A Short Revisit to Tight-binding Model

Taper

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Contents

Note: After reading chapter 7.9 of [Par09], I think that book provides a much clearer understanding of what tight-binding model is, and therefore I recommend a first reading of that book, before go into [AM76].

To me, Tight-binding model is almost synonym of the following 2nd-quantized Hamiltonian:

$$H = \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma} - t \sum_{\langle i,j\rangle,\sigma} \left(c^\dagger_{i,\sigma} c_{j,\sigma} + \text{h.c.} \right) \tag{0.0.1}$$

But actually there is much more that just this. I here give a short note about some key points in chapter 10, The Tight-Binding Method, in [AM76].

The aim of Tight-binding model, is to deal

> " with the case in which the overlap of atomic wave functions is enough to require corrections to the picture of isolated atoms, but not so much as to render the atomic description completely irrelevant "

For this purpose, we start with a set of states:

$$\psi_n(\mathbf{r}) \tag{0.0.2}$$

that satisfy two conditions:

1. They model a wave function localized at each lattice points. Here, they are taken to be the bound levels of atomic Hamiltonian which are well localized:
$$H_{\text{at}} \psi_n(\mathbf{r}) = E_n \psi_n(\mathbf{r}) \tag{0.0.3}$$
2. They are orthonormal with respect to each other (which is quite reasonable a requirement).

With this states, we test if the following wave function is a good wavefunction of the system:

$$\psi_k = \sum_R e^{ikR} \phi(r - R) \tag{0.0.4}$$

where k ranges through the N values in the first Brillouin zone consistent with the Born-von Karman periodic boundary condition. And

$$\phi(r) = \sum_n b_n \psi_n(\mathbf{r}) \tag{0.0.5}$$

Exactly how many n should be summed in the above expression will depend on the situation (explained below).

It is easy to see that ψ_{nk} satisfy the Bloch condition. So we could assume that:

$$H\psi(\mathbf{r}) = (H_{\text{at}} + \Delta U(\mathbf{r}))\psi(\mathbf{r}) = \varepsilon(\mathbf{r})\psi(\mathbf{r}) \tag{0.0.6}$$

Using the orthonormal condition and some techniques, we have (see pp.179 to 180 of [AM76]):

$$\begin{aligned}(\varepsilon(k) - E_m)b_m = &-(\varepsilon(k) - E_m)\sum_n \left(\sum_{R\neq 0}\int \psi_m^*(r)\psi_n(r-R)e^{ikR}\,\mathrm{d}r\right) b_n \\ &+ \sum_n \left(\int \psi_m^*(r)\Delta U(r)\psi_n(r)\,\mathrm{d}r\right) b_n \\ &+ \sum_n \left(\sum_{R\neq 0}\int \psi_m^*(r)\Delta U(r)\psi_n(r-R)e^{ikR}\,\mathrm{d}r\right) b_n \end{aligned} \tag{0.0.7}$$

eq:tb-model-eq

Now we argue that the right hand side of this equation should be small because there are small overlap between those localized ψ_n. Therefore, the left hand side should also be small. Therefore:

$$\varepsilon(k) \approx E_0,\ b_m \approx 0 \text{ unless } E_m \approx E_0 \tag{0.0.8}$$

where E_0 is energy of one atomic level. However, the above is only an approximate analysis. To get more details, we would let n only summed over those levels with energies either degenerate with or very close to E_0, our anticipated atomic energy level. This would make 0.0.7 for different ms into a matrix equation. (see more at p.181 of [AM76]). The solution to this equation gives us coefficients b_m, the wavefunction ψ_k, and the energy $\varepsilon(k)$.

Wannier function The Tight-binding model is related to Wannier function, since any Bloch function $\psi_{nk}(r)$ can be expended

$$\psi_{nk} = \sum_r f_n(r-R)e^{iRk} \tag{0.0.9}$$

where

$$f_n(R,r) = \frac{1}{v_0}\int \mathrm{d}k\, e^{-iRk}\psi_{nk}(r) \tag{0.0.10}$$

and v_0 is the volume in k-space of the first Brillouin zone, and the integral is taken over the 1st BZ. f_n are the so called Wannier functions and they could be

well localized (see p.188 of [AM76]) and is orthonormal (see problem 3 of chapter 10, [AM76]). Therefore they may be substituted as the atomic eigenstates $\psi_n(r)$ in the above steps.

How to proceed them?

Also, this article [MMY+12] that reviews Wannier functions is a very good resource to understand why we need Wannier functions and that Wannier and Bloch functions both provide complete information for the system we studied.

References

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