

An Introduction to Second Quantization

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January 27, 2010

1 Introduction

We all know single particle quantum mechanics very well. The state of a system can be represented by a ket $|\psi\rangle$ and the space in which these states lie is called the *Hilbert space*. This Hilbert space contains states which can accommodate one particle. Thus, there is no room for more than one particles! What do we do to accommodate more guests? The answer is simple and that is to EXPAND!

$$\Rightarrow \mathcal{H}^N = \underbrace{\mathcal{H} \otimes \cdots \otimes \mathcal{H}}_{n\text{-copies}}$$

The idea is pretty similar to the idea of extension from 1-dimension to 2-dimensions. A point in 1-dimension is represented in \mathbb{R} as x or y . If we take two copies of \mathbb{R} , we get the space $\mathbb{R} \otimes \mathbb{R}$ in which we can represent a 2-dimensional point i.e. we go from $x \rightarrow (x, y)$. The operation \otimes is known as direct product.

Let us now examine how we can write a two particle state using two single particle states $|1\rangle$, $|2\rangle$. Suppose the particle 1 is in the state $|1\rangle$ and particle 2 is in the state $|2\rangle$. Using the above idea, we can straight away write a state $|1\rangle \otimes |2\rangle$ in $\mathcal{H} \otimes \mathcal{H}$. What is the meaning of this state?

$$\langle r_1, r_2 | 1\rangle \otimes |2\rangle = \langle r_1 | 1\rangle \langle r_2 | 2\rangle = \phi(r_1)\phi(r_2) \quad (1)$$

If the particle 2 is in the state $|1\rangle$ and particle 1 is in the state $|2\rangle$, the two particle state can be written as $|2\rangle \otimes |1\rangle$ and

$$\langle r_1, r_2 | 2\rangle \otimes |1\rangle = \langle r_1 | 2\rangle \langle r_2 | 1\rangle = \phi(r_2)\phi(r_1) \quad (2)$$

Thus, a general two particle state in \mathcal{H}^2 can be written as

$$|\psi\rangle_2 = \alpha|1\rangle \otimes |2\rangle + \beta|2\rangle \otimes |1\rangle \quad (3)$$

We know that the particles in quantum mechanics are *indistinguishable* and occur only in two possibilities

	Fermions	Bosons
Wavefunction	Anti-symmetric	Symmetric
Allowed	$ \psi\rangle_2^f = (1\rangle \otimes 2\rangle - 2\rangle \otimes 1\rangle)$	$ \psi\rangle_2^b = (1\rangle \otimes 2\rangle + 2\rangle \otimes 1\rangle)$

Consider the anti-symmetric state. We can drop \otimes for brevity: $|\psi\rangle_2^f = \frac{1}{\sqrt{2}}(|1\rangle|2\rangle - |2\rangle|1\rangle)$. The real space representation is given by

$$\begin{aligned} \langle r_1, r_2 | \psi\rangle_2^f &= \frac{1}{\sqrt{2}} (\phi_1(r_1)\phi_2(r_2) - \phi_2(r_1)\phi_1(r_2)) \\ &= \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_1(r_1) & \phi_1(r_2) \\ \phi_2(r_1) & \phi_2(r_2) \end{vmatrix} \\ &\equiv |1, 2\rangle \end{aligned} \quad (4)$$

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This form $|1, 2|$ is known *Slater determinant* and is used to represent anti-symmetric wavefunctions. The generalization to the N -particle anti-symmetric wavefunction is trivial. If we have N states $|n\rangle$, ($n = 1, 2, \dots, N$). Then the slater determinant $|1, 2, \dots, N|$ is given by

$$|\psi\rangle_N^f = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(r_1) & \cdots & \phi_1(r_N) \\ \vdots & \vdots & \vdots \\ \phi_N(r_1) & \cdots & \phi_N(r_N) \end{vmatrix} \quad (5)$$

The subspace spanned by these anti-symmetric states is known as *Fock's space* for fermions.

There is an ambiguity in the way we have defined (4). There is nothing which prevents us from writing a slater determinant as

$$\langle r_1, r_2 | \psi \rangle_2^f = \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_2(r_1) & \phi_2(r_2) \\ \phi_1(r_1) & \phi_1(r_2) \end{vmatrix} \quad (6)$$

Thus, we need a convention. If we have a two particle slater determinant $|l, m|$, then

$$\langle r_1, r_2 | \psi \rangle_{l,m}^f = |l, m| = \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_l(r_1) & \phi_l(r_2) \\ \phi_m(r_1) & \phi_m(r_2) \end{vmatrix} \quad (7)$$

for $l < m$.

For bosons, we get a space of symmetrized states which is the Fock's space for bosons. The bosonic wavefunctions are represented by *permanents*.

2 Occupation number formalism

Instead of writing Slater determinant state (7) as $|\psi\rangle_{l,m}^f$, we can write it as

$$|\psi\rangle_{l,m}^f \equiv |0, \dots, 0, \underbrace{1}_l, 0, \dots, 0, \underbrace{1}_m, 0, \dots\rangle \quad (8)$$

i.e. we write '1's at positions l and m corresponding to participating single particle states in the slater determinant and '0's at all other positions. This is known as occupation number representation. Note that we have written (8) for a fermionic state. The same representation can be used to describe bosonic states as well. It is easy to see that, by construction, the state written in occupation number representation contains the information about the nature of particles (symmetry or anti-symmetry).

Since, we are interested in situations where particle number is not fixed, we want operators which can take us from one Fock space to another Fock space with different particle number, say from \mathcal{F}_{n-1} to \mathcal{F}_n . Thus, the states in a Fock space can be obtained by successively applying such operators on the vacuum state (the state with no particles).

2.1 Fermionic Operators

Let us define operator c_n^\dagger to be the operator which creates a particle in state $|n\rangle$. This is known as creation operator. There is a conjugate operator c_n as well that destroys a particle from state $|n\rangle$ and hence called an annihilation operator. Now we can create $|\psi\rangle_{l,m}^f$ from the vacuum state by operator of c_l^\dagger and c_m^\dagger successively.

$$\begin{aligned} |0\rangle &= |0, \dots, 0, \underbrace{0}_l, 0, \dots, 0, \underbrace{0}_m, 0, \dots\rangle \\ c_m^\dagger |0\rangle &= |0, \dots, 0, \underbrace{0}_l, 0, \dots, 0, \underbrace{1}_m, 0, \dots\rangle \\ c_l^\dagger c_m^\dagger |0\rangle &= |0, \dots, 0, \underbrace{1}_l, 0, \dots, 0, \underbrace{1}_m, 0, \dots\rangle \equiv |\psi\rangle_{l,m}^f \end{aligned} \quad (9)$$

Now consider

$$c_m^\dagger c_l^\dagger |0\rangle = |\psi\rangle_{m,l}^f = -|0, \dots, 0, \underbrace{1}_l, 0, \dots, 0, \underbrace{1}_m, 0, \dots\rangle \quad (10)$$

Thus

$$\begin{aligned} (c_l^\dagger c_m^\dagger + c_m^\dagger c_l^\dagger) |0\rangle &= 0 \\ (c_l^\dagger c_m^\dagger - c_m^\dagger c_l^\dagger) &= 0 \end{aligned} \quad (11)$$

We get the anti-commutation relation as a result of the anti-symmetry of the state. Using this, we can define the operation of c_l^\dagger on any state $|n_1, n_2, \dots\rangle$

$$c_l^\dagger |n_1, \dots, n_{l-1}, n_l, \dots\rangle \propto (-1)^{n_1+n_2+\dots+n_{l-1}} |n_1, \dots, n_{l-1}, n_l+1, \dots\rangle \quad (12)$$

The proportionality constant is fixed using normalization condition which give

$$c_l^\dagger |n_1, \dots, n_{l-1}, n_l, \dots\rangle = (-1)^{\sum_{i=0}^{l-1} n_i} \sqrt{n_l+1} |n_1, \dots, n_{l-1}, n_l+1, \dots\rangle \quad (13)$$

For fermions, n_l+1 has to be considered modulo 2 due to Pauli exclusion principle. Similarly, the conjugate of this operator is defined as

$$c_l |n_1, \dots, n_{l-1}, n_l, \dots\rangle = (-1)^{\sum_{i=0}^{l-1} n_i} \sqrt{n_l} |n_1, \dots, n_{l-1}, n_l-1, \dots\rangle \quad (14)$$

Using these relations, we can check that, for fermions,

$$\begin{aligned} c_l c_m + c_m c_l = \{c_l, c_m\} &= 0 \\ c_l c_m^\dagger + c_m^\dagger c_l = \{c_l, c_m^\dagger\} &= \delta_{lm} \end{aligned} \quad (15)$$

2.2 Bosonic Operators

Bosonic creation and annihilation operators can be defined as

$$\begin{aligned} b_l^\dagger |n_1, \dots, n_{l-1}, n_l, \dots\rangle &= \sqrt{n_l+1} |n_1, \dots, n_{l-1}, n_l+1, \dots\rangle \\ b_l |n_1, \dots, n_{l-1}, n_l, \dots\rangle &= \sqrt{n_l} |n_1, \dots, n_{l-1}, n_l-1, \dots\rangle \end{aligned} \quad (16)$$

Bosonic operators follow commutation relations

$$\begin{aligned} b_l b_m - b_m b_l = [b_l, b_m] &= 0 \\ b_l^\dagger b_m^\dagger - b_m^\dagger b_l^\dagger = [b_l^\dagger, b_m^\dagger] &= 0 \\ b_l b_m^\dagger - b_m^\dagger b_l = [b_l, b_m^\dagger] &= \delta_{lm} \end{aligned} \quad (17)$$

Irrespective of the nature of particles, one can check that $\{|n_1, n_2, \dots\rangle\}$ forms a orthonormal basis for a N -particle system.

$$\langle n'_1, n'_2, \dots | n_1, n_2, \dots \rangle = \delta_{n'_1, n_1} \delta_{n'_2, n_2} \dots \quad (18)$$

Also, a general state $|n_1, n_2, \dots\rangle$ can be written as

$$|n_1, n_2, \dots\rangle = \frac{(a_1^\dagger)^{n_1}}{\sqrt{n_1!}} \frac{(a_2^\dagger)^{n_2}}{\sqrt{n_2!}} \dots |0\rangle \quad (19)$$

where a^\dagger 's can be either bosonic or fermionic creation operators.

3 Observables

Does it make sense to talk of the momentum \vec{p}_i of a single particle i ? The answer is NO, since the particles are indistinguishable. We can only talk about sums such as $\sum_i \vec{p}_i$

3.1 Single Particle Operators

The operators which involve sum over only single particles are known as single particle operators

$$\hat{F}_1 = \sum_i \hat{f}_1(\vec{r}_i, \vec{p}_i) \quad (20)$$

In second quantization, this operator can be written as

$$\hat{F}_1 = \sum_{l,l'} \langle l | \hat{f}_1 | l' \rangle a_l^\dagger a_{l'} \quad (21)$$

where,

$$\langle l | \hat{f}_1 | l' \rangle = \int_r \phi_l^*(r) \hat{f}_1(r, p) \phi_{l'}(r) \quad (22)$$

3.2 Two Particle Operators

The operators which involve sum over two particles are known as two particle operators

$$\hat{F}_2 = \frac{1}{2} \sum_{i \neq j} \hat{f}_2(\vec{r}_i, \vec{p}_i; \vec{r}_j, \vec{p}_j) \quad (23)$$

In second quantization, this operator can be written as

$$\hat{F}_2 = \sum_{l_1, l_2, l_3, l_4} \langle l_1 l_2 | \hat{f}_2 | l_4 l_3 \rangle a_{l_1}^\dagger a_{l_2}^\dagger a_{l_3} a_{l_4} \quad (24)$$

where,

$$\langle l_1 l_2 | \hat{f}_2 | l_4 l_3 \rangle = \int_{r_1, r_2} \phi_{l_1}^*(r_1) \phi_{l_2}^*(r_2) \hat{f}_2(r_1, p_1; r_2, p_2) \phi_{l_4}(r_1) \phi_{l_3}(r_2) \quad (25)$$

The good thing about this representation is that it is independent of the nature of the particles.

4 Change of Basis

Suppose we have creation operators a_λ^\dagger corresponding to the basis $\{|\lambda\rangle\}$. Now we want to go to a different basis $\{|\tilde{\lambda}\rangle\}$. What are $a_{\tilde{\lambda}}^\dagger$ s in terms of a_λ^\dagger s?

Since $\{|\lambda\rangle\}$ is a basis, we can write a state $|\tilde{\lambda}\rangle$ as

$$|\tilde{\lambda}\rangle = \sum_\lambda \langle \lambda | \tilde{\lambda} \rangle |\lambda\rangle \quad (26)$$

Thus,

$$a_{\tilde{\lambda}}^\dagger |0\rangle = \sum_\lambda \langle \lambda | \tilde{\lambda} \rangle a_\lambda^\dagger |0\rangle \quad (27)$$

This gives

$$a_{\tilde{\lambda}}^\dagger = \sum_{\lambda} \langle \lambda | \tilde{\lambda} \rangle a_{\lambda}^\dagger \quad (28)$$

Taking conjugate of the above equation, we get

$$a_{\tilde{\lambda}} = \sum_{\lambda} \langle \tilde{\lambda} | \lambda \rangle a_{\lambda} \quad (29)$$

Example: Suppose a_i^\dagger creates a particle at site i on a lattice. What is operator a_k^\dagger in the momentum space? Using the above formula, we have

$$\begin{aligned} a_k^\dagger &= \sum_i \langle i | k \rangle a_i^\dagger \\ &= \frac{1}{\sqrt{N}} \sum_i e^{ik \cdot R_i} a_i^\dagger \end{aligned} \quad (30)$$

5 Applications of Second Quantization

5.1 Single spin- $\frac{1}{2}$ operator

A spin- $\frac{1}{2}$ can be represented as

$$\{\hat{S}^i\}_{\alpha, \alpha'} = \frac{1}{2} \{\hat{\sigma}^i\}_{\alpha, \alpha'} \quad (31)$$

where, $\hat{\sigma}^i$ s are Pauli matrices

$$\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma^y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad (32)$$

The basis states here are eigen states of S^z i.e. $|\uparrow\rangle$ and $|\downarrow\rangle$. This operator in second quantized language can be written as

$$\begin{aligned} \hat{S}^i &= \sum_{\alpha, \alpha'} c_{\alpha}^\dagger \hat{S}_{\alpha, \alpha'}^i c_{\alpha} \\ &= \frac{1}{2} \sum_{\alpha, \alpha'} c_{\alpha}^\dagger \hat{\sigma}_{\alpha, \alpha'}^i c_{\alpha} \end{aligned} \quad (33)$$

which gives

$$\begin{aligned} S^x &= \frac{1}{2} (c_{\uparrow}^\dagger c_{\downarrow} + c_{\downarrow}^\dagger c_{\uparrow}) \\ S^y &= \frac{1}{2i} (c_{\uparrow}^\dagger c_{\downarrow} - c_{\downarrow}^\dagger c_{\uparrow}) \\ S^z &= \frac{1}{2} (c_{\uparrow}^\dagger c_{\uparrow} - c_{\downarrow}^\dagger c_{\downarrow}) \end{aligned} \quad (34)$$

5.2 Local Density Operator

Local density $\rho(r)$ is defined as

$$\rho(r) = \sum_i \delta(r - r_i) \quad (35)$$

In second quantized language, it is written as

$$\begin{aligned}\rho(r) &= \int d^d r' a^\dagger(r') \delta(r - r') a(r') \\ &= a^\dagger(r) a(r)\end{aligned}\quad (36)$$

Total number of particles are given by

$$\hat{N} = \int d^d r a^\dagger(r) a(r) \quad (37)$$

5.3 Free Electrons

If the potential is constant, then we have free particles. The free particle Hamiltonian is given by

$$\mathcal{H}_0 = \sum_{k\sigma} \frac{k^2}{2m} c_{k\sigma}^\dagger c_{k\sigma} \quad (38)$$

The ground state of such system can be easily determined. For a system of size $L_x \times L_y \times L_z$, the allowed momentum states \vec{k} have components $k_i = 2\pi n_i / L_i$ where $n_i \in \mathbb{Z}$. Each such state because of Pauli exclusion principle can accomodate two electrons (\uparrow, \downarrow). Thus, if we have N electrons, all states upto an energy E_F , called *Fermi energy*, are occupied. The momentum k_F corresponding to Fermi energy ($\frac{k_F^2}{2m}$) is called *Fermi momentum*. All the k points which have smaller momentum than Fermi momentum forms the *Fermi surface*. In second quantized language, the ground state can be written as

$$|FS\rangle = \prod_{|k| < k_F, \sigma} c_{k\sigma}^\dagger |0\rangle \quad (39)$$

In most of the problems, we are interested in excitations about this state. For example, destroying a electron inside Fermi surface and creating one outside. Can we define operators such that this state is the "physical vacuum" of the theory?

$$\tilde{c}_{k\sigma}^\dagger = \begin{cases} c_{k\sigma}^\dagger & \text{if } k > k_F \\ c_{k\sigma} & \text{if } k \leq k_F \end{cases} \quad \tilde{c}_{k\sigma} = \begin{cases} c_{k\sigma} & \text{if } k > k_F \\ c_{k\sigma}^\dagger & \text{if } k \leq k_F \end{cases} \quad (40)$$

We can see that if we apply $\tilde{c}_{k\sigma}$ on $|FS\rangle$, we will get zero.

5.4 Free electrons in a magnetic field

Suppose we have N electrons in a magnetic field. The Hamiltonian for such a system is given by

$$\mathcal{H} = \sum_i \frac{1}{2m} \left(\vec{p}_i - \frac{e\vec{A}(r_i)}{c} \right)^2 - \gamma \sum_i \vec{\sigma}_i \cdot \vec{B}(r_i) \quad (41)$$

The Hamiltonian in the second quantization language can be written as

$$\mathcal{H} = \sum_\sigma \int d^d r \frac{1}{2m} c_\sigma^\dagger(r) \left(-i\vec{\nabla}_r - \frac{e\vec{A}(r)}{c} \right)^2 c_\sigma(r) - \gamma \sum_{\alpha, \alpha'} \int d^d r \left(c_\alpha^\dagger(r) \vec{\sigma}_{\alpha, \alpha'} c_{\alpha'}(r) \right) \cdot \vec{B}(r) \quad (42)$$

5.5 Non-interacting particles

Consider spinless non-interacting particles. The Hamiltonian is given by

$$\mathcal{H} = \sum_i \left[\frac{\hat{p}_i^2}{2m} + V(r_i) \right] \quad (43)$$

In real space basis, the second quantized Hamiltonian can be written as

$$\mathcal{H} = \int d^d r a^\dagger(r) \left[\frac{\hat{p}^2}{2m} + V(r) \right] a(r) \quad (44)$$

where $\hat{p} = -i\vec{\nabla}_r$

5.6 Electrons in a periodic potential

Eigen-states of a periodic Hamiltonian are the Bloch states which are represented as

$$\psi_{kn}(r) = e^{ik \cdot r} u_{kn}(r) \quad (45)$$

where $u_{kn}(r)$ has the same periodicity as $V(r)$. k is the crystal momentum which takes values inside the Brillouin zone and n is the band index. Let us assume that the bands are well separated and we are interested in the lowest band only. The Hamiltonian in the momentum space can be written as

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} \quad (46)$$

5.7 Coulomb Interaction

The term corresponding to Coulomb interaction is given by

$$\mathcal{H}_{ee} = \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|r_i - r_j|} \quad (47)$$

In momentum basis, this can be written as

$$\mathcal{H}_{ee} = \frac{1}{2} \sum_{\{k_i\}, \{\sigma_i\}} \langle k_1 \sigma_1, k_2 \sigma_2 | \frac{e^2}{|r_i - r_j|} | k_4 \sigma_4, k_3 \sigma_3 \rangle c_{k_1 \sigma_1}^\dagger c_{k_2 \sigma_2}^\dagger c_{k_3 \sigma_3} c_{k_4 \sigma_4} \quad (48)$$

Then, the overlap matrix element is given by

$$\begin{aligned} & \langle k_1 \sigma_1, k_2 \sigma_2 | \frac{e^2}{|r_i - r_j|} | k_4 \sigma_4, k_3 \sigma_3 \rangle \\ &= \int d^3 r \int d^3 r' \frac{e^{-ik_1 \cdot r}}{\sqrt{V}} \cdot \frac{e^{-ik_2 \cdot r'}}{\sqrt{V}} \cdot \frac{e^2}{|r - r'|} \cdot \frac{e^{ik_4 \cdot r}}{\sqrt{V}} \cdot \frac{e^{ik_3 \cdot r'}}{\sqrt{V}} \delta_{\sigma_1 \sigma_4} \delta_{\sigma_2 \sigma_3} \\ &= \frac{\delta_{\sigma_1 \sigma_4} \delta_{\sigma_2 \sigma_3}}{V^2} \int d^3 r \int d^3 r' e^{-i(k_1 + k_2 - k_3 - k_4) \cdot r'} e^{-i(k_1 - k_4) \cdot (r - r')} \frac{e^2}{|r - r'|} \\ &= \frac{\delta_{\sigma_1 \sigma_4} \delta_{\sigma_2 \sigma_3}}{V^2} \underbrace{\int d^3 r' e^{-i(k_1 + k_2 - k_3 - k_4) \cdot r'}}_{V \delta(k_1 + k_2 - k_3 - k_4)} \underbrace{\int d^3 \rho e^{-i(k_1 - k_4) \cdot \rho} \frac{e^2}{\rho}}_{\text{Change of variable: } \vec{r} - \vec{r}' = \vec{\rho}} \\ &= \frac{\delta_{\sigma_1 \sigma_4} \delta_{\sigma_2 \sigma_3}}{V^2} \times V \delta(k_1 + k_2 - k_3 - k_4) \times \frac{e^2}{(k_1 - k_4)^2} \\ &= \frac{\delta_{\sigma_1 \sigma_4} \delta_{\sigma_2 \sigma_3}}{V} \delta(k_1 + k_2 - k_3 - k_4) \end{aligned} \quad (49)$$

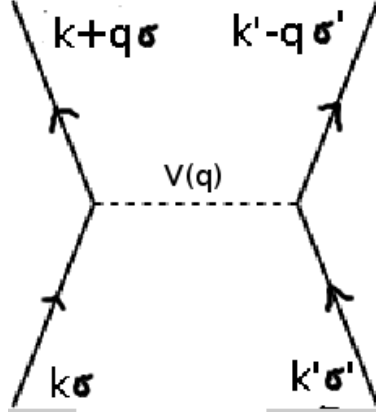


Figure 1: Feynman diagram depicting the interaction of two particles via Coulomb interaction.

We see that the Coulomb interaction conserves the total momentum. Thus,

$$\mathcal{H}_{ee} = \frac{e^2}{2} \sum_{k, k', q, \sigma, \sigma'} c_{(k+q)\sigma}^\dagger c_{(k'-q)\sigma'}^\dagger \left(\frac{1}{q^2} \right) c_{k'\sigma'} c_{k\sigma} \quad (50)$$

This interaction of two particles via Coulomb interaction is shown in the Feynman diagram in fig. 1. Note that for $q = 0$, the matrix element diverges but this term in a lattice is cancelled by the uniform background of positive ionic charge. This model is known as *Jellium model*.

5.8 Tight Binding Model

5.8.1 Wannier States

Suppose we have atomic orbitals localized at atomic sites in a lattice. Let's assume that the "physical extent" of such orbitals is smaller than the inter-atomic spacing. In such cases, we say that the orbitals are tightly bound to the lattice centers. It is thus, convenient to work in the local basis that corresponds to the atomic orbital states of the isolated ion. Wannier state localized at site R_i is defined as

$$|\psi_i\rangle = \frac{1}{\sqrt{N}} \sum_k e^{-ik \cdot R_i} |\psi_k\rangle \quad (51)$$

where $|\psi_k\rangle$'s are the Bloch states. It is easy to see that this set of states forms an orthogonal basis. Thus,

$$|r\rangle = \sum_i \langle \psi_i | r \rangle |\psi_i\rangle \quad (52)$$

This gives us

$$c_{\sigma}^\dagger(r) = \sum_i \psi_i^*(r) c_{i\sigma}^\dagger \quad (53)$$

Similarly, invertng (51) gives us

$$c_{k\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{ik \cdot R_i} c_{i\sigma}^\dagger \quad (54)$$

Thus, Bloch Hamiltonian (46) in this basis becomes

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} = \frac{1}{N} \sum_{ij} \sum_{k\sigma} e^{ik \cdot (R_i - R_j)} \epsilon_k c_{i\sigma}^\dagger c_{j\sigma} \equiv \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} \quad (55)$$

where $t_{ij} = \frac{1}{N} \sum_k e^{ik \cdot (R_i - R_j)} \epsilon_k$ is known as *hopping amplitude* for the electron to go from site i to site j .