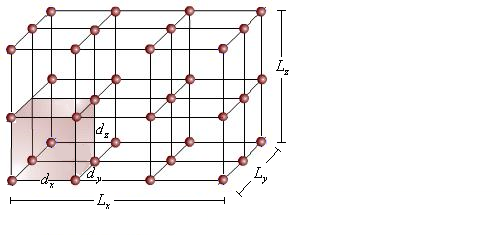
**2nd quantization**

Last one…

**Some operators in tight binding ‘basis’**

In the conceit of the tight binding model, we have a crystal composed of a bunch of molecules/atoms centered at sites Rj.



Let φ­ν­σ(r-Rj) be the set of functions on site j which are eigenfunctions of that site’s molecular Hamiltonian, and εν be their energies. ν stands for orbital d.o.f., and σ denotes spin. The set of site functions φνσ(r-Rj) are orthonormal to each other on that site. In other words φνσ(r-Rj) is orthonormal to φν´σ´(r-Rj). But φνσ(r-Rj) isn’t really going to be orthonormal to φν´σ´(r-Rk) if j ≠ k. However, in order to use the 2nd quantization formalism, we must assume the overlap is small enough to be negligible, and we will. To be clear, we aren’t presuming the site wavefunctions are non-zero only within their unit cell, just that the inner product between two wavefunctions from different sites is zero. Under this approximation, we can associate each wavefunction with a site creation/annihilation operator. What follows is basically equivalent to the use of a variational principle calculation, valid to only zeroth order in the overlap of adjacent site wavefunctions (see Quantum Mechanics/Variational Principle). But this is usually a good approximation.

**Hamiltonian with single particle potential**

So, the typical single particle H would be:



where the sum runs over all lattice sites. And let’s introduce states |jνσ> = φνσ(r-Rj), taken to be eigenstates of:



with eigenvalues εν. Let cjνσ† create such states, and cjνσ annihilate them. And so the 2nd quantized H would be:



where we have defined:



which is the potential at site j coming from all the other sites’s potentials. And by the notation |jν>, we mean to indicate just the spatial part of the single particle ket. Now ΔUj(r) shouldn’t actually depend on j, due to the crystal’s periodicity. And further, the expectation <jν|ΔUj(r)|kν´> should only depend on the relative position of the two sites, i.e., on **R**k – **R**j = **R**δ. So I’m going to reparameterize |k> as |j+δ>, and write:



So going back to:



So then we have:



**Hamiltonian with two-particle potential**

What about a two-particle operator? We’ll assume it doesn’t explicitly depend upon spin. In that case, we’ll have:



So,



The overlap integrals are usually quite small. The largest term would be nearest neighbor interactions and onsite interactions. So for instance, one possibility is keeping just the direct interaction between sites (set n = k, m = ℓ) (but not equal to each other).



Since the ck’s won’t equal the cℓ’s, they anticommute, and we can write this as:



One could suppose that the wavefunctions φ(r-R) are relatively isolated about R, and are quasi-delta function like, at least from the perspective of neighboring atoms. In that case, we could probably say, in a phenomenological manner, that:



So,



where nk = Σσnkσ. And I expect 2 is pretty close to V2 itself. Another possibility, besides the off-site interaction, is retaining just the interaction between e-‘s on the same sight.



So we have, not much of a simplification,



So putting the two together, we’d have approximately,



Now let’s simplify further,

**Only spin degrees of freedom**

Let’s say there is only spin d.o.f. on each site [this could be appropriate, even if we have multiple orbitals, if we feel that the crystal potential will only mix electron energy levels within the *same* orbital]. And we’ll of course presume the crystal potential doesn’t itself mix orbitals with different spin. Then we can say:



[note δ can be 0] ΔU0 is defined to be the correction to the orbital energy. ΔUδ≠0 is called a hopping term, meaning that the e- can hop from site to site perhaps. Note the kinetic energy operator was included already, as we saw, so the hopping term doesn’t serve the purpose of ‘including’ KE in the Hamiltonian. The hopping refers to there being V(r) overlap between adjacent site’s wavefunctions…and this alters the form of the wavefunction from a localized to delocalized state, and gives the energy band curvature, which gives the electron states a mean velocity (see Condensed Matter/Metals/Electrons/Crystal Excitations Properties file) whereas before it wouldn’t have had a mean velocity. If there is no overlap, then there is no chance that the e‑ can ooze onto the other site. Moving on to the two-particle potential, since the interaction should be spin-independent, we’ll have:



The approximation to the offsite potential doesn’t change. We still have:



Again, we can postulate that:



where (R) is just some phenomenologically determined function, in which case we’ll have:



Then specializing to the onsite interaction, we have:



where,



As written, the model would exclude self-interaction terms. So that having a single spin onsite wouldn’t have an associated potential energy, as it shouldn’t. At this point one often specializes to the case where the spins are opposite (σ,σ´) = (↑,↓), (↓,↑). Well, in fact they can only be opposite because otherwise ckσckσ will anihilate whatever state it’s acting on. Then we can anti-commute the last c to bring it next to the first one:



and then since the sum is symmetric we have:



Then altogether,



Keeping just the last term is called the Hubbard Model.

**Some more operators in special only-spin-d.o.f. case**

Some more operators of interest are the density,



and its Fourier transform,



and this can be written as:



where,



The current can be written as:



We can use a shortcut through:



formulating P, and commuting it with H to get the time-derivative, we’ll find [at least for the one with V2offsite, not sure about the V2onsite]:



(where J is total current – so I guess that makes it I) We’ll observe that if we set the overlap between adjacent wavefunctions to be 0, meaning that we set δ = 0, then the current must vanish, as there is no way for the e- to go from one site to the other. Last I guess, let’s do the spin operator. Let’s not do spin density per se´, but the operator which represents the spin on site.



We may take ciσ†ciσ**S**σσ´ as the onsite spin operator. Working out these formulas for the case of multiple orbitals is not hard.