**Physical Behavior**

**Electron States**

Want to characterize the electron states according to the various models we have of them.

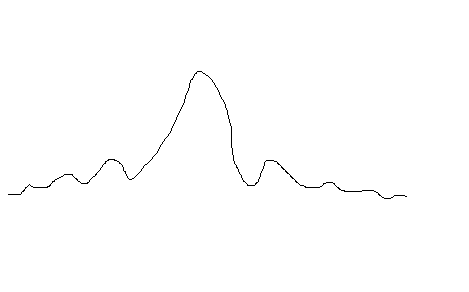
***Classical***

Classical electrons are point particles that more or less float unimpeded (except by the surface) across the metal lattice. And so it is presumed that we could have electron states with a non-zero average velocity in the pure metal. When we add impurities then scattering would cause these states’ average velocity to drop to zero. Nonetheless we would presume these states to be ‘extended’ in that they are free to diffuse though the entire sample. As we increase disorder, we would still expect the states to be extended I believe, as long as there were any energetic path between the ends of the sample. What if we have an electric or magnetic field present? What if we have magnetic impurities? If non-zero temperature, then they ought to get bumped around more, but otherwise…

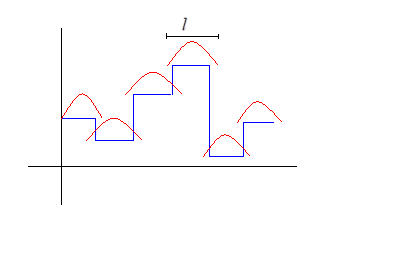
***Semiclassical-quantum***

In semi-classical picture, the electrons are extended k-states. The energy spectrum will take a band structure as all the individual quantum well states will join in harmonically to lift the degeneracies. Some band crossing is possible. As a consequence of the band structure there will be band gaps, and the density of states will take a periodic hump like structure. These states will have non-zero average velocity, just as their classical counterparts do, thanks to their ability to resonate in between the wells (which causes all the reflected waves to perfectly cancel) and hence perfectly transmit.

If there is disorder, then we’d expect them to elastically scatter, in a perhaps diffusive manner. Looked at differently, to first order, the impurity perturbations ought to mix the various unperturbed eigenstates. A mix of these states would still be extended, but with zero average velocity. And so that’s what we expect to zeroth order – extended states with no average velocity, though yet an average kinetic energy of course. Perhaps in fact, the phase φ´(x) of the wavefunction will be somewhat chaotically distributed through the sample, in analogy to how the velocity vector of a diffusing particle would be directed. Unexpectedly, however, these states won’t necessarily extend over the entire sample, due to the same phase coherence that allows them to penetrate the regular lattice structure. They will rather be confined to some localization length ξ. This seems reasonable if we have attractive disorder, but odd if we have repulsive disorder, or just a dislocation. But I think that electrons can be localized regardless of the background potential – just as light can be localized without an ‘attractive’ potential per se´, and free electrons can be localized too. This ought to be because pure transmission of electrons (either to the left or to the right) through the sample requires cancelation of all the reflected waves (either to the left or to the right), which can only happen if all the potentials are regularly spaced, etc. Any disorder (repulsive or attractive) will disrupt the rolling ‘gear’ motion of the electron through the periodic potential wells. It is the periodicity of the wells that allows the electron to escape being localized by them. And just like if we put a pebble in the way of a rolling cylinder, the electron can be jarred and by the disruption, and then get out of sync with the potentials and end up trapped by them. Come to think of it, this is what would happen if we did this to a real gear and periodic lattice. So we kind of expect something like:



Now it turns out that *all* states in 1D and 2D are localized. But in 3D not necessarily. This seems queer since an arbitrarily small 1D potential cannot localize a state with *any* energy – there are 1D free states given any single potential well. But perhaps the scenario we’re considering is one rather where we have a multitude of random potentials, rather than just one, albeit of possibly *very* small strength. And then in this case, the repeated destructive interference (though small) may eventually result in localization. Why do we need a sufficient potential in 3D though? This can be fairly readily explained by analogy with a free electron subjected to a central potential – a case studied in the QM notes. We calculated that we can have localized electrons in 1D, 2D for any strength of potential, but it required a certain strength to localize in 3D. And the qualitative reason we gave was that localizing a wavefunction causes a dramatic shift in curvature. This shift in curvature produces kinetic energy by well-known association. In general, localizing a wavefunction produces more kinetic energy in higher dimensions since KE ~ Σd ∂2/∂x2 ~ d∙∂2/∂x2. Apparently the shift in curvature isn’t severe enough to liberate the electron in the lower dimensions, but in 3D it is, and a certain strength of potential/disorder is required to grab hold of the electron. Another perspective on this, from the path integral point of view is that in 3D, the particle has more room for maneuver and so is less likely to classically return to its initial point upon scattering, and so is less likely to constructively interfere with itself there and form a bound state. We can take another perspective for the strong disorder case. Continuing this line of thought, suppose that we have *a lot* of impurities in our crystalline solid – so strong disorder case. Then the potential landscape can be thought of as looking like,



We’d like to ascertain the actual eigenstates of the sample. The unperturbed eigenstates will just be those eigenstates of the individual wells. These unperturbed states are something like the bound well states we had in the localized approximation (tight-binding approximation) of the Kronig-Penny model. The bound states will overlap a bit, or a lot, as before. But the difference here is basically that they’ll all be at different, randomized, energies. Consider a given bound state |nwell(0)>. What will it evolve into as we turn on the potential? Well up to 1st order…



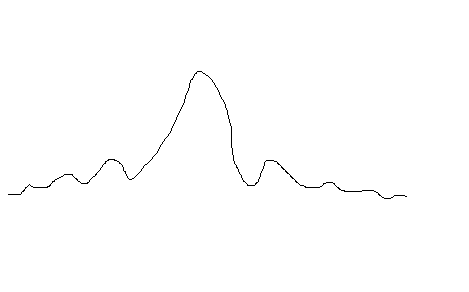
where |n(0)> is the linear combination of the |nwell(0)> that diagonalizes H at the given degenerate energy level. So what would |n(0)> look like? Is the it likely extended or exponentially damped? That depends on how far separated are the eigenstates |nwell(0)> at of the same energy. Let’s consider a model where we have sites of volume V0. And let’s say that the energies are randomly distributed between –W/2 and W/2 in units of δE. The number of sites within radius r would be N ~ Vdrd/V0. The probability that none will have the same energy would be



So when can we expect one to show up? Certainly when the exponent is zero. But a little less fastidiously, I guess at the characteristic radius:



Clearly the radius increases with disorder (but it decreases with dimension so that localization would be suppressed at higher dimensions). I would say that if ℓ < r, then we can expect the zeroth order states to be still localized. If ℓ > r, then extended. But so far we’ve considered mixing only between states at the same energy. And while this 0th order mixing would give the first contribution to the exact wavefunctions, at next order in perturbation theory we’d have to consider mixing from say E → E´ → E. So what about these contributions to the exact states at first order, after we’ve diagonalized the subspaces. Here we can get contributions from any other energy state, and so in a sense the actual eigenstates are going to be extended, but probably only in an exponentially damped sense, like this (which still counts as localized therefore):



since nearby states contribute, but only a little because they are unlikely to have same energy and are therefore suppressed by the energy denominator, whereas far away states (some of which at least are more likely to have same energy) are suppressed by the numerator. A more precise accounting could be made, but I’m gonna leave it off for now. We can also elaborate on how the state energy affects its localization. For instance, suppose we start a state off at position r and energy E. This is presumably not an eigenstate of H and so it would decay. If there is a state of nearby energy then it would hop to (mix with) that state (with probability depending on the matrix element connecting the two states I suppose). What is the probability that such a state will be found? Well this would be related to the density of states (per unit volume). Near band edges is where the density of states is low and so we should expect these to be localized first. At the critical disorder we would have all states up to the Fermi-level localized. After this, we’re in the insulating regime, and the conducting state can only *tunnel* through the sample.

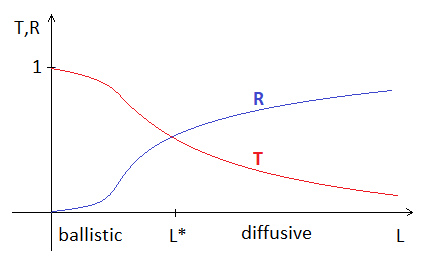
**Time-dependence**

We’d like to consider the motion of electrons through the lattice.

***Classical***

If we consider no disorder first. If we simply shot them into the sample, they would continue with the same average velocity, unabated. If there were a field, then they would accelerate. We might note that we had a source of electrons, then they ought to string out, like water from a faucet so that the current density j = ρv remains the same.

Suppose we have electrons at T = 0 initially, in a 1D lattice with disorder, and that all collisions with the impurities are elastic. Such collisions might preferentially favor small angles, θ. When we fire an electron into the lattice with velocity v, then it periodically make collisions with the impurities (we would say with any atom it comes into contact with, but quantum mechanics would say otherwise). It might immediately reflect, or continue into the lattice. But in any event its mechanical energy, (1/2)mve2, will be converted to random () ‘internal’ energy (in a time-averaged sense) pretty rapidly no doubt. How ve changes as a function of time probably depends on the initial velocity, and perhaps angle of incidence, and but in any event, this ve ought to diminish exponentially, as the Brownian motion formulas below would predict. While its entropic velocity is still finite, the electron will be in the ballistic regime. And I would suspect that the probability of transmission exceeds that of reflection so far. Once ve has dropped to zero, then it will be behaving diffusively, all of its mechanical energy will have been converted to ‘internal’ energy, and it will be in ‘thermal’ equilibrium with the lattice so to speak. At this point it would be equaly likely to go right or left in a time averaged sense, and if the end of the lattice is much further than the beginning, then I imagine the probability of transmission will be smaller than reflection. I’d imagine a graph like this:



I imagine the two curves cross somewhere near (or a little after really) the point where the motion becomes diffusive. And I’d also suspect that the shape of the curve changes to 1/L dependence somewhere after that point. Of course upon reflection or transmission, it will have the same velocity, v, it started with. In 2D/3D, a similar situation would prevail, except that the reflected or transmitted velocity could be different than the incoming one, while the speed would certainly be the same. If we had multiple particles, perhaps all sent in with a certain set of trajectories, perhaps even completely random, then we may say that there is some initial average velocity ve along with a sort of internal energy. The reflected particles would all have the same speed as the incident ones, but they may be more disordered than the incident ones (or not), and so the average velocity along the wire of the aggregate reflected particles may be different than the incident. As the transmitted cloud progresses, its velocity ve will certainly decrease and its energy converted to internal. When this is complete then we’ll have entered the diffusive regime. The final transmitted beam of particles may have a different aggregate average velocity along the wire after the disordered region, even as each individual particle has same speed, as well as some residual ‘internal’ energy. Of course the net current in/out must be the same.

If we set up an E field, then the e’s will accelerate forward until they strike an impurity and are knocked backwards elastically. We may imagine that the collisions completely randomize the orientation of the velocity. But more realistically, again, there would be some velocity preference, especially if we’re not dealing with a spherical hard wall potential. Eventually they should settle (could be accelerated up to, or down to – depending on whether initial injection velocity is below/above the drift velocity ve) on an average-ish velocity ve described by equation below. Before this happens, I would call this the ballistic regime, and afterwards the diffusive regime, again.



where τ is the mean collision time, and α is the fractional velocity that is lost when a collision happens. Now according to a classical peg model of collisions, it would seem that α is close to 1. But if we model the impurities as Coulomb wells, then we know that collisions are preferentially in the forward direction, and so α may be much less than 1. And moreover, that it is a decreasing function of v. But now we also know that τ ought to be a decreasing function of v too. So then as long as αv/τ is an increasing function of v at the electron’s velocity range we ought to get sensible results that (1) the rate of velocity loss will increase with velocity, and (2) the rate will be linear in v (at least least for velocities near the typical – Taylor series) so that the equilibrium velocity will be proportional to the field (so that current doubles when E doubles). But still, if collisions are elastic, then the electron cloud will be building up internal energy as its forward momentum is blunted. Would this affect ve? It seems plausible that it would, but also plausible that it wouldn’t (at least linearly in time; maybe as tsmall power?), and that the rate at which ‘directed’ energy is created via work done by the field is equal to the rate at which the collisions ‘internalize’ it. It seems that it is mathematically possible for the the velocity to even out, at least at the level of energy conservation.



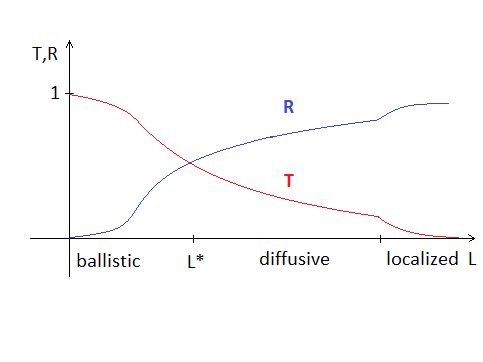
So now with a driving electric field, of course we ought to get the majority of electrons to transmit, since they certainly would mostly transmit past L\* and by the time they reach L\*, they’ll be in the diffusive regime and so the electric field will give them a drift velocity to the right and so they should make it through then. In the limit of zero impurity concentration, the drift velocity (and mean free time) would approach infinity, and so the conductivity, would approach that as well. More impurities would mean greater frequency of collisions, and therefore slower average velocity.

If we add a magnetic field, suppose a crossed one, then the electrons would be pushed, say, upwards, which would reduce their effective dimensionality. And this ought to increase the probability of collisions, and so the resistivity.

If we add in thermal interactions, then I imagine the electron cloud, which is heating up, would relax to the temperature of the lattice (or well, they’d both settle on some equilibrium temperature in between). Or they’d both settle at the temperature of the bath, T, if one is applied. Or, another way to say this (to kind of put both collision + relaxation steps into one) is that the electrons will emerge from the collisions with a speed equal to the equilibrium temperature of the electrons and lattice. And now, if the temperature of the electron cloud is held constant, then one might expect that the drift velocity certainly will not increase. An even more acute analysis of this equilibration processes would be the recognition of density oscillations in lattice, which would result in charge density oscillations in the lattice, which would allow for interactions with the electrons. And I think that these can be cast as collisions between the electron and phonons (which would be responsible for the equilibration process). Not sure why the phonons would impede motion since it seems they’d be just as likely to accelerate electrons forward as knock them backwards. Well it does seem that if you are equally likely to absorb energy in any ‘direction’, you will be on the net regressed in your velocity since an elastic collision in the forward direction doesn’t increase velocity as much as an elastic collision in the negative direction decreases it. And, if we inject an electron into a thermal bath of other electrons, we certainly wouldn’t expect it to continue it’s average drift velocity to the otherside of bath – rather it would come to equilibrium with the bath, and end up diffusing. So it makes sense that we’d treat phonons as extra impurities. And so the process of equilibration doesn’t merely bring the temperature of the electrons back down to that of the bath, but it also affects their ability to propagate through the lattice.

***Semiclassical***

Again, we’ll consider their motion through the lattice. So if a bunch of electrons are injected into a sample w/o impurities then they would penetrate the sample entirely due to their resonance with the crystalline structure (at least if their wavefunction resembles an eigenstate). If there are impurities, then they will collide of course. But collisions cannot kick an electron into any arbitrary state due to Pauli-exclusion principle (it seems this would in fact *force* the collisions to be elastic, if they’re not *explosive*). But also according to QM, the collisions should happen elastically (this follows from the first order perturbation results, and I think we can use first order perturbation theory because t is small – the collisions happen quickly) at a rate given by that Γ ~ |V|2δ(E-E´) formula. If the electrons are injected at the Fermi-surface then certainly they can only be scattered backwards/sideways into states near the Fermi surface that are unoccupied. It also might be the case that the collisions disprefer backward scattering, as the Coulomb potential does, and so collisions might be less common since there are fewer states available. So when they’re injected, some will reflect, and some will penetrate into the sample. Those penetrating will slink through at some ever decreasing average velocity ve until it eventually, pretty quickly, comes to rest, and all its directed energy converted to ‘internal’ energy. At this point of course it will have passed from the balistic to diffusive mode. We’d expect the transmission probability to behave as classically, but instead we’d find that there is a precipitous drop at a certain length. I don’t think that the curve will look so disjointed but you get the idea.

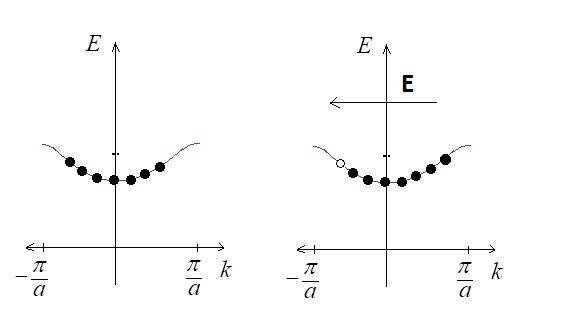
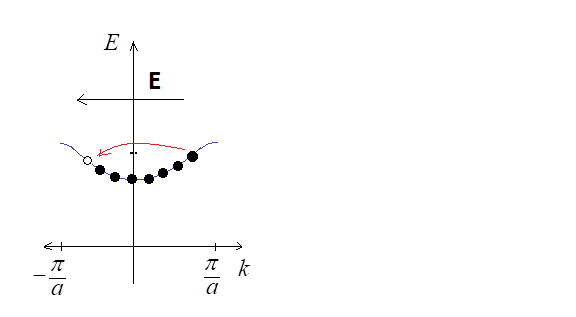


This length is called the ‘localization length’, and is caused by trapping of the electrons. The localization comes about due to the multitude of phase-coherent reflections off of impurities. Due to nature of its entrance into the sample, I imagine that its kind of biased towards the injection side of the sample, so that it might be able to diffuse backwards, but would only be able to *transmit* by tunneling more or less. Turning on B ought to lift the exponential damping and restore to power law decay in the infinite B limit.

When we turn on the E field, in an impurity-less environment, it will (adiabatically?) drive the electrons through their k-states, according to the equations:



(note we cannot always make this argument that ∂ε/∂t = ∂ε/∂χ∙∂χ/∂t, where χ is some parameter in ε, because sometimes none of those χ’s are changing – like with an electric field pushing a ground state harmonic oscillator). Without band structure, this would just predict an ever accelerating current. And if we have impurities, then the collisions will cause electrons directed energy to be blunted into thermal energy of cource. When we have an E field, the electrons will be displaced according to the dynamics discussed earlier. And so we see that this will create a net current to the right.

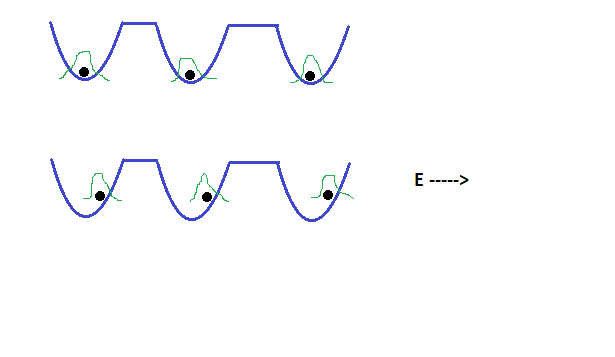
 

But with impurities the electrons will be kicked back into an unoccupied part of the Fermi sphere. And then the next highest energy on the right will inch upwards (and the rest of the electrons with it), and then be kicked to the back of the line. I imagine this process will repeat itself: each subsequent electron being kicked to the back. And so slowly the electrons will inch forward. We can see from this picture that only the electrons near the so-called Fermi surface will contribute to the conductivity.

They will settle on a velocity, ve, where the rate of energy input by the field is equal to the rate of directed energy output by the collisions. Note that unlike in the classical case, this drift velocity ve would be dependent on the energy of the electrons (or their original kinetic energy before injection). This is because the higher their energy, the higher their transmission probability through the impurity wells. And we’ll note that σ is energy-dependent anyway; it’s value at the Fermi surface is just what we use when T = 0. So as a result of the energy loss, the temperature of the cloud will increase. If we don’t allow the electrons to shed energy to the lattice then I imagine the electron temperature would just continue to increase, and so the edge of the electron distribution would continue to increase and so the ‘Fermi velocity’ might continue to increase, and so vF, and perhaps σ would continue to increase. But perhaps these effects would show up at larger times, or higher orders, at which first order PT is invalid. Or maybe they wouldn’t happen at all? But at a certain impurity concentration, the conductivity would drop to zero abruptly (which would imply that ve isn’t proportional to E, but perhaps to E2 or something, who knows). So σ shows how ve depends on E. If a Taylor series expansion is always valid, we may suppose we can write ve as a function of E as:



Each of these coefficients: σ, σ2, σ3, etc., would depend on the impurity concentration. Generally they decrease with impurity concentration ni. But apparently σ abruptly goes to zero when ni = some critical value. A bound state model below could illustrate.



Since if the electric field isn’t strong enough to push the charges past the hump, then application of the field to first order will just shift the equilibrium position. For instance the drift velocity would be:



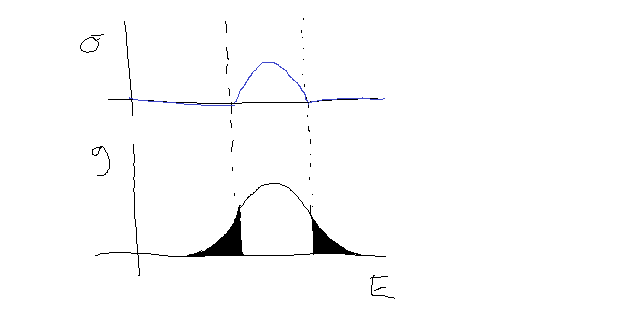
where a is the radius of the well.

If we include thermal interactions, then the electron cloud will exchange energy with the lattice, to settle back down into a thermodynamic equilibrium state at temperature (slightly above) T. Then the lattice/electrons as a whole would shed this extra thermal energy to the bath. So the whole repetetive process: E induced acceleration to create forward momentum---collisions to eliminate the momentum and dissipate the mechanical energy into internal energy—resettling into thermodynamic equilibrium state at the temperature of the lattice (now slightly higher)---shedding energy to the bath: results in a net average drift velocity of the electron cloud. The new distribution function that we find in the semi-classical approach, f = f0 + χE∙ve just takes into account the acceleration and scattering parts, and it’s time-independent by design, but I think that this is only because we’re considering f out to first order. Anyway, the greater the number of impurities, the greater the frequency of collisions, and so the lesser the conductivity. If the number of impurities is great enough then we find that conductivity vanishes.

***Quantum***

Moving on…we’re going to add impurities now. These ‘impurities’ don’t even have to be actual atoms I don’t think, but could even be dislocations, or density fluctuations, i.e., any disruption of periodicity? These states have no velocity expectation in any dimension (perhaps because its phase φ´(x) is chaotically distributed throughout space), but will be extended or not based on their energy/velocity level. If we simply inject electrons into the metal, their dynamics will be controlled by the states at the same energy. Of course, none of these states has a velocity expectation so I’d expect that the velocity expectation of the injected electron to decay pretty quickly to zero, and their projected energy φ´2 would be converted more or less to fluctuation energy A´´/A (but I have doubts about this discription now). And once this is done, they are more likely to reflect than transmit, due to their random velocity orientation. If the energy of these electrons matches localized states, however, then we’d expect the vast majority of electrons to reflect if the sample size is greater than that energy’s localization length.

If we apply an E field, then how do these states evolve? In the GF approach, we take the impurities into account via the disorder averaged GF. And it turns out we only need the scattering time in the calculation – we ignore the impurities’ contribution to the real part of the self-energy. So apparently turning on the field causes a brief acquisition of a velocity expectation (perhapse the phase φ´(x) acquires a constant average part). Like before, the energy of the system will continue to increase (perhaps it continues to acquire A´´/A energy, φ´2 energy being held constant – but again, doubts). This increasing energy is basically all internal therefore, and perhaps this would result in a build up of the effective EF. And perhaps we expect the localized states to behave the same way, but with an obviously exponentially decaying envelope? The conductance of these states apparently goes as σ = (E – Ec)ν for energies greater than the Ec, but ~ exp(-L/ξ) for energies less than. So generally something like this:



If we allow thermal interactions, then this energy will be dissipated into the lattice.

Need to figure out relationship between elastic scattering and thermodynamic equilibration

**Phenomenology of Conduction**

Have a problem between the conduction formulas….

* Eigenstates would not change entropy because they aren’t changing with time. Require time-dependence to have entropy change.
* Does ve increase when dragging with E-field. It seems like it must with semi-classical picture, but seems it might not with classical picture. Well in semi-classical picture, it might continually increase kF, but that doesn’t mean that the *average* velocity is necessarily changing.
* In eigenfunction view, the wavefunction will penetrate the well, and reflect off boundary, etc. The reflection will slow the net velocity down (as that previous wavefunction analysis kind of indicates), and so perhaps overall, there will be a net constant velocity through the lattice. Also, these reflections correspond to the reflections of the classical and semi-classical particle and also to the sort of ‘entropic expansion’ of the wavefunction, and classical/semi-classical trajectories.