

Solid State Physics

Lecture 41

Tridiagonal Matrices and Continued Fraction

(Refer Slide Time: 00:23)

Now, if we work out the Hamiltonian matrix, we will find a tridiagonal matrix here because we are considering only nearest neighbor hopping's beyond nearest neighbor the hopping elements are 0; that is what we are assuming. (Refer Slide Time: 00:45)

With tridiagonal matrix, it offers certain advantages, let us see what kind of advantages we have towards our side with this tridiagonal matrix. A matrix whose non-vanishing elements occur only on the principal diagonal and the next upper and lower ones is called the tridiagonal; called the tridiagonal matrix. And the crystal Hamiltonian that we have here in this context can be written, represented in terms of localized orbitals as the basis. So, we will have basis elements like $|f_n\rangle$, these are our basis elements which are nothing, but our local orbitals $|\phi_a(x - t_n)\rangle$. So, if we have this kind of basis elements, then the Hamiltonian operator can be expressed in terms of these basis elements as $H = E_0 \sum_n$ all the diagonal elements of the operator $|f_n\rangle\langle f_n| + \gamma \sum_n [|f_n\rangle\langle f_{n+1}| + |f_{n+1}\rangle\langle f_n|]$, this would be the expression of the Hamiltonian operator in terms of this $|f_n\rangle$ basis which are localized orbital basis. Now, one-dimensional tight binding Hamiltonian with one orbital per site and only nearest neighbor hopping is the simplest example that we can describe using a tridiagonal Hamiltonian and let us represent this. So, the general form of this tridiagonal Hamiltonian is instead of E_0 and γ , we will write just generic representation $\sum_n a_n |f_n\rangle\langle f_n| + \sum_n b_n [|f_n\rangle\langle f_{n+1}| + |f_{n+1}\rangle\langle f_n|]$ with appropriate values of the diagonal and off-diagonal matrix elements a_n and b_n . We have the Hamiltonian operator as a Hermitian operator, it must be Hermitian. If H is Hermitian, a_n must be real because the diagonal elements have to be real of a Hermitian matrix. The off-diagonal elements can be complex in general, but we can absorb the complex part of it in appropriate phase factor associated with the basis elements and if we do that, we can make b_n also real by absorbing the phase factor into the basis elements itself. (Refer Slide Time: 05:28)

Now let us see how we can invert a tridiagonal matrix that is actually pretty easy, inversion of a tridiagonal matrix. Inverting the tridiagonal matrix would give us the advantage of being able to calculate various quantities quite easily. So, let us consider a tridiagonal matrix of the form $M =$

$$\begin{pmatrix} \alpha_0 & \beta_1 & 0 & 0 & \dots \\ \beta_1 & \alpha_1 & \beta_2 & 0 & \dots \\ 0 & \beta_2 & \alpha_2 & \beta_3 & \dots \\ 0 & 0 & \beta_3 & \alpha_3 & \dots \\ \vdots & \vdots & \vdots & \ddots & \vdots \end{pmatrix}. \text{ We are considering a big matrix of finite size. We have this kind of a}$$

big matrix at hand. For simplicity, we consider the rank of the matrix to be finite, but arbitrarily large. If we call the inverse of this matrix to be M^{-1} , then we are primarily interested in finding the explicit expression of the elements in here. Let us consider the first element $(M^{-1})_{00}$. If we consider how to find this element, then we can indicate the $\det(M) = D_0$ this and then, we write D_1 is the determinant suppressing the 1st row and column. Similarly, we can calculate D_2, D_3 and so on. So, $D_0 = \alpha_0 D_1 - \beta_1^2 D_2$. So, $(\frac{1}{M})_{00} = \frac{D_1}{D_0}$. (Refer Slide Time: 09:11)

Similarly, with this expression, we can write $(\frac{1}{M})_{00} = \frac{1}{D_0/D_1} = \frac{1}{\alpha_0 - \beta_1^2 \frac{1}{D_1/D_2}}$, you can see that it becomes an iterative process and if we iterate like this, we can write an expression of iteration like $(\frac{1}{M})_{00} = \frac{1}{\alpha_0 - \frac{\beta_1^2}{\alpha_1 - \frac{\beta_2^2}{\dots}}}$. So, we have written continued fraction expression for the elements of the inverse matrix. Now, in this case, we have $\beta_0 = 0$, then we obtain the previous equation that we have discussed earlier. So, this method; using this method, we can obtain any of the diagonal

elements of the inverse matrix, also there is a formalism to get the off-diagonal elements of the inverse matrix, similar formalism. And this using this continued fraction expressions which does not go to infinity because we are considering matrices of finite size, it will, it can be easily evaluated using a computer, there is no problem with this. Now, let us consider the density of states. If we consider a system described by a Hamiltonian, the Hamiltonian is H and let us say it has ψ_m , normalized eigenfunctions corresponding to E_m eigenvalue, then the total density of states can be defined as $D(E) = \sum_m \delta(E - E_m)$. Consider this definition, think about it carefully and you will be able to reconcile its meaning with whatever we understand from our previous notion of density of states, this is consistent with that. So, if we integrate the density of states, then we are going to get the number of states. If we $\int_{E_1}^{E_2} D(E) dE$ we get the number of states in this energy range. (Refer Slide Time: 14:03)

The density of states if we consider it projected onto any arbitrary state of interest, let us consider $|f_0\rangle$ to be the arbitrary state of interest. Usually, local orbitals happen to be our states of interest, then we can project the density of state onto this orbital that means, we can get the local density of states provided this $|f_0\rangle$ is a local orbital. So, the density of state projected on any arbitrary state of interest, if we normalize it to unity, we can define it as $n_0(E) = \sum_m |\langle f_0 | \psi_m \rangle|^2 \delta(E - E_m)$ provided ψ_m is normalized, f_0 is the arbitrary basis elements so, this is also arbitrary state of interest, this is also normalize so, this quantity inner product squared would be a fraction less than 1 usually and this gives us something less than the density of states that is also a function of energy. So the projected or local density of states gives information uniquely on the spectral region investigated by the orbital f_0 ; that means, if we want to find out the contribution at a particular energy of certain orbitals, contribution of that orbital into the density of state, we can perform this projection and see what is the contribution coming from that particular orbital in the density of states at that particular energy and a spectrum can be plotted varying the energy that is the idea. And if we $\int n_0(E) dE = 1$ just because $|f_0\rangle$ is normalized. The total density of states is just the sum of the projected density of state over the complete orthonormal basis set. So, if we consider the entire orthonormal basis set $|f_n\rangle$ and project the density of state onto each elements and sum them for a particular energy, then we will get the total density of states.