**Conservation of Crystal Momentum**

This applies to more than just the free e and free ions. We can add interactions between electrons and interactions between electrons and ions. But I guess I’ll put this here, in the free file anyway. So the periodic structure of a crystal endows it with a sort of translational symmetry. And associated with any symmetry of the Hamiltonian/Lagrangian is a conservation law. Since the symmetry has to do with translation, we might suspect that the conservation law has to do with momentum, and we’d be right. But it’s a restricted kind of conservation of momentum. So consider the following Hamiltonian,



If we take all the electrons and shift them forward by a lattice vector **a**, and simultaneously replace all the ionic displacements **x**(**R**) by **x**(**R** – **a**), and ionic momenta **P**(**R**) by **P**(**R**-**a**), the Hamiltonian will remain invariant.



Note it wouldn’t have been invariant had we a Hamiltonian where Mion were R-dependent, though this would still have preserved overall translational momentum. However we would still have crystal momentum conservation if we had a single-particle ionic potential V = (k/2)ΣRx(R)2. Okay well now we need the operators which effectuate this transformation. Apropos the electrons, this is:



What about for the ions? Turns out we want something similar. Let the lattice be in some state with specified phonon occupation numbers |{nq}>. Then define the operator,



which is sort of like a crystal momentum operator. Then we can say,



And the product will be the total transformation operator.



Let’s work out the action of Ti on the creation the lattice x and p operators. So these are:



It suffices to work out the action of Ti on the creation/annihilation operators. So let’s do that. We’ll implicitly act on a random eigenstate of the free Hamiltonian |{nq}>, which suffices because any arbitrary state is simple a linear combination of such eigenstates. So,



and,



So altogether we have



Now let’s see what happens when we operate on x,



And we’ll get similar result for **(R)**. So now we know T = TiTe commutes with H. This means that if we’re in an eigenstate |λ> of these operators, with eigenvalue λ, then as time evolves we will continue to remain in an eigenstate (not *necessarily* the same one), with the same eigenvalue (see Quantum Mechanics/Foundations/General Consequences). Consider starting off in a state:



where |{niki}> is a many-body Bloch eigenstate comprising a bunch of electrons, and |{nq}> an eigenstate of the ion Hamiltonian comprising a bunch of phonon occupation numbers. This is an eigenstate of T, since,



So this means as time evolves, we must have:



So one possibility is:



where k´i, n´q are crystal momentum, and crystal momentum occupation numbers at some later time, say after some collision between electrons and phonons or electrons with electrons, or phonons with phonons, etc. This would be a so-called ‘normal’ process. But the most general possibility is:



where **G** is any reciprocal lattice vector, since **G**·**a** = 2πm, for some m. So crystal momentum is *almost* preserved during collisions between these particles – just up to a reciprocal lattice vector. When **G** ≠ 0, this is called Umklapp scattering, or U-process. Should note that **k** and **q** are restricted to the 1st BZ, and **G** is the reciprocal lattice vector that makes this possible. Here’s a picture I’m probably going to use ad infinitum. It shows two electrons’ orange k-vectors, undergoing a collision. They are both going rightwards. But after the collision, we can see they actually end up going to the left (well at least it’s plausible they’re both going to the left – all that’s certain is the sum of the final k-vectors must end up at the tip of the blue arrow).

A diagram of a complex geometry

Description automatically generated with medium confidence

I read somewhere that during any such collision where a **G** is generated, -**G** crystal momentum gets absorbed by the entire lattice itself. And if you were to properly include the *sliding*/*translational* d.o.f. (rather than just the oscillatory d.o.f.) of the lattice, which would be described by a state with no phonon occupation numbers, then you’d find crystal momentum, overall, *is* conserved. Finally, if we added external photons or neutrons (say doing optical/acoustical scattering measurements) to our system, then ascribing the neutron and photon to the free state eip·r (where p is real momentum), and repeating our analysis, with a Hamiltonian that includes these guys (which would be of the same form, just with extra terms), we would find:

