# (17) A SPIN-OSCILLATOR COUPLED APPROXIMATION FOR THE STATICS AND DYNAMICS OF A FOURTH ORDER ANHARMONIC LATTICE

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We derive the dynamic correlation matrix for a fourth order anharmonic lattice. A self-consistent Ising spin-oscillator coupled approximation is introduced and shown to yield a static susceptibility in qualitative agreement with the exact result for a non-interacting system. Extensions of the approximation to dynamics, and to a $d$-dimensional lattice of interacting oscillators are discussed.

**Introduction**:

As a model for physical systems undergoing a structural phase transition with a scalar order parameter is often used the fourth order anharmonic lattice defined by the Hamiltonian [1]

$$H=\sum_{\ell}\{\frac{1}{2}P_{\ell}^{2}+\frac{1}{2}AX_{\ell}^{2}+\frac{1}{4}BX_{\ell}^{4}-C\sum_{\langle\ell'\rangle}X_{\ell}X_{\ell'}\}\equiv\sum_{\langle\ell'\rangle}H_{\ell}\,. \tag{1}$$

Here $X_{\ell}$ and $P_{\ell}$ are local scalar displacements and their conjugate momenta. The sum extends over a $d$-dimensional hypercubic lattice, and the interaction is restricted to nearest neighbors. $B>0$, $C\geqslant 0$, while $A$ can take arbitrary values. This model has been studied in extensive computer simulations by Schneider and Stoll, and by Koehler et al. [1–5]. Their main results can be summarized as:

i) Static critaical behavior consistent with a $d$-dimensional Ising model.

ii) Second sound in a temperature window below $T_c$.

iii) A sharp central peak (CP) in the dynamic structure factor close to $T_c$, even in the high-temperature phase.

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iv) Damped phonon-like exitations which undergo incomplete softening near $T_c$.

Following Schneider and Stoll, we derive the dynamic correlation matrix,

$$C_{AB}(z) = (A | \frac{i}{z - \mathscr{L}} | B) \tag{2}$$

where the scalar product is

$$(A | B) = \langle A^* B\rangle - \langle A\rangle\langle B\rangle, \tag{3}$$

angular brackets denoting equilibrium average and $\mathscr{L}$ the Liouville operator. As relevant variables we take the displacement fluctuations,

$$X_{\boldsymbol{q}} = N^{-1/2} \sum_{\ell} (X_\ell - \langle X_\ell\rangle)\, e^{i\boldsymbol{q}\cdot\boldsymbol{R}_\ell} \tag{4}$$

and the energy density fluctuations,

$$H_{\boldsymbol{q}} = N^{-1/2} \sum_{\ell} (H_\ell - \langle H_\ell\rangle)\, e^{i\boldsymbol{q}\cdot\boldsymbol{R}_\ell} \tag{5}$$

and their time derivatives. Since the total energy is conserved, there is a heat conduction mode in the energy density correlation function. But the cross-correlation functions $\langle X_{-\boldsymbol{q}} H_{\boldsymbol{q}}\rangle$ and $\langle \dot{X}_{-\boldsymbol{q}} \dot{H}_{\boldsymbol{q}}\rangle$ are proportional to the order parameter $\langle X\rangle$, so the CP above $T_c$ must be due to some mechanism other than linear coupling to heat conduction. Several mechanisms have been proposed, like domain wall motion [1, 6], and nonlinear coupling to the energy density [7].

The correlation matrix takes the standard form

$$C(z) = i(k_B T)[z1 - \Omega + i\Sigma(z)]^{-1}\chi \tag{6}$$

where

$$\chi_{AB} = (k_B T)^{-1}(A | B) \tag{7}$$

is the static susceptibility,

$$\Omega = \omega\chi^{-1},$$

$$\omega_{AB} = i(k_B T)^{-1}(\dot{A} | B) \tag{8}$$

is the Mori-type frequency matrix, and

$$\Sigma(z) = \sigma(z)\,\chi^{-1},$$

$$\sigma_{AB}(z) = (k_B T)^{-1} (\dot{A} \,|\, \frac{i}{z - O\mathscr{L}O} \,|\, \dot{B}) \tag{9}$$

is the damping matrix. $O$ is the projector onto the irrelevant subspace. $\sigma(z)$ has the four nonzero elements $\sigma_{\dot{X}\dot{X}}$, $\sigma_{\dot{X}\dot{H}} = \sigma_{\dot{H}\dot{X}}{}^*$ and $\sigma_{\dot{H}\dot{H}}$. $\sigma_{\dot{X}\dot{X}}$ must contain the CP above $T_c$.

In the mode-decoupling approximation all the terms in the frequency matrix are functions of the static displacement susceptibility

$$\chi_T(\boldsymbol{q}) = (k_B T)^{-1} \langle X_{-\boldsymbol{q}} X_{\boldsymbol{q}} \rangle. \tag{10}$$

**Spin-oscillator approximation:**

In order to approximate $X_T$ and the damping matrix we introduce the spin-oscillator coupled approximation by the transformation

$$X_\ell = Q_\ell + S_T\, \varepsilon_\ell . \tag{11}$$

$\epsilon_\ell$ is an Ising spin variable and $Q_\ell$ is an oscillatory variable whose average conditionally on $\epsilon_\ell$, vanishes:

$$\varepsilon_\ell = \pm 1, \qquad S_T \geqslant 0, \qquad \langle Q_\ell \,|\, \varepsilon_\ell \rangle = 0. \tag{12}$$

This approximation resembles the two-Gaussian approximation employed by A. D. Bruce et al. to EPR results from $SrTiO_3$ [8]. The transformation (11) increases the state space of the model by a factor $2^N$, but at low temperatures where $\langle Q_\ell^2 \rangle \ll S_T^2$, the additional unphysical states are very improbable.

$S_T$ is determined by requiring the average forces conditionally on $\epsilon_\ell$, to vanish:

$$\langle B X_\ell^3 + (A - 4dC) X_\ell \,|\, \varepsilon_\ell \rangle = 0, \tag{13}$$

which, with (11), (12) and the simplifying assumption

$$< Q_\ell^{\;3} \mid \varepsilon_\ell > = 0, \tag{14}$$

yields

$$S_T \cdot ( S_T^2 + 3 <Q_\ell^{\;2}>_T - S_0^2 ) = 0, \tag{15a}$$

or

$$S_T^2 = \begin{cases} 0 \\ S_0^2 - 3 <Q^2>_T \end{cases} \tag{15b}$$

where $S_0$ is the order parameter at $T = 0$,

$$S_0^2 = ( 4\,dC - A )/B. \tag{16}$$

**Non-interacting case**:

In the non-interacting case, $dC = 0$, the results of the spin-oscillator approximation can be checked against the high- and low temperature expansions of Onodera's exact susceptibility [9], and against the numerical values for $< X^2 >$, computed from the Boltzmann distribution $P(X) = e^{-\beta H(X)}/\mathrm{Tr}\,e^{-\beta H(X)}$. Using (11) and (15) we write the non-interacting single particle Hamiltonian as the sum of an effective harmonic oscillator and a nonlinear term:

$$H = H_{\mathrm{E}} + H_{\mathrm{A}}, \tag{17a}$$

$$H_{\mathrm{E}} = \frac{1}{2} ( P^2 + \omega_{\mathrm{E}}^2 (T)\, Q^2 ) \tag{17b}$$

$$H_{\mathrm{A}} = ( B/4 ) ( Q^4 - 6 <Q^2>_T Q^2 ) + B S_T ( Q^3 - 3 <Q^2>_T Q ) \,\varepsilon\,. \tag{17c}$$

The effective frequency is

$$\omega_{\mathrm{E}}^2 (T) = \begin{cases} 2 B S_T^2 = 2 B ( -A/B - 3 <Q^2>_T ), & S_T > 0 \\ A + 3 B <Q^2>_T \qquad\qquad\qquad\quad , & S_T = 0. \end{cases} \tag{18}$$

The $Q\epsilon$ coupling term vanishes from $H_E$ because of (15). $\omega_E^2(T)$ is a function of $T$ only through $<Q^2>_T$, which thus can be determined self-consistently from the relation

$$\omega_E^2\,(<Q^2>_T)\cdot<Q^2>_T = k_B T\,, \tag{19}$$

yielding for the mean square displacement $<X^2>_T$:

$A>0$ (single well):

$$<X^2>_T = <Q^2>_T = \frac{A}{6B}\sqrt{\frac{T_0+2T}{T_0}}\,, \qquad k_B T_0 = A^2/6B\,. \tag{20}$$

$A<0$ (double well):

$$<X^2>_T = S_T^2 + <Q^2>_T = \begin{cases} -\dfrac{A}{3B}\left[2+\sqrt{\dfrac{T_0-T}{T_0}}\right], & T<T_0 \\[2ex] -\dfrac{A}{6B}\left[1+\sqrt{\dfrac{T_0+2T}{T_0}}\right], & T>T_0\,. \end{cases} \tag{21}$$

For $A>0$, $S_T \equiv 0$, while for $A<0$, it drops discontinuously to zero at $T_0$. $<X^2>_T$ also has a finite discontinuity at $T_0$ for $A<0$, as seen from (21). This discontinuity is clearly an artifact of the selfconsistent approximation used to determine $<Q^2>_T$. But the high- and low temperature expansions of (20) and (21) agree reasonably well with the series expansions of Onodera's exact result, $<X^2>_E$:

High-$T$ expansions:

$$\begin{aligned} <X^2>_E &= 2\delta\sqrt{\frac{k_B T}{B}} + \frac{1-4\delta^2}{2}\left(-\frac{A}{B}\right) + 4\delta^3\left(-\frac{A}{B}\right)^2\sqrt{\frac{B}{k_B T}} + O\left(-\frac{A}{B}\right)^3\left(\frac{B}{k_B T}\right)^1 \\ &= (\,0.676\cdots\cdots\,)\sqrt{\frac{k_B T}{B}} + (\,0.271\cdots\,)\left(-\frac{A}{B}\right) \\ &\quad + (\,0.154\cdots\,)\left(-\frac{A}{B}\right)^2\sqrt{\frac{B}{k_B T}} + O\left(-\frac{A}{B}\right)^3\left(\frac{B}{k_B T}\right)^1, \end{aligned}$$

where $\delta \equiv \Gamma(3/4)/\Gamma(1/4) = 0.3380\ldots$ .

$$<X^2>_T = \frac{1}{\sqrt{3}}\sqrt{\frac{k_B T}{B}} + \frac{1}{6}\left(-\frac{A}{B}\right) + \frac{1}{24\sqrt{3}}\left(-\frac{A}{B}\right)^2\sqrt{\frac{B}{k_B T}} + O\left(-\frac{A}{B}\right)^4\left(\frac{B}{k_B T}\right)^{3/2}$$

$$= (0.577\cdots)\sqrt{\frac{k_B T}{B}} + (0.166\cdots)\left(-\frac{A}{B}\right)$$

$$+ (0.024\cdots)\left(-\frac{A}{B}\right)^2\sqrt{\frac{B}{k_B T}} + O\left(-\frac{A}{B}\right)^4\left(\frac{B}{k_B T}\right)^{3/2} .$$

Low-$T$ expansions:

$A > 0$ (single well):

$$<X^2>_E = \frac{k_B T}{A} - \frac{3B}{A}\left(\frac{k_B T}{A}\right)^2 + \frac{8}{3}\left(\frac{3B}{A}\right)^2\left(\frac{k_B T}{A}\right)^3 + O\left(\frac{3B}{A}\right)^3\left(\frac{k_B T}{A}\right)^4$$

$$<X^2>_T = \frac{k_B T}{A} - \frac{3B}{A}\left(\frac{k_B T}{A}\right)^2 + 2\left(\frac{3B}{A}\right)^2\left(\frac{k_B T}{A}\right)^3 + O\left(\frac{3B}{A}\right)^3\left(\frac{k_B T}{A}\right)^4.$$

$A < 0$ (double well):

$$<X^2>_E = -\frac{A}{B} + \frac{k_B T}{A} + O(T^2)$$

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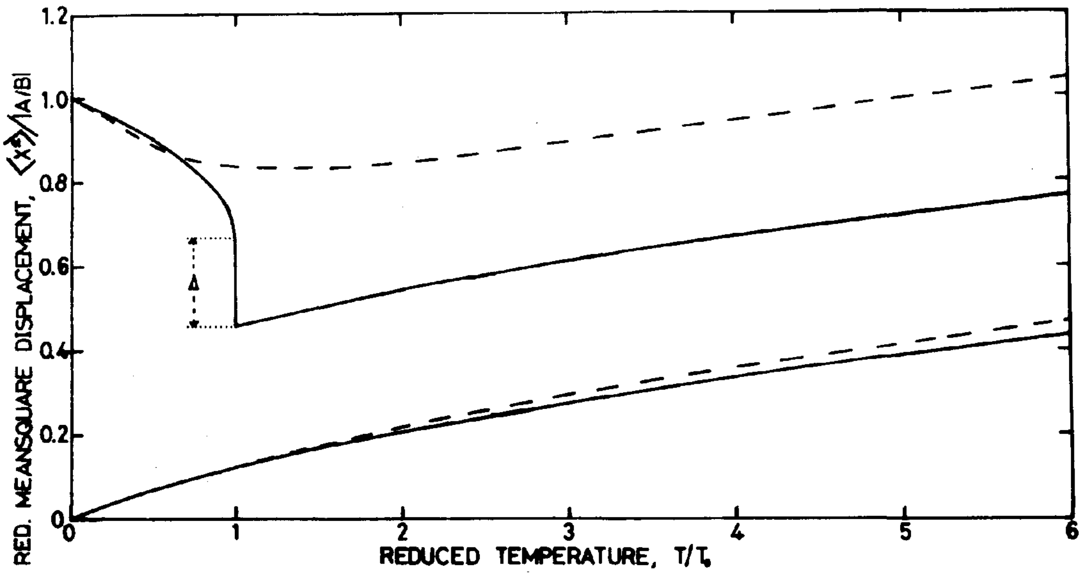


**Figure caption:**

Fig. 1 Reduced mean square displacement, $<X^2>/|A/B|$, for noninteracting anharmonic oscillators as function of reduced temperature, $T/T_0$. Upper curves: double well case, $A < 0$. Lower curves: single well case, $A > 0$. Solid lines give the self-consistent spin-oscillator approximation. Broken lines are the correct values, obtained by numerical integration of the Boltzman distribution. The gap size in the self-consistent approximation is $\Delta = 2/3 - (1 + \sqrt{3})/6$.

Fig. 1 shows the solutions (20) and (21) together with the correct numerical values, obtained by numerical integration of the Boltzmann distribution. The exact result in the double well case has a shallow dip with minimum slightly above $T_0$. Thus the spin-oscillator coupled model shows qualitative agreement with the exact statics, even in the case of a single oscillator. It is reasonable to assume that in the case of higher-dimensional interacting systems, where fluctuations are less important, the agreement will be still better.

It seems natural to try to use the approximation to account also for the dynamics. In order to do this it is necessary to construct a kinetic equation for the Ising variables. I hope to work out an extension in this direction.

**Interacting system:**

In the case of a $d$-dimensional interacting system ($dC > 0$) the analogue of (17) becomes

$$H_{\mathrm{E}} = \sum_{\ell} \{ \frac{1}{2} P_{\ell}^{2} + \frac{1}{2} (\mathrm{A} + 3BS_T^2 - 3B \langle Q^2 \rangle_T)\; Q_{\ell}^{2} - 2C \sum_{\alpha=1}^{d} Q_{\ell}\, Q_{\ell+u_\alpha}$$

$$- 2CS_T \sum_{\alpha=1}^{d} Q_{\ell}\, ( \varepsilon_{\ell+\boldsymbol{u}_\alpha} - 2\,\varepsilon_{\ell} + \varepsilon_{\ell-\boldsymbol{u}_\alpha} ) - 2\,CS_T^2 \sum_{\alpha=1}^{d} \varepsilon_{\ell}\, \varepsilon_{\ell+\boldsymbol{u}_\alpha} \} , \qquad (22)$$

where $\boldsymbol{u}_\alpha$ is the unit vector in the $\alpha$-direction, and we have used (11) and (15). The remaining $Q\epsilon$-interaction couples $Q$ to the discrete analogue of $\nabla^2 \epsilon$, which differes from zero only near a kink in the spin configuration. The formulation becomes similar to that of Mazenko and Sahni for the analogous field theoretic problem [10]. $H_{\mathrm{A}}$ is the sum of single-particle terms of the form (17c).

With the standard spatial Fourier transform,

$$H_{\mathrm{E}} = \sum_{\boldsymbol{q}} \{ \frac{1}{2} P_{-\boldsymbol{q}} P_{\boldsymbol{q}} + \frac{1}{2} \omega_{\boldsymbol{q}}^{2}(T)\, Q_{-\boldsymbol{q}} Q_{\boldsymbol{q}} - I_{\boldsymbol{q}}(T)\, Q_{-\boldsymbol{q}} Q_{\boldsymbol{q}} - CS_T^2 F_{\boldsymbol{q}}\, \varepsilon_{-\boldsymbol{q}} \varepsilon_{\boldsymbol{q}} \} , \qquad (23\mathrm{a})$$

where

$$F_{\boldsymbol{q}} = 2 \sum_{\alpha=1}^{d} \cos q_\alpha \; , \qquad (23\mathrm{b})$$

$$I_{\boldsymbol{q}} = - 2CS_T\, ( F_0 - F_{\boldsymbol{q}} ) \sim \boldsymbol{q}^2 \qquad (23\mathrm{c})$$

$$\omega_{\boldsymbol{q}}^2(T) = \omega_0^2(T) + 2C(F_0 - F_{\boldsymbol{q}}), \tag{23d}$$

and

$$\omega_0^2(T) = \begin{cases} 2BS_T^2\,, & S_T = S_0^2 - 3\langle Q^2\rangle_T \\ B(3\langle Q^2\rangle_T - S_0^2)\,, & S_T = 0. \end{cases} \tag{23e}$$

$H_{\mathrm{E}}$ is diagonalized by transformation to displace oscillator coordinates [11, 12],

$$\hat{Q}_{\boldsymbol{q}} = Q_{\boldsymbol{q}} - \frac{I_{\boldsymbol{q}}(T)}{\omega_{\boldsymbol{q}}^2(T)}\,\varepsilon_{\boldsymbol{q}} = Q_{\boldsymbol{q}} + S_T\frac{C(F_0 - F_{\boldsymbol{q}})}{BS_T^2 + C(F_0 - F_{\boldsymbol{q}})}\,\varepsilon_{\boldsymbol{q}}\,. \tag{24}$$

In the order-disorder limit, $A \ll -4dC$, this is very close to $Q_q$ for all $q$. Near the displacive limit, $4dC-A \ll 1$, it is approximately $X_q$, except for $q \ll 1$. $H_{\mathrm{E}}$ becomes

$$H_{\mathrm{E}} = \sum_{\boldsymbol{q}}\{\frac{1}{2}P_{-\boldsymbol{q}}P_{\boldsymbol{q}} + \frac{1}{2}\omega_{\boldsymbol{q}}^2(T)\,\hat{Q}_{-\boldsymbol{q}}\hat{Q}_{\boldsymbol{q}} - \frac{1}{2}J_{\boldsymbol{q}}(T)\,\varepsilon_{-\boldsymbol{q}}\varepsilon_{\boldsymbol{q}}\}\,, \tag{25}$$

where the total effective spin-spin interaction is

$$\begin{aligned} J_{\boldsymbol{q}}(T) &= [1 - N^{-1}\sum_{\boldsymbol{q}}]\frac{I_{\boldsymbol{q}}^2(T)}{\omega_{\boldsymbol{q}}^2(T)} + 2CS_T^2F_{\boldsymbol{q}} \\ &= 4B^2S_T^6\,[\,\omega_{\boldsymbol{q}}^{-2}(T) - N^{-1}\sum_{\boldsymbol{q}}\omega_{\boldsymbol{q}}^{-2}(T)\,]\,. \end{aligned} \tag{26}$$

The sum over $q$-space can be performed exactly for $d = 1$, and in the Debye approximation for $d > 1$.

The selfconsistency equation becomes

$$\langle Q_{-\boldsymbol{q}}\hat{Q}_{\boldsymbol{q}}\rangle = k_{\mathrm{B}}T/\omega_{\boldsymbol{q}}^2(T)\,, \tag{27}$$

or, with (23) and (24),

$$<Q^2>_T - S_T^2 N^{-1} \sum_{\boldsymbol{q}} \left[ \frac{2C(F_0 - F_{\boldsymbol{q}})}{\omega_0^2(<Q^2>_T) + 2C(F_0 - F_{\boldsymbol{q}})} \right]^2 < \varepsilon_{-\boldsymbol{q}} \varepsilon_{\boldsymbol{q}} >$$

$$= N^{-1} \sum_{\boldsymbol{q}} \left[ \frac{k_B T}{\omega_0^2(<Q^2>_T) + 2C(F_0 - F_{\boldsymbol{q}})} \right] , \tag{28}$$

which requires an estimate of the spin correlation function $< \epsilon_{-\boldsymbol{q}} \epsilon_{\boldsymbol{q}} >$ under the interaction $J_{\boldsymbol{q}}(T)$. In the limit $\omega_0^2(T) >> 8dC$ we can ignore the second term on the l. h. s. We have done this for $d = 1$, and obtained a solution which is qualitatively similar the non-interacting case.

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