# Conservation of Crystal Momentum

Associated with every symmetry of a Hamiltonian is a conservation law. The Hamiltonian of a crystal possesses a symmetry, closely related to the translational symmetry of the Bravais lattice, that leads to a very general conservation law known as the conservation of *crystal momentum*. Consider the Hamiltonian:

$$H = \sum_{\mathbf{R}} \frac{\mathbf{P(R)}^2}{2M} + \frac{1}{2} \sum_{\mathbf{R}\mathbf{R'}} \phi[\mathbf{R} + \mathbf{u(R)} - \mathbf{R'} - \mathbf{u(R')}]$$
$$+ \sum_{i=1}^{n} \frac{p_i^2}{2m_i} + \frac{1}{2} \sum_{i \neq j} v_{ij}(\mathbf{r}_i - \mathbf{r}_j)$$
$$+ \sum_{\mathbf{R}, i} w_i(\mathbf{r}_i - \mathbf{R} - \mathbf{u(R)}). \tag{M.1}$$

The first two terms are the Hamiltonian of the ion cores. Note that we have not made the harmonic approximation,[1] but have represented the ion-ion interaction by a general sum of pair potentials.[2] The next two terms are the Hamiltonian of $n$ additional particles, and the last term gives the interaction of these particles with the ions. To keep the discussion general, we do not specify the nature of the $n$ particles, though the following possibilities are of interest:

1. If $n = 0$, we are discussing an isolated insulating crystal.
2. If $n = 1$, we can apply the discussion to the scattering of a single particle, say a neutron, by an insulating crystal.
3. If we wish to discuss an isolated metal, we can let the $n$ particles be the conduction electrons ($n \approx 10^{23}$), in which case all the $m_i$ would be the electron mass $m$ and the $v_{ij}(\mathbf{r})$ would all be the same function of $\mathbf{r}$.
4. We can let the $n$ particles be the conduction electrons and an incident external particle, if we wish to discuss neutron scattering by a metal.

Note that the Hamiltonian (M.1) is invariant under the uniform translation:

$$\mathbf{r}_i \to \mathbf{r}_i + \mathbf{r}_0, \qquad i = 1, \dots, n,$$
$$\mathbf{u(R)} \to \mathbf{u(R)} + \mathbf{r}_0, \qquad \text{for all } \mathbf{R}. \tag{M.2}$$

This familiar symmetry leads to conservation of the total *momentum* of the ions and particles, and is not the symmetry we are interested in. *Crystal momentum* conservation arises from the fact that when the translation vector $\mathbf{r}_0$ is a Bravais lattice vector $\mathbf{R}_0$, then it is possible to simulate the translation of the ions by a simple permutation of the

[1] We shall, however, be introducing operators defined in terms of the phonon operators $a$ and $a^\dagger$ (Appendix L). These will not be well defined, if the system is so unlike a harmonic crystal with Bravais lattice $\{\mathbf{R}\}$ as to lie in a completely different Hilbert space. Thus although the procedure we shall follow makes formal sense for any system (e.g., a liquid, or a crystal with a Bravais lattice different from that specified by the $\{\mathbf{R}\}$), the conclusions can be meaningfully applied only to the case of a crystal with the Bravais lattice $\{\mathbf{R}\}$.

[2] Even the assumption of pair interactions is unnecessary. It is made only to give $H$ a concrete form that is not too complex to obscure the argument.

$$\mathbf{r}_i \to \mathbf{r}_i + \mathbf{R}_0, \qquad i = 1, \dots, n,$$
$$\mathbf{u(R)} \to \mathbf{u(R - R}_0), \qquad P(\mathbf{R}) \to P(\mathbf{R - R}_0), \quad \text{for all } \mathbf{R}, \tag{M.3}$$

as can be verified explicitly by direct substitution into (M.1). To emphasize the difference between symmetry (M.2) (with $\mathbf{r}_0 = \mathbf{R}_0$) and symmetry (M.3), consider the following two symmetry-breaking terms one might add to the Hamiltonian (M.1):

1. We might add a term:

$$\frac{1}{2} K \sum_{\mathbf{R}} [\mathbf{u(R)}]^2, \tag{M.4}$$

which ties each ion to its equilibrium site with a harmonic spring. This term destroys the translational symmetry (M.2) of the Hamiltonian, and momentum will not be conserved in its presence. However, the term (M.4) is invariant under the permutation symmetry (M.3), so its addition will not destroy the conservation of crystal momentum.

2. Suppose, on the other hand, we alter the Hamiltonian (M.1) so as to maintain the translational symmetry but destroy the permutation symmetry. We might, for example, give each ion a different mass, replacing the ionic kinetic-energy term by:

$$\sum_{\mathbf{R}} \frac{\mathbf{P(R)}^2}{2M(\mathbf{R})}. \tag{M.5}$$

The resulting Hamiltonian will continue to be invariant under the spatial translation (M.2) so total momentum will continue to be conserved. However, it will no longer be invariant under the permutation (M.3), and *crystal* momentum will not be conserved.

Of the two conservation laws, crystal momentum conservation is by far the more important. In practice, crystals are not free to recoil as a whole, and even if they were, the minute changes in the total momentum of the entire crystal produced by the scattering of a single neutron would be impossible to measure directly.

## DERIVATION OF THE CONSERVATION LAW

To derive the conservation law implied by the symmetry (M.3) we must describe the quantum-mechanical operators that produce this transformation. That part of the transformation affecting the particle coordinates, $\mathbf{r}_i \to \mathbf{r}_i + \mathbf{R}_0$, is effected by the particle translational operator $T_{\mathbf{R}_0}$ (see Chapter 8). It is a fundamental result of quantum mechanics that this transformation can be written as a unitary transformation involving the total momentum operator for the particles:[3]

$$\mathbf{r}_i \to \mathbf{r}_i + \mathbf{R}_0 = T_{\mathbf{R}_0} \mathbf{r}_i T_{\mathbf{R}_0}{}^{-1} = e^{(i/\hbar)\mathbf{P} \cdot \mathbf{R}_0} \mathbf{r}_i \, e^{-(i/\hbar)\mathbf{P} \cdot \mathbf{R}_0},$$
$$\mathbf{P} = \sum_{i=1}^{n} \mathbf{P}_i. \tag{M.6}$$

[3] See, for example, K. Gottfried, *Quantum Mechanics*, vol. I, W. A. Benjamin, Menlo Park, Calif., 1966, p. 245.

In addition, we need the operator that produces the transformation (M.3) on the ionic variables. Crystal momentum conservation takes on a simple form primarily because this transformation has a structure very much like Eq. (M.6):

$$\mathbf{u}(\mathbf{R}) \to \mathbf{u}(\mathbf{R} - \mathbf{R}_0) = \mathfrak{I}_{\mathbf{R}_0}\,\mathbf{u}(\mathbf{R})\,\mathfrak{I}_{\mathbf{R}_0}^{-1} = e^{i\mathcal{K}\cdot\mathbf{R}_0}\,\mathbf{u}(\mathbf{R})\,e^{-i\mathcal{K}\cdot\mathbf{R}_0},$$
$$\mathbf{P}(\mathbf{R}) \to \mathbf{P}(\mathbf{R} - \mathbf{R}_0) = \mathfrak{I}_{\mathbf{R}_0}\,\mathbf{P}(\mathbf{R})\,\mathfrak{I}_{\mathbf{R}_0}^{-1} = e^{i\mathcal{K}\cdot\mathbf{R}_0}\,\mathbf{P}(\mathbf{R})\,e^{-i\mathcal{K}\cdot\mathbf{R}_0}, \qquad (M.7)$$

The operator $\mathcal{K}$ is not related in any way to the total momentum operator $\mathbf{P} = \sum\mathbf{P}(\mathbf{R})$ for the ions, but is specified[4] by taking the eigenstates of $\mathcal{K}$ to be the eigenstates of the harmonic part of the ion-ion Hamiltonian, and its eigenvalue in a state with phonon occupation numbers $n_{\mathbf{k}s}$ to be given by

$$\mathcal{K}|\{n_{\mathbf{k}s}\}\rangle = \left(\sum_{\mathbf{k}s}\mathbf{k}n_{\mathbf{k}s}\right)|\{n_{\mathbf{k}s}\}\rangle. \qquad (M.8)$$

To verify that the operator $\mathcal{K}$ defined by (M.8) does produce the transformation (M.7), we must use the representation (L.14) that gives $\mathbf{u}(\mathbf{R})$ and $\mathbf{P}(\mathbf{R})$ in terms of the oscillator raising and lowering operators for each normal mode:

$$\mathbf{u}(\mathbf{R}) = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}s}\sqrt{\frac{\hbar}{2M\omega_s(\mathbf{k})}}\,(a_{\mathbf{k}s} + a^\dagger_{-\mathbf{k}s})e^{i\mathbf{k}\cdot\mathbf{R}}\,\boldsymbol{\epsilon}_s(\mathbf{k}). \qquad (M.9)$$

(We consider explicitly only the $\mathbf{u}(\mathbf{R})$. The argument for the $\mathbf{P}(\mathbf{R})$ is virtually the same.) Since the only operators in (M.9) are $a_{\mathbf{k}s}$ and $a^\dagger_{-\mathbf{k}s}$, we have

$$e^{i\mathcal{K}\cdot\mathbf{R}_0}\,\mathbf{u}(\mathbf{R})\,e^{-i\mathcal{K}\cdot\mathbf{R}_0}$$
$$= \frac{1}{\sqrt{N}}\sum_{\mathbf{k}s}\sqrt{\frac{\hbar}{2M\omega_s(\mathbf{k})}}\,(e^{i\mathcal{K}\cdot\mathbf{R}_0}a_{\mathbf{k}s}e^{-i\mathcal{K}\cdot\mathbf{R}_0} + e^{i\mathcal{K}\cdot\mathbf{R}_0}a^\dagger_{-\mathbf{k}s}e^{-i\mathcal{K}\cdot\mathbf{R}_0})e^{i\mathbf{k}\cdot\mathbf{R}}\,\boldsymbol{\epsilon}_s(\mathbf{k}). \qquad (M.10)$$

We will therefore have established (M.7) when we prove that

$$e^{i\mathcal{K}\cdot\mathbf{R}_0}a_{\mathbf{k}s}e^{-i\mathcal{K}\cdot\mathbf{R}_0} = e^{-i\mathbf{k}\cdot\mathbf{R}_0}a_{\mathbf{k}s},$$
$$e^{i\mathcal{K}\cdot\mathbf{R}_0}a^\dagger_{-\mathbf{k}s}e^{-i\mathcal{K}\cdot\mathbf{R}_0} = e^{-i\mathbf{k}\cdot\mathbf{R}_0}a^\dagger_{-\mathbf{k}s}, \qquad (M.11)$$

for substitution of (M.11) into (M.10) reduces it back to the form (M.9) with $\mathbf{R}$ replaced by $\mathbf{R} - \mathbf{R}_0$.

Both results in (M.11) will follow if we can establish the single identity:

$$e^{i\mathcal{K}\cdot\mathbf{R}_0}a^\dagger_{\mathbf{k}s}e^{-i\mathcal{K}\cdot\mathbf{R}_0} = e^{i\mathbf{k}\cdot\mathbf{R}_0}a^\dagger_{\mathbf{k}s}, \qquad (M.12)$$

for the first of (M.11) is just the adjoint of (M.12) and the second follows from letting $\mathbf{k} \to -\mathbf{k}$. Equation (M.12) will be established if we can demonstrate that the operators on both sides of the equation have the same effect on a complete set of states, for they will then have the same effect on any linear combination of states from the complete set, and thus on any state whatsoever. We again choose the complete set to be the eigenstates of the harmonic Hamiltonian. The operator $a^\dagger_{\mathbf{k}s}$ being an oscillator-

---

4 An operator is defined by giving a complete set of eigenstates and the corresponding eigenvalues, since any state can be written as a linear combination of eigenstates. Note that here the subtle assumption that the solid is actually crystalline with Bravais lattice {R} appears; if it were not, its states could not be written as linear combinations of eigenstates of a harmonic crystal with Bravais lattice {R}.

raising operator for the $\mathbf{k}s$ normal mode, simply acts on a state with a particular set of phonon occupation numbers to produce (to within a normalization constant) a state in which the occupation number for the $\mathbf{k}s$ normal mode is increased by one, and all other occupation numbers remain the same. We may, to begin with, write

$$e^{i\mathcal{K}\cdot\mathbf{R}_0}a^\dagger_{\mathbf{k}s}e^{-i\mathcal{K}\cdot\mathbf{R}_0}|\{n_{\mathbf{k}s}\}\rangle = \exp\left(-i\sum_{\mathbf{k}'s}\mathbf{k}'n_{\mathbf{k}'s}\cdot\mathbf{R}_0\right)e^{i\mathcal{K}\cdot\mathbf{R}_0}a^\dagger_{\mathbf{k}s}|\{n_{\mathbf{k}s}\}\rangle, \qquad (M.13)$$

which simply exploits (M.8). Since the state $a^\dagger_{\mathbf{k}s}|\{n_{\mathbf{k}s}\}\rangle$ differs from $|\{n_{\mathbf{k}s}\}\rangle$ only in that the occupation number of mode $\mathbf{k}s$ is increased by one, it will also be an eigenstate of $\mathcal{K}$ with eigenvalue $\sum\mathbf{k}'n_{\mathbf{k}'s} + \mathbf{k}$. Therefore every term in the eigenvalue of $e^{-i\mathcal{K}\cdot\mathbf{R}_0}$ cancels the corresponding term in the eigenvalue of $e^{i\mathcal{K}\cdot\mathbf{R}_0}$ except for the single extra term $e^{i\mathbf{k}\cdot\mathbf{R}_0}$, and we have:

$$\exp\left(-i\sum_{\mathbf{k}'s}\mathbf{k}'n_{\mathbf{k}'s}\cdot\mathbf{R}_0\right)e^{i\mathcal{K}\cdot\mathbf{R}_0}a^\dagger_{\mathbf{k}s}|\{n_{\mathbf{k}s}\}\rangle = e^{i\mathbf{k}\cdot\mathbf{R}_0}a^\dagger_{\mathbf{k}s}|\{n_{\mathbf{k}s}\}\rangle. \qquad (M.14)$$

Equations (M.13) and (M.14) establish (M.12), and therefore $\mathcal{K}$ gives the desired transformation. The operator $\hbar\mathcal{K}$ is called the crystal momentum operator.

## APPLICATIONS

We illustrate the workings of crystal momentum conservation in several cases:

**1. Isolated Insulator** If only the ions are present, then the invariance (M.3) implies that the Hamiltonian commutes with the operator $e^{i\mathcal{K}\cdot\mathbf{R}_0}$, since

$$e^{i\mathcal{K}\cdot\mathbf{R}_0}H(\{\mathbf{u}(\mathbf{R}),\mathbf{P}(\mathbf{R})\})e^{-i\mathcal{K}\cdot\mathbf{R}_0} = H(\{\mathbf{u}(\mathbf{R}-\mathbf{R}_0),\mathbf{P}(\mathbf{R}-\mathbf{R}_0)\}) \equiv H,$$
$$\text{or} \quad e^{i\mathcal{K}\cdot\mathbf{R}_0}H = He^{i\mathcal{K}\cdot\mathbf{R}_0}. \qquad (M.15)$$

This means that the operator $\mathfrak{I}_{\mathbf{R}_0} = e^{i\mathcal{K}\cdot\mathbf{R}_0}$ is a constant of the motion; i.e., if the crystal is in an eigenstate of $\mathfrak{I}_{\mathbf{R}_0}$ at time $t = 0$, it will remain in an eigenstate at all subsequent times. In particular, suppose that the crystal is in an eigenstate of the harmonic Hamiltonian at $t = 0$ with phonon occupation numbers $n_{\mathbf{k}s}$. Because the full Hamiltonian is not harmonic this will not be a stationary state. However, crystal momentum conservation requires that it remain an eigenstate of $\mathfrak{I}_{\mathbf{R}_0}$ for all Bravais lattice vectors $\mathbf{R}_0$. This means that the state at future times can only be a linear combination of eigenstates of the harmonic Hamiltonian with phonon occupation numbers $n'_{\mathbf{k}s}$ leading to the same eigenvalue of $\mathfrak{I}_{\mathbf{R}_0}$ as the original state:

$$\exp(i\sum\mathbf{k}n'_{\mathbf{k}s}\cdot\mathbf{R}_0) = \exp(i\sum\mathbf{k}n_{\mathbf{k}s}\cdot\mathbf{R}_0). \qquad (M.16)$$

Since this must hold for *arbitrary* Bravais lattice vectors $\mathbf{R}_0$ (the $\mathfrak{I}_{\mathbf{R}_0}$ commute with one another for different $\mathbf{R}_0$) we have

$$\exp\{i\sum(\mathbf{k}n'_{\mathbf{k}s} - \mathbf{k}n_{\mathbf{k}s})\cdot\mathbf{R}_0\} = 1 \quad \text{for all } \mathbf{R}_0, \qquad (M.17)$$

which requires that

$$\sum\mathbf{k}n_{\mathbf{k}s} = \sum\mathbf{k}n'_{\mathbf{k}s} + \text{reciprocal lattice vector}. \qquad (M.18)$$

Thus the total phonon wave vector in an anharmonic crystal is conserved to within an additive reciprocal lattice vector.

**Scattering of a Neutron by an Insulator** Suppose that at the start of the experiment the crystal is in an eigenstate of the harmonic Hamiltonian with phonon occupation numbers $n_{\mathbf{k}s}$ and the neutron is in a state with real momentum $\mathbf{P}$, satisfying:

$$T_{\mathbf{R}_0}\psi(\mathbf{r}) = e^{(i/\hbar)\mathbf{p}\cdot\mathbf{R}_0}\psi(\mathbf{r}) \qquad (\text{i.e., } \psi(\mathbf{r}) = e^{(i/\hbar)\mathbf{p}\cdot\mathbf{R}_0}), \qquad (\text{M.19})$$

where $T_{\mathbf{R}_0}$ is the neutron translation operator. The invariance of the total neutron-ion Hamiltonian under (M.3) implies that the product of the neutron translation and ion permutation operators commutes with $H$ for any $\mathbf{R}_0$:

$$[T_{\mathbf{R}_0}\mathfrak{I}_{\mathbf{R}_0}, H] = 0. \qquad (\text{M.20})$$

In the initial state $\Phi$ we have:

$$T_{\mathbf{R}_0}\mathfrak{I}_{\mathbf{R}_0}\Phi = \exp\left[i(\mathbf{p}/\hbar + \Sigma\mathbf{k}n_{\mathbf{k}s})\cdot\mathbf{R}_0\right]\Phi, \qquad (\text{M.21})$$

and therefore subsequent states must continue to be eigenstates with the same eigenvalue. They can therefore be represented as linear combinations of states in which the neutron has momentum $\mathbf{p}'$ and the crystal has occupation numbers $n'_{\mathbf{k}s}$ with the restriction that

$$\mathbf{p}' + \hbar\sum{}'\mathbf{k}n'_{\mathbf{k}s} = \mathbf{p} + \hbar\sum{}'\mathbf{k}n_{\mathbf{k}s} + \hbar \times \text{reciprocal lattice vector.} \qquad (\text{M.22})$$

Thus *the change in the momentum of the neutron must be balanced by a change in the crystal momentum[5] of the phonons, to within an additive reciprocal lattice vector times $\hbar$.*

**Isolated Metal** If the particles are conduction electrons then we can consider at $t = 0$ a state in which the electrons are in a specified set of Bloch levels. Now each Bloch level (see Eq. (8.21)) is an eigenstate of the electron translation operator:

$$T_{\mathbf{R}_0}\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{R}_0}\psi_{n\mathbf{k}}(\mathbf{r}). \qquad (\text{M.23})$$

If, in addition, the crystal is in an eigenstate of the harmonic Hamiltonian at $t = 0$, then the combined electron translation and ion permutation operator $T_{\mathbf{R}_0}\mathfrak{I}_{\mathbf{R}_0}$ will have the eigenvalue

$$\exp\left[i(\mathbf{k}_e + \Sigma\mathbf{k}n_{\mathbf{k}s})\cdot\mathbf{R}_0\right]. \qquad (\text{M.24})$$

where $\mathbf{k}_e$ is the sum of the electronic wave vectors of all the occupied Bloch levels (i.e., $\hbar\mathbf{k}_e$ is the total electronic crystal momentum). Since this operator commutes with the electron-ion Hamiltonian, the metal must remain in an eigenstate at all subsequent times. Therefore *the change in the total electronic crystal momentum must be compensated for by a change in the total ionic crystal momentum to within an additive reciprocal lattice vector.*

1. **Scattering of a Neutron by a Metal** In the same way, we can deduce that when neutrons are scattered by a metal, the change in the neutron momentum must be

balanced by a change in the total crystal momentum of the electrons and ions, to within an additive reciprocal lattice vector times $\hbar$. Neutrons, however, interact only weakly with electrons, and in practice it is only the lattice crystal momentum that changes. This case is therefore essentially the same as case 2. Note, however, that X rays do interact strongly with electrons, so crystal momentum can be lost to the electronic system in X-ray scattering.

[5] The eigenvalue $\hbar\Sigma\mathbf{k}n_{\mathbf{k}s}$ of the crystal momentum operator $\hbar\mathfrak{K}$, is called the crystal momentum. cf. page 472).