body Bose- or Fermi-system. Classical source fields are introduced by this method into the partition function to generate the Green's functions. These can be generated by taking the functional derivatives of the generalized free energy.

Our aim is to get definite information on the partition function for an anharmonic quantum or classical crystal. We will show that for an A^4-theory the phase transition cannot occur at finite temperature if the dynamical matrix of the A^4-phonon theory does not depend on the temperature T. In this case the phase transition occurs only in the ground state. Further it follows from the quantum mechanical model, that the classical one is also unstable if the harmonic matrix has negative portions in the Brillouin zone.

In order to construct a closed form for the partition function we write down the quantum lattice dynamical model Hamiltonian

$$H = \frac{1}{2}\sum_{l_1} P^2(l_1) + \sum_{l_1 l_2} \omega^2(l_1 l_2)A(l_1)A(l_2) + \frac{V}{4}\sum_{l_1} A^4(l_1) \tag{1.1}$$

where $A(l_1)$ is the displacement field and $P(l_1)$ its canonical conjugate momentum at site l_1 of a d-dimensional lattice. $A(l_1)$ and $P(l_2)$ fulfil the Heisenberg-commutation relations, $[P(l_1), A(l_2)] = \hbar/i\ \delta_{l_1,l_2}$. Here δ_{l_1,l_2} denotes the Kronecker's δ-function. We assume periodic boundary conditions, that means the Fourier transform of the dynamical matrix

$$\hat{\omega}^2(\mathbf{q}) = \sum_{l_1} \exp\{-i\mathbf{q}\cdot(\mathbf{R}_{l_1} - \mathbf{R}_{l_2})\}\omega^2(l_1 l_2) \tag{1.2}$$

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of the Hamiltonian equation (1.1) does exist and is periodic with respect to the reciprocal lattice vectors **K**. The Fourier transforms of $A(l_1)$ and $P(l_2)$ are also periodic in **K**.

(2) Under these conditions we prove the following theorem:

Theorem. *If the dynamical matrix $\hat{\omega}^2(\mathbf{q})$ is negative definite for a portion of wave vectors $\mathbf{q}$ in the Brillouin zone B and $\hat{\omega}^2(\mathbf{q})$ does not depend on the temperature T, then the model phonon system equation (1.1) is unstable and it exhibits a ground state instability which is present at all temperatures $T > 0$.*

To prove this we study the partition function Z (or the free energy F) of the model system equation (1.1), which leads to the construction of the 'S-matrix' of Z in the imaginary time interval $[0, \beta]$. The construction of the 'S-matrix' requires that we split up the model Hamiltonian equation (1.1) into a Harmonic part

$$H_0 = \frac{1}{2}\sum_{l_1} P^2(l_1) + \frac{1}{2}\sum_{l_1 l_2} \Omega^2(l_1 l_2) A(l_1) A(l_2) \tag{2.1}$$

with positive definite $\Omega^2(l_1 l_2) > 0$ and into a perturbation

$$H_1 = -a\sum_{l_1} A^2(l_1) + \frac{v}{4}\sum_{l_1} A^4(l_1), \tag{2.2}$$

where we assumed

$$\omega^2(l_1 l_2) = \Omega^2(l_1 l_2) - 2a\,\delta_{l_1,l_2}, \quad a > 0, \tag{2.3}$$

The partition function Z can be written as

$$Z = \mathrm{Tr}\,\{\exp(-\beta H)\} = Z_0 \langle S[H_1]\rangle_0, \tag{2.4}$$

where

$$\langle S[H_1]\rangle_0 = \mathrm{Tr}\left\{\frac{\exp(-\beta H_0)}{Z_0} S[H_1]\right\},$$

$$S[H_1] = T\exp\left(-\int_0^\beta d\tau H_1(\tau)\right). \tag{2.5}$$

T denotes the imaginary time ordering operator. $H_1(\tau)$ is in the interaction representation, $H_1(\tau) = \exp(\tau H_0) H_1 \exp(-\tau H_0)$. The free partition function Z_0 is given by

$$Z_0 = \prod_{\mathbf{q}\in B}\left[2\cdot Sh\left(\frac{\beta\hbar}{2}\hat{\Omega}\mathbf{q}\right)\right]^{-1}, \quad \hat{\Omega}\mathbf{q} \geq 0. \tag{2.6}$$

Notice that the expectation value of the S-matrix equation (2.5) should be real to have well-defined thermodynamics. We prove the contrary for the model equation (1.1), that means $\langle S[H_1]\rangle_0$ is complex for $a > 0$ and $v > 0$ and the instability of the system is always present in the parameter space $\{a, v\}$.

To do so, we introduce at first a generalized partition function by

$$Z_{u,j} = Z_0 \langle T S_u S_j S[H_1]\rangle_0 \tag{2.7}$$

with

$$S_u = T\exp\left[-\frac{1}{2}\int_0^\beta d\tau_1\int_0^\beta d\tau_2 \sum_{l_1 l_2} u(l_1\tau_1, l_2\tau_2)A(l_1\tau_1)A(l_2\tau_2)\right], \tag{2.8}$$

$$S_j = T\exp\left[i\int_0^\beta d\tau_1 \sum_{l_1} j(l_1\tau_1)A(l_1\tau_1)\right]. \tag{2.9}$$

In $S[H_1]$, S_u and S_j the displacement fields are in interaction representation. $U(l_1\tau_1, l_2\tau_2)$ and $j(l_1\tau_1)$ denote classical source fields such that $U(l_1\tau_1, l_2\tau_2) = U(l_1\tau_1)\cdot\delta_{l_1 l_2}\cdot\delta(\tau_1 - \tau_2)$. It is easy to show that the generalized partition function can be written with help of functional derivatives as

$$\begin{aligned} Z_{u,j} &= Z_0\cdot\exp(\Delta_v + \Delta_a)\langle TS_u S_j\rangle_0 \\ &= Z_0\cdot\exp(\Delta_v + \Delta_a + \Delta_u)\langle S_j\rangle_0 \end{aligned} \tag{2.10}$$

where

$$\Delta_v = -\frac{v}{4}\int_1 \frac{\delta^4}{\delta j(1)^4}, \tag{2.11a}$$

$$\Delta_a = -a\int_1 \frac{\delta^2}{\delta j(1)^2}, \tag{2.11b}$$

$$\Delta_u = \frac{1}{2}\int_1\int_2 u(1,2)\frac{\delta^2}{\delta j(1)\,\delta j(2)}. \tag{2.11c}$$

Here the sign $\int_1$ denotes the sum over the lattice points $\sum_{l_i}$ and the integral over the imaginary time interval $[0,\beta]$: $\int_i = \sum_{l_i}\beta\int_0 d\tau_i$, $i = [l_i, \tau_i]$. One gains the partition function Z equation (2.4) after performing the functional derivatives in equation (2.7) and then putting the source fields equal zero.

To get information about the stability of the system we compute $\langle TS_u S_j S[H_1]_0\rangle$ at $u = j = 0$. One evaluates the quantity $\langle S_j\rangle_0$ at first:

$$\langle S_j\rangle_0 = \exp\left[-\frac{1}{2}\int_1\int_2 j(1)\,D_2^0(1,2)j(2)\right]. \tag{2.12}$$

Here $D_2^0(1,2)$ denotes the imaginary time ordered two point, free phonon Green's function, which is real. The space Fourier transform of $D_2^0(1,2)$ is

$$D_2^0(\mathbf{q},\tau) = \frac{1}{2}\cdot\frac{\hbar}{\hat{\Omega}\mathbf{q}}\cdot\frac{Ch[(\beta/2 - |\tau|)\hbar\hat{\Omega}\mathbf{q}]}{Sh[\beta/2\hbar\hat{\Omega}\mathbf{q}]} \tag{2.13}$$

where $\hat{\Omega}\mathbf{q}$ is given by the Fourier transform of $\Omega^2(l_1, l_2)$. We define

$$F_0[u,j] = \langle TS_u S_j\rangle_0 = \exp(\Delta_u)\langle S_j\rangle_0. \tag{2.14}$$

To evaluate this expression, we make the 'ansatz'

$$F_0[u,j] = C[u]\cdot\exp\left[-\frac{1}{2}\int_1\int_2 j(1)\,D_2^0(1,2\mid u)j(2)\right] \tag{2.15}$$

and the two point phonon Green's function is defined by

$$D_2^0(1,2\mid u) = \langle T\{A(1)A(2)S_u\}\rangle_0/\langle S_u\rangle_0. \tag{2.16}$$

Now from equation (2.14) it follows

$$\frac{\delta}{\delta u(1,2)} F_0[u,j] = \frac{1}{2}\cdot\frac{\delta^2}{\delta j(1)\,\delta j(2)} F_0[u,j] \tag{2.17}$$

which with equation (2.15) permits to write the identity

$$\delta \ln C[u] = -\frac{1}{2}\int_1\int_2 D_2^0(1,2\mid u)\,\delta u(2,1). \tag{2.18}$$

The integration of this equation gives

$$C[u] = \det{}^{-1/2}\,[\mathbb{1} + D_2^0 u] \tag{2.19}$$

in the notation of matrices. In the determinant D_2^0 is given by equation (2.13). Using the local u-source field the generalized partition function $Z_{u,j}$ can be written at $j = 0$ as

$$\begin{aligned} Z_{u,0} &= Z_0\cdot\exp(\Delta_{1u} + \Delta_{au})\det{}^{-1/2}(\mathbb{1} + D_2^0 u) \\ &= Z_0\cdot\exp(\Delta_{1u})\cdot\det{}^{-1/2}[\mathbb{1} + D_2^0(u - 2a\mathbb{1})] \end{aligned} \tag{2.20}$$

with

$$\Delta_{1u} = -\frac{v}{4}\int_1 \frac{\delta^2}{\delta u(1)^2}, \tag{2.21a}$$

$$\Delta_{au} = -2a\int_1 \frac{\delta}{\delta u(1)}. \tag{2.21b}$$

Therefore the expectation value of the S-matrix $\langle S[H_1]\rangle_0$ can be written as

$$\begin{aligned} \langle S[H_1]\rangle_0 &= \exp(\Delta_{1u})\cdot\det{}^{-1/2}[\mathbb{1} + D_2^0(u - 2a\mathbb{1})]\big|_{u=0} \\ &= f[\hat{\Omega}\mathbf{q}, v, a]\cdot\exp[-\tfrac{1}{2}\operatorname{Tr}\{\ln(\mathbb{1} - 2a\,D_2^0)\}]. \end{aligned} \tag{2.22}$$

Here $f[\hat{\Omega}_{\mathbf{q}}, v, a]$ is a functional only of $[(D_2^0)^{-1} - 2a]^{-1}$ and a function only of v. Further

$$[(D_2^0)^{-1} - 2a]^{-1}(\mathbf{q},\tau) = \frac{\hbar}{2\hat{\omega}_{\mathbf{q}}}\cdot\frac{Ch[(\beta/2 - |\tau|)\hbar\hat{\omega}_{\mathbf{q}}]}{Sh[\beta/2\hbar\hat{\omega}_{\mathbf{q}}]} \tag{2.23}$$

remains always real for real or imaginary frequencies $\hat{\omega}_{\mathbf{q}}$, see equation (2.3), it follows immediately that $f[\hat{\Omega}_{\mathbf{q}}, v, a]$ is real. However the exponential of equation (2.22) $\exp[-\frac{1}{2}\operatorname{Tr}\{\ln(1 - 2a\,D_2^0)\}]$ is complex for all positive $a > 0$. Therefore the instability in the model system equation (1.1) starts to occur at $a = 0$ which proves the theorem.

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REFERENCES

[1] P. C. Martin and J. Schwinger, Phys. Rev. *115*, 1342 (1958), see also K. Symanzik in *Local Quantum Theory*, Enrico Fermi School, Course XLV, ed. by R. Jost (1969).