Conditions for Rotational Invariance of a Harmonic Lattice

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The conditions for rotational invariance of a Born–von Karman lattice model are re-examined. It is found that the Born–Huang conditions for rotational invariance are necessary but not sufficient. Some additional conditions are obtained which, together with the Born-Huang conditions, constitute a set of necessary and sufficient conditions.

I. INTRODUCTION

IT is well known that the force constants associated with a lattice medium must satisfy certain relationships in order for the potential energy to remain invariant under a coordinate transformation corresponding to a rigid motion of the medium. A set of such conditions has been given by Born and Huang[1] and repeated by Leibfried[2] and Maradudin *et al.*[3] in their comprehensive treatments of the subject of lattice dynamics. It has been suspected for some time that the Born-Huang conditions did not tell the complete story of invariance under rigid motion. One notable example has been the case of the Montroll-Potts-Rosenstock-Newell (MPRN)[4,5] lattice model, one of the first to include noncentral forces. If the lattice is infinite, this model satisfies the Born-Huang relationships, but has some unhealthy features: First, the long-wave approximation produces two different sets of relationships between the force constants and the elastic constants,[6] depending on whether one compares the potential energy or the equations of motion given by the lattice and continuum theories; and, second, a bounded lattice fails to satisfy the Born-Huang relationship of rotational invariance, even though the infinite lattice does. In a recent paper, Ludwig and Lengeler[7] suggested, as a method for restoring the rotational invariance of a bounded lattice, introducing some additional interactions near the surface. This, of course, does not correct the ambiguity regarding the force-constant–versus–elastic-constant relationship in the long-wave approximation.

In this paper, it is shown that the Born-Huang relationships, while necessary, are not sufficient for rotational invariance. They guarantee that the resultant force on any particle remains invariant under a small rotation, but do not guarantee that the same is true of the potential energy. Some additional relationships are obtained which, together with the Born-Huang relationships, form a set of necessary and sufficient conditions for rotational invariance, in the harmonic approximation. Similar conditions are, of course, needed for anharmonic lattices.

The new conditions are not satisfied by the MPRN model, either in its original form or as modified by Ludwig and Lengeler, both in the bulk and near the surface of a bounded lattice. This is because a small rotation produces a zero resultant force but a nonzero moment acting on every atom, and consequently, a nonzero change in potential energy.

A safe method for constructing a potential-energy function which is invariant under rigid motion is to write it as a function of invariant quantities, such as distances between atoms and angles formed by sets of three atoms. This has been done in two previous papers[8,9] in constructing models of simple cubic- and body-centered-cubic lattices including noncentral forces.

II. THE INVARIANCE CONDITIONS

We shall give a concise derivation of the complete set of necessary and sufficient conditions of invariance under rigid motion, including the Born-Huang conditions, after a remark regarding the contrast between bounded and unbounded lattices. In solving a problem for a bounded lattice region one may take one of two points of view. The first one is that taken by Ludwig and Lengeler,[7] namely, that a bounded lattice is an inhomogeneous medium with a discontinuity in the force constants near the surfaces. The second point of view is that the solution for the bounded lattice is one obtained for the unbounded lattice with the displacements satisfying certain constraints so that the bounded

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region of interest is not influenced by the motion of the atoms outside of it. The two points of view must, of course, give the same solution to a physical problem. It is the second point of view which is taken in the classical formulation of boundary-value problems in continuous media, as well as in our own formulation of boundary-value problems in lattices.[8] This observation allows us to confine our attention to an unbounded lattice and obtain conditions of invariance which will also be appropriate for a bounded region of this lattice.

The potential energy of a lattice Φ is assumed to be a function of the displacements $\mathbf{u}(lk)$, where l distinguishes the various lattice cells and k the different atoms in the unit cell. In the harmonic approximation, the function Φ is further assumed to be a quadratic function of the components of displacement, namely,

$$\Phi=\Phi_0+\sum_{l,k,\alpha}\Phi_\alpha(lk)u_\alpha(lk)+\tfrac{1}{2}\sum_{\substack{l,k,\alpha\\ l',k',\beta}}\Phi_{\alpha\beta}(lk,l'k')u_\alpha(lk)u_\beta(l'k'). \quad (1)$$

In Eq. (1), Φ_0 is the equilibrium potential energy and

$$\Phi_\alpha(lk)=\partial\Phi/\partial u_\alpha(lk)\,|_0,\qquad \Phi_{\alpha\beta}(lk,l'k')=\partial^2\Phi/\partial u_\alpha(lk)\partial u_\beta(l'k')\,|_0, \quad (2)$$

where the subscript 0 means that the derivatives are evaluated in the equilibrium configuration. From the second of Eqs. (2) we see that $\Phi_{\alpha\beta}(lk,l'k')$ satisfies the symmetry condition

$$\Phi_{\alpha\beta}(lk,l'k')=\Phi_{\beta\alpha}(l'k',lk). \quad (3)$$

In addition, the first-order constant $\Phi_\alpha(lk)$ is seen to be equal to the negative of the force acting in the α direction on the atom (lk) in the equilibrium configuration, which must be zero, i.e.,

$$\Phi_\alpha(lk)=0. \quad (4)$$

The invariance conditions further express the requirement that the potential energy must remain invariant under a coordinate transformation corresponding to a rigid displacement of the lattice, while the forces acting on each atom must transform as vectors.

It may readily be seen that a necessary and sufficient condition for invariance under translation is that the force acting on each atom as a result of an arbitrary translation be zero. The force components are given by

$$F_\alpha(lk)=-\frac{\partial\Phi}{\partial u_\alpha(lk)}=-\sum_{l',k',\beta}\Phi_{\alpha\beta}(lk,l'k')u_\beta(l'k') \quad (5)$$

and they are zero for arbitrary $u_\beta(l'k')=\epsilon_\beta$, where the vector ϵ_β is constant, if and only if

$$\sum_{l',k'}\Phi_{\alpha\beta}(lk,l'k')=0. \quad (6)$$

Using Eq. (6) we can write the potential energy and the force components in the form

$$\Phi=\Phi_0+\tfrac{1}{2}\sum_{\substack{l,k,\alpha\\ l',k',\beta}}\Phi_{\alpha\beta}(lk,l'k')u_\alpha(lk,l_0k_0)u_\beta(l'k',l_0k_0),$$
$$F_\alpha(lk)=-\sum_{l',k',\beta}\Phi_{\alpha\beta}(lk,l'k')u_\beta(l'k',lk), \quad (7)$$

where $u_\alpha(lk,l_0k_0)$ denote the components of relative displacements between the atoms (lk) and (l_0k_0); i.e.,

$$u_\alpha(lk,l_0k_0)=u(lk)-u(l_0k_0) \quad (8)$$

and (l_0k_0) is an arbitrary reference atom.

Let us now assume that the whole lattice undergoes a small rotation about a position of equilibrium; hence, the relative displacements are given by

$$u_\alpha(lk,l_0k_0)=\sum_\beta\omega_{\alpha\beta}X_\beta(lk,l_0k_0), \quad (9)$$

where $\omega_{\alpha\beta}$ are the components of an antisymmetric tensor and

$$X_\beta(lk,l_0k_0)=X_\beta(lk)-X_\beta(l_0k_0) \quad (10)$$

denotes the relative positions of the two atoms. It is again necessary that the resultant force on each atom due to this rotation be zero. But this condition is no longer sufficient because the atoms may be acted upon by moments in addition to forces. If these moments have a nonzero resultant per unit cell, then they will result in a nonzero change in potential energy after a small rotation described by Eqs. (9) and (10). The requirement of zero forces due to an arbitrary small rotation yields the well-known conditions[1–3]

$$\sum_{l'k'}[\Phi_{\alpha\beta}(lk,l'k')X_\gamma(lk,l'k')-\Phi_{\alpha\gamma}(lk,l'k')X_\beta(lk,l'k')]=0. \quad (11)$$

The requirement of zero change in potential energy yields some additional invariance conditions, namely,

$$\sum_{\substack{l,k\\ l',k'}}\{[\Phi_{\alpha\gamma}(lk,l'k')X_\beta(lk,l_0k_0)-\Phi_{\beta\gamma}(lk,l'k')X_\alpha(lk,l_0k_0)]X_\delta(l'k',l_0k_0)+[\Phi_{\beta\delta}(lk,l'k')X_\alpha(lk,l_0k_0)-\Phi_{\alpha\delta}(lk,l'k')X_\beta(lk,l_0k_0)]\times X_\gamma(l'k',l_0k_0)\}=0. \quad (12)$$

These conditions are obtained by writing the potential energy corresponding to the displacements given in Eq. (9), and setting the coefficients of each product $\omega_{\alpha\beta}\omega_{\gamma\delta}$ equal to zero. It may be ascertained that these conditions are independent of the Born-Huang conditions given in Eq. (11). Therefore, the Born-Huang conditions are not sufficient for rotational invariance.

It is of interest to consider the class of lattice models

which satisfy the additional symmetry relationship

$$\Phi_{\alpha\beta}(lk,l'k')=\Phi_{\beta\alpha}(lk,l'k'). \quad (13)$$

Such models are, for example, all central-force models and all models in which each atom is a center of cubic symmetry. In this case, the potential energy may be written in the form

$$\Phi=\Phi_0+\tfrac{1}{4}\sum_{\substack{l,k,\alpha\\ l',k',\beta}}\Phi_{\alpha\beta}(lk,l'k')u_\alpha(lk,l'k')u_\beta(l'k',lk). \quad (14)$$

The condition of zero forces after a small rotation [Eq. (11)] remains unchanged. However, instead of the condition (12) we now obtain the condition

$$\sum_{l',k',k}\{[\Phi_{\alpha\gamma}X_\beta-\Phi_{\beta\gamma}X_\alpha]X_\delta +[\Phi_{\beta\delta}X_\alpha-\Phi_{\alpha\delta}X_\beta]X_\gamma\}=0, \quad (15)$$

where the identification $(lk,l'k')$ is the same for all values of Φ_{ij} and X_i and has been omitted. The index of summation l has been suppressed before arriving at Eq. (15) because all lattice cells in an unbounded lattice give an identical contribution.

We now consider the case of a monatomic cubic lattice, which includes the MPRN model. In this case, the conditions (15) are further simplified because the coefficients of all the cross products of the components $\omega_{\alpha\beta}$ are zero. The remaining conditions are

$$\sum_{l',k',k}[\Phi_{\alpha\alpha}X_\beta{}^2+\Phi_{\beta\beta}X_\alpha{}^2-2\Phi_{\alpha\beta}X_\alpha X_\beta]=0 \quad (16)$$

and they are obtained from the requirement that the coefficients of the squares of $\omega_{\alpha\beta}$ be zero.

III. THE MPRN MODEL

The MPRN model is a model of a simple cubic lattice which, in addition to central-force interactions, includes shear-force interactions.[4,5] If l_i, l_j, and l_k denote a lattice position in a monatomic lattice and i, j, k the corresponding axes, then the force constants corresponding to these shear-force interactions are

$$\Phi_{\alpha\alpha}(l_\beta, l_\beta\pm1)=\Phi_{\alpha\alpha}(l_\beta,l_\beta)=\gamma, \quad \alpha\neq\beta \quad (17)$$

while all the other noncentral-force constants are zero. For simplicity, only that one of the indices l_i, l_j, l_k which is different for a pair of interacting atoms has been included in Eq. (17).

All the invariance conditions are obviously satisfied by the central-force constants. The noncentral-force constants satisfy the conditions (6) and (11) if the lattice is unbounded. They violate the conditions (11) near the surface of a bounded lattice, and conditions (16) everywhere, since the quantity inside the bracket of Eq. (16) is always positive. The revised model of Ludwig and Lengeler[7] contains some additional noncentral-force interactions corresponding to force constants

$$\Phi_{ik}(l_i, l_i\pm1)=\pm\gamma/2 \quad (18)$$

which are associated with atoms at the boundary, for which $l_k=0$. With these additional force constants, the conditions (11) are satisfied for a semi-infinite lattice. However, the conditions (16) are, of course, still violated, and hence the model is not rotationally invariant.

IV. CONSTRUCTION OF ROTATIONALLY INVARIANT MODELS

It is in principle possible to verify the rotational invariance of an arbitrary lattice model using the relationships given in the preceding sections. However, a more convenient method for constructing an invariant model is by writing the potential energy as a function of invariant quantities. Recently, Keating[10] used inner products of vectors of displacement and equilibrium positions in obtaining invariant contributions to the potential energy. Other invariant quantities are the distances between atoms and the angles formed by sets of three atoms. Interactions proportional to changes of distances and angles are physically plausible and do not depend on the orientation of the coordinate axes. Such interactions were included in two papers[8,9] in constructing models of simple cubic and body-centered-cubic lattices. Only nearest- and next-nearest-layer interactions were included in these models. Longer range interactions may be introduced in two ways: by considering sets of farther removed atoms, and by introducing in the potential-energy difference approximations to the space derivatives of these distance and angle changes, with the differences taken between lattice points. These additional terms would be analogous to strain-gradient terms, such as those included in the Cosserat[11] "couple-stress" theory which has recently been revived and extended by Mindlin and Tiersten[12] and by Toupin.[13]

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