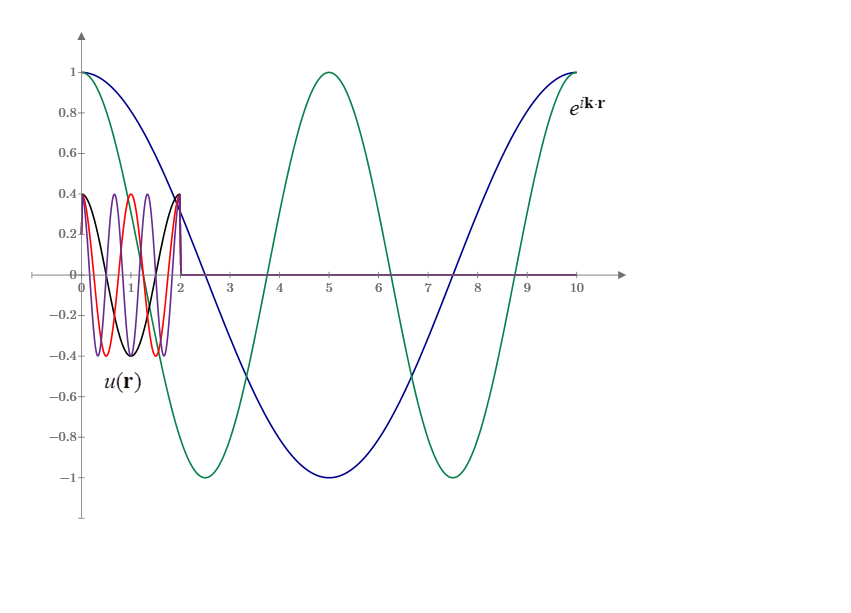
**Crystal Excitations**

**Trying to put a physical picture to Bloch’s theorem**

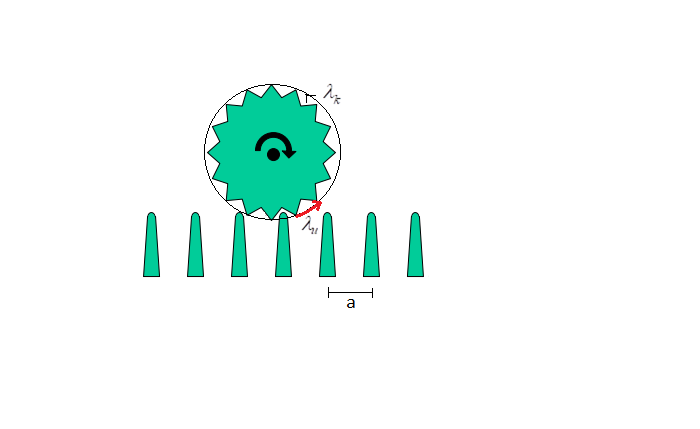
So I’d like to put a physical picture to these states. The previous calculations all bear out Bloch’s theorem, so we know the wavefunction looks like this:



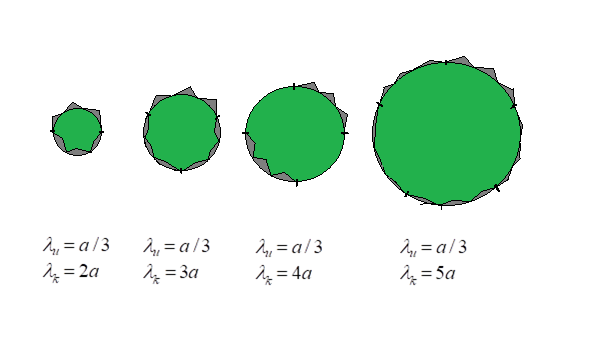
where ei**k**∙**r** is a wavefunction periodic over the sample and u(**r**) is a wavefunction periodic over the primitive cell. So **k** will be comprised of vectors that satisfy ei**k**∙(**r**+**L**) = ei**k**∙**r** → ei**k**∙**L** = 1 → k = 2πn/L (in 1D anyway). But these will be restricted to a BZ for uniqueness. And u(**r**), being periodic over the primitive cell, can be Fourier decomposed into waves with **G**’s such that ei**G**∙(**r**+**a**) = ei**G**∙**r** 🡪ei**G**∙**a** = 1 🡪 G = 2πn/a (again, in 1D). So we can write u(**r**) = ΣGuGei**G**∙**r**. Note that **k** is small, meaning small curvature, meaning wavelength λ = 2π/k never gets smaller than size of primitive cell. And **G** is large, meaning large curvature. So the ei**k**∙**r** function is just a way to ‘transport’ the u(**r**) function into other cells. The u(**r**) functions ‘ride the wave of the eikr guys’. Could roughly say that the wavefunction is u(r) repeated from cell to cell, but with an amplitude and phase given by eikr.



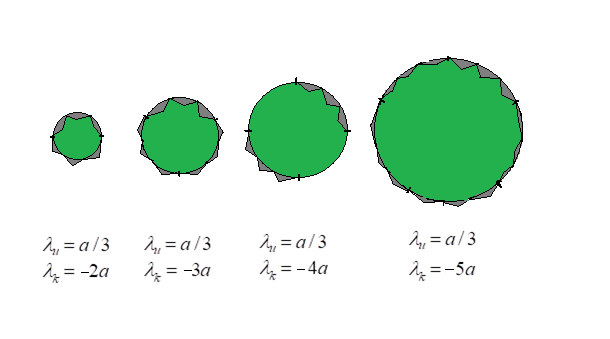
Another nice mental picture is afforded below. An electron wavefunction can sort of roll along the lattice potential without dispersion, like a finely tuned gear. The individual wavefunctions are extended of course, but we can write a ‘physical’ wavefunction as a linear combination with some group velocity, that would remain coherent for a long time presumably (and you can think of the teeth in the gear as being the u(r) themselves). We can sort of think of the distance between spikes on the gear as the wavelength of the periodic function u(R). So the possibilities for λu are a, a/2, a/3, a/4, …., a/∞. In the diagram λu = a/2. And the circumference of the gear can be taken as the wavelength λk in the prefactor eikr. And as such, this would be: ±2a, ±3a, …, ±Na = ±L. In the diagram λk = 16a/2 = 8a.



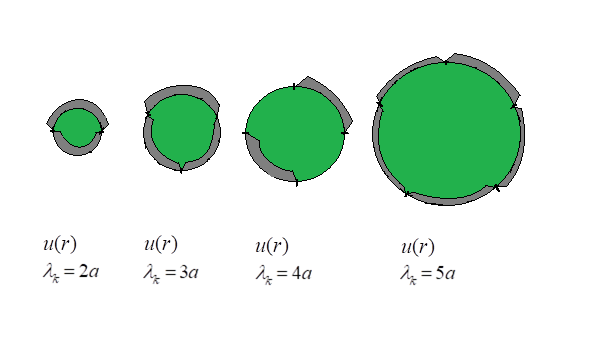
But one thing the gear doesn’t illustrate is the fact that the wavefunction isn’t periodic over a, but rather changes phase over a by amount φ = ka. The wavefunction is only periodic over the whole circumference rather. Below I’ve attempted to illustrate this effect.



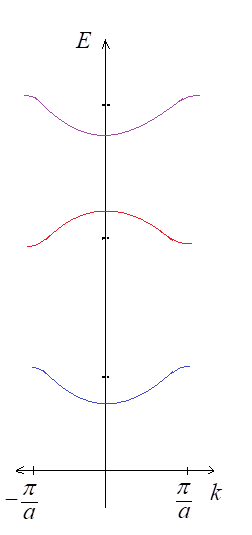
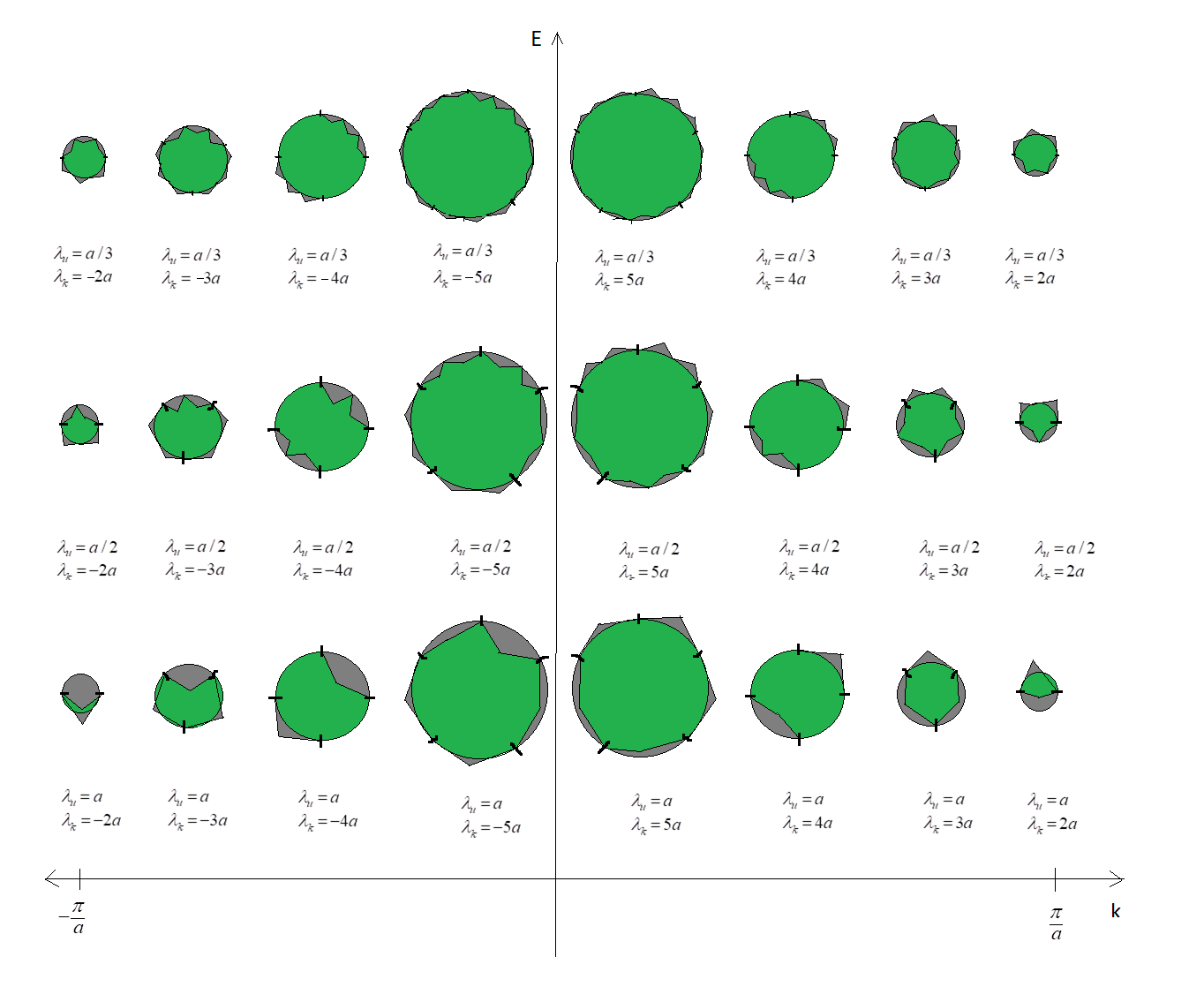
I suppose that λk = -2a, -3a, -4a, -5a would look like those above, but with displacements multiplied by -1.



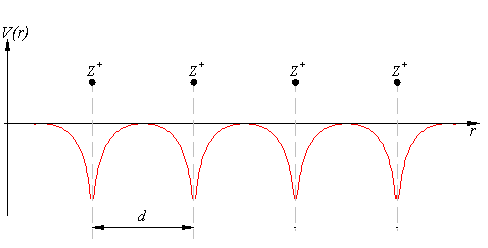
Technically our gear picture only depicts a free electron, but in a real metal the nature of u(r) would be different. I suppose we could accommodate a non-zero periodic potential by modifying the structure of the gear to simply make the spoky structure stuff that happens w/in the space of a to be kind of arbitrary, but still necessarily replicating over the distance a, modulo the phase factor. And we would still have an infinite # of such spoky-structures, corresponding to the infinite # of possible wavelengths λu. We can still see that such a gear would still roll unimpeded over the lattice. I tried to draw that below.



But if disorder is present then of course it will be impeded. I’d like to relate the energy diagram to the wavefunctions (below). So k = 0 corresponds to λk = ∞, and k = π/a → λ = 2a. So for a given energy band, we have the largest (in circumference) gear in the center, and then they get smaller out towards the edges. But the ‘# of spikes’ within the distance *a* is the same for each gear – though u(r) does technically change for each k b/c of that phase factor attached to the ψ(r-R) – this I haven’t pictured. In the lowest band, the # of spikes is ~ 1, and at the next band ~ 2, etc. I say ~ because of course the functions u(r) are not free so the band doesn’t correspond to the number of wavelengths fitting within a. Still, the higher the band, the curvier the u(r) most likely.



I flipped the bands upside down, as I was previously arguing I should’ve. We can make sense of the humps. Note the k = 0 (isn’t such a term, really, but k = 2π/L would be closest) term would correspond to a simple straight up sum of all the ψs(r-Ri)’s. This would be like the symmetric combination of the individual well eigenstates for the double well potential. Such a state would spend must of its time in the interstitial regions, which would seem to rather *raise* its energy. But in fact it *lowers* it because the symmetric state has much lower curvature, and so much less kinetic energy than typical states. The k = π/a and -π/a states would correspond to a completely antisymmetric sum of the ψs(r-Ri)’s. These states will spend more of their time in the potential regions and so will have much *lower* potential energy than the symmetric state, but as a consequence of it’s highly curvy state, it will have commensurately much *greater* kinetic energy, and so it will actually be a higher energy state. As we’ll see in a minute, the states in the middle and edges of the band may have low/high kinetic energy, but that doesn’t mean the kinetic energy is *directed* anywhere, i.e. <v> = 0 still.



Seems we can interpret the energy bands εn(k) as sort of giving the set of wavevectors that can freely propagate through the material, i.e., k = √2mεn(k), is a wavevector that can propagate through the material, ala Ramsauer effect in scattering theory.