A NEW MODEL OF A STRUCTURAL PHASE TRANSITION

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The dynamics of structural phase transitions is usually described by a model based on the Hamiltonian $H_1 = T_1+V_1$, $2T_1 = \sum_n p_n^2/m$,

$$V_1 = \sum_n \{ -Ay_n^2 + By_n^4 + C(y_n-y_{n-1})^2 \} , \qquad A,B,C > 0 .$$

$n=1,..,N$: particle number

y_n : displacement of the n-th particle $(y_0:=y_N)$

or on its generalization to more dimensions [1]. Although invariant under lattice translations $(y_n \to y_{n-1})$ and the lattice reflection $(y_n \to -y_{N-n})$ H_1 is not invariant under rigid translations $(y_n \to y_n+c)$ since it describes the motion of N interacting particles relative to a static lattice of infinite mass [2]. This motion has been discussed in various approximation schemes [1]; the most successful one seems to be the continuum version (= field theory) of [3].

The aim of this note is to generalize the above model so that the motion of all lattice constituents is included. The simplest model of this kind considers a system which is composed of two N-particle subsystems. The particles of each subsystem are assumed to form at any time a (slightly distorted) sublattice with lattice constant 1, but there is no restriction on the relative position of the two sublattices. The relative motion of the 2N particles is then governed by the Hamiltonian $H_2 = T_2 + V_2$, $2T_2 = p^2 + \sum_{hq} p_{hq}p_{h,-q}$,

$$V_2 = A(z) + \sum_{hq} B_q^h(z) z_q^h + \sum_{hh'qq'} C_{qq'}^{hh'}(z) z_q^h z_{q'}^{h'} + \text{cubic and quartic terms.}$$

$h=1,2$: index of the subsystem

$q=(2\pi/N)k$, $k=\text{integer}\neq 0$, $-N<2k<N$: wave vector $(\neq 0)$

$$p = [m_1m_2(m_1+m_2)N]^{-1/2} \sum_n (m_2p_n^1-m_1p_n^2)$$

$$z = [m_1m_2/(m_1+m_2)N]^{1/2} \sum_n (y_n^1-y_n^2)$$

} relative motion of the two rigid sublattices

$$p_q^h = (m_hN)^{-1/2} \sum_n e^{iqn} p_n^h$$

$$z_q^h = (m_h/N)^{1/2} \sum_n e^{iqn} y_n^h$$

} normal coordinates of the two subsystems

The potential V_2 can be obtained from an interaction V depending on the 2N positions x_n^h by expressing V as a function of the 2N-1 variables z and z_q^h, expanding this function into a Taylor series in the z_q^h's (but not in z) and truncating this series after the quartic terms. Because of this construction V_2 should approximate V within a cylinder C_ε containing all configurations for which $\sum_{hq} (z_q^h)^2 < \varepsilon$ holds.

Since V (and hence also V_2) is a real function and the z_q^h's commute the functions A,B,.. have to satisfy relations such as $A=A^*$, $B_q^h=B_{-q}^{h*}$, etc. Further relations, e.g.

$$A(z) = A(-z) = A(z+\zeta), \quad \zeta = [m_1 m_2 N/(m_1+m_2)]^{1/2} ,$$

$$B(z) = 0 ,$$

$$C_{qq'}^{hh'}(z) = C_{-q,-q'}^{hh'}(-z) = C_{qq'}^{hh'}(z+\zeta)\ e^{i(q'\delta_{h'1} - q\delta_{h1})} = 0 \text{ if } q+q'\neq 0 \text{ modulo } N ,$$

follow from the fact that V_2 is assumed to be invariant under the transformations

$$(1)\ z \to -z,\ z_q^h \to -z_{-q}^h \qquad (2)\ z \to z,\ z_q^h \to e^{-iq} z_q^h \qquad (3)\ z \to z+\zeta,\ z_q^h \to e^{-iq\delta_{h1}} z_q^h .$$

Using the relations $y_n^h = x_n^h - n$ one can show that the symmetry group of V_2 generated by the transformations (1)-(3) contains all transformations which can be generated by the transformations

$$(1')\ x_n^h \to x_n^h + c \qquad (2')\ x_n^h \to -x_n^h \qquad (3')\ x_n^h \to x_{n'}^h,\ (n \to n' : \text{permutation of } 1..N)$$

$$(4')\ x_n^h \to x_n^h + Ng_n^h ,\quad g_n^h \text{ integer}$$

and leave the cylinder C_ε invariant. The transformations (1')-(3') correspond to rigid motions and permutations of particles of the same kind and are therefore natural symmtries of any realistic potential V. The periodicity of V showing up in its invariance under the translations (4') is, on the other hand, only an approximate one and restricted to a certain part of the domain of V. The potential approximated by V_2 in C_ε is therefore not V but a potential $\bar{V}$ strictly invariant under (1')-(4') and approximating V within a region containing C_ε. The use of $\bar{V}$ instead of V means roughly speaking that periodic boundary conditions are introduced just from the beginning. As has been shown elsewhere [4] this procedure ensures that finite homomorphic images of space groups appear as symmetry groups of 'local' approximations such as the usual harmonic approximation or the series expansion considered here.

If V is a sum of short-range 2-body interactions the corresponding potential $\bar{V}$ can be obtained by periodic continuation of these functions. For

$$\bar{V} = V_{(1)} + V_{(2)} + W ,\quad V_{(h)} = 1/2 \sum_{n\neq 1} v_{(h)}(x_n^h - x_1^h) ,\quad W = \sum_{n1} w(x_n^1 - x_1^2)$$

$$v_{(h)}(x) = v_{(h)}(-x) = v_{(h)}(x+N)\ , \quad v_{(h)}(x) = 0 \ \text{ for } \ 3/2 < x < N - 3/2$$

$$W(x) = w(-x) = w(x+N)\ , \quad w(x) = 0 \ \text{ for } \ 1/2 < x < N - 1/2$$

and $|z| < 1$ one finds

$$A(z) = N \{ v_{(1)}(1) + v_{(2)}(1) + w(z/\zeta) \}$$

$$c^{hh'}_{q,-q}(z) = (m_h m_{h'})^{-1/2} \{ \delta_{hh'} 4\sin^2(q/2) v''_{(h)}(1) + (3\delta_{hh'} - 2)(1/2) w''(z/\zeta) \}$$

and similar expressions for the coefficients of the cubic and quartic terms.

The next step is to approximate the classical equations of motion obtained from H_2 by

$$d^2z/dt^2 = -A'(z)$$

$$d^2z^h_q/dt^2 = -\sum_{h'} \langle c^{hh'}_{q,-q}(z) \rangle z^h_q + \text{quadratic and cubic terms}$$

$\langle F(z) \rangle$ = time average for z being a solution of the first equation

and to look for semiclassical solutions of these equations. This program can be carried out for an interaction

$$w(x) = \gamma^2\{(\alpha+\cos 2\pi x)^2 - (\alpha-1)^2\} \quad \text{for } |x|<1/2\ , \quad 0 < \alpha < 1$$

yielding a double-well potential in each interval of length ζ and the corresponding periodic solutions of z $(0<|z|<\zeta)$. Because of the specific form of w the period of this motion, the Bohr-Sommerfeld integral needed for the determination of the allowed energies, and the average of the coefficients of the z^h_q's can be calculated by means of elliptic integrals [5]. For energies where z varies in one well only $\langle w'' \rangle$ is positive and the z^h_q's vibrate in the usual way since their motion is essentially determined by the positve definite dynamical matrix $\langle C \rangle$. If however the energy is so high that the quasiparticle with coordinate z is just able to pass the hump between the two wells and spends most of its time near $z=\zeta/2$ $\langle w'' \rangle$ is negative and the matrix $\langle C \rangle$ no more positive definite if q is sufficiently small. The motion of these z^h_q's is then stabilized by the quartic contribution of W since the cubic contribution of W has a vanishing average and the cubic and quartic contributions of the $V_{(h)}$'s are neglegted as it is done in the usual model. There exist then linear combinations of these z^h_q's which are (nearly) constant in time and resemble to the clusters found in the usual model.

References

[1] see e.g. H.Beck, J.Phys.C9(1976)33 and the references cited there

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