Tight-Binding Model in the Second Quantization Formalism

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Contents

1 Second quantization

1.1 Representations and bases

Consider a lattice with N sites labeled by the positions $\mathbf{r}_j$ ($n = 1, \ldots, N$). We can express the state of the lattice in terms of the number of particles at each site:

$$\text{Occupation number representation:} \quad |n_1, \ldots, n_N\rangle \ . \tag{1}$$

We can define creation and annihilation operators in position space that create or annihilate a particle in the jth site:

$$\begin{aligned} \hat{c}_j^\dagger |n_1, \ldots, n_j, \ldots, n_N\rangle &= \sqrt{n_j + 1}\, |n_1, \ldots, n_j + 1, \ldots, n_N\rangle \ , \\ \hat{c}_j |n_1, \ldots, n_j, \ldots, n_N\rangle &= \sqrt{n_j}\, |n_1, \ldots, n_j - 1, \ldots, n_N\rangle \ , \end{aligned} \tag{2}$$

where fermions satisfy the anticommutation relations

$$\text{Fermions:} \qquad \begin{aligned} &\{\hat{c}_{i\sigma}, \hat{c}_{j\sigma'}^\dagger\} = \delta_{ij}\delta_{\sigma\sigma'} \ , \\ &\{\hat{c}_{i\sigma}, \hat{c}_{j\sigma'}\} = \{\hat{c}_{i\sigma}^\dagger, \hat{c}_{j\sigma'}^\dagger\} = 0 \, , \end{aligned} \tag{3}$$

where σ, σ' denote the spin state of the fermions (which we will ignore for simplicity in these notes), and bosons satisfy the commutation relations

$$\text{Bosons:} \qquad \begin{aligned} &[\hat{c}_i, \hat{c}_j^\dagger] = \delta_{ij} \ , \\ &[\hat{c}_i, \hat{c}_j] = [\hat{c}_i^\dagger, \hat{c}_j^\dagger] = 0 \, . \end{aligned} \tag{4}$$

For fermions, the fact that they anticommute means that we need to establish a convention for how we are defining states. For example, we can choose the convention

$$|r_1, r_2, r_3\rangle \equiv \hat{c}_1^\dagger \hat{c}_2^\dagger \hat{c}_3^\dagger |0\rangle \ , \tag{5}$$

so if we permuted one of the creation operators, we would get a minus sign:

$$\hat{c}_1^\dagger \hat{c}_3^\dagger \hat{c}_2^\dagger |0\rangle = -|r_1, r_2, r_3\rangle \ . \tag{6}$$

We can also express the state of the lattice in terms of the number of particles containing different momenta:

$$\text{Momentum space representation:} \quad |\mathbf{k}\rangle \ . \tag{7}$$

In this momentum space representation, we can define creation and annihilation operators in position space that create or annihilate a particle with momentum $\mathbf{k}$:

$$\begin{aligned} \hat{c}_{\mathbf{k}}^\dagger |0\rangle &= |\mathbf{k}\rangle \ , \\ \hat{c}_{\mathbf{k}} |\mathbf{k}\rangle &= |0\rangle \ , \end{aligned} \tag{8}$$

where $|0\rangle$ is the vacuum state.

We can change of basis by inserting the identity $\sum_\alpha |\alpha\rangle\langle\alpha| = \mathbb{1}$ (where α labels the states in any given basis):

$$|\beta\rangle = \sum_\alpha \langle\alpha|\beta\rangle\,|\alpha\rangle\ . \tag{9}$$

In terms of creation and annihilation operators, this is

$$\hat{c}^\dagger_\beta\,|0\rangle = \sum_\alpha \langle\alpha|\beta\rangle\,\hat{c}^\dagger_\alpha\,|0\rangle\ , \tag{10}$$

so we can see that we can also transform from one set of creation and annihilation to another through the relation

$$\hat{c}^\dagger_\beta = \sum_\alpha \langle\alpha|\beta\rangle\,\hat{c}^\dagger_\alpha\,. \tag{11}$$

Using

$$\langle\mathbf{k}|j\rangle = \psi^*_\mathbf{k}(\mathbf{r}_j) = \frac{1}{\sqrt{N}}e^{-i\mathbf{k}\cdot\mathbf{r}_j}\ , \tag{12}$$

where $|j\rangle = \hat{c}^\dagger_j\,|0\rangle$ is the state in which we have a particle in the jth site, we can thus express the creation and annihilation operators in position space in terms of those in momentum space:

$$\begin{aligned}\hat{c}^\dagger_j &= \frac{1}{\sqrt{N}}\sum_\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{r}_j}\,\hat{c}^\dagger_\mathbf{k}\,,\\ \hat{c}_j &= \frac{1}{\sqrt{N}}\sum_\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{r}_j}\,\hat{c}_\mathbf{k}\,.\end{aligned} \tag{13}$$

We can invert these expressions to obtain

$$\begin{aligned}\hat{c}^\dagger_\mathbf{k} &= \frac{1}{\sqrt{N}}\sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j}\,\hat{c}^\dagger_j\,,\\ \hat{c}_\mathbf{k} &= \frac{1}{\sqrt{N}}\sum_j e^{-i\mathbf{k}\cdot\mathbf{r}_j}\,\hat{c}_j\,.\end{aligned} \tag{14}$$

The total number of particles is also conserved going from position space to momentum space, and vice versa:[1]

$$\sum_j \hat{n}_j = \sum_\mathbf{k} \hat{c}^\dagger_\mathbf{k}\hat{c}_\mathbf{k}\,. \tag{15}$$

The following orthogonality relations are also useful:

$$\sum_\mathbf{r} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} = \sum_i e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i} = N\delta_{\mathbf{k}\mathbf{k}'}\ , \tag{16}$$

$$\sum_\mathbf{k} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} = N\delta_{\mathbf{r}\mathbf{r}'}\ . \tag{17}$$

[1] This can also be verified explicitly.

1.2 Single-particle operators (side note)

In first quantization, single-particle operators are operators that can be written as a sum over operators acting on single particles:

$$\hat{F} = \sum_i \hat{f}_i \, , \tag{18}$$

where the operator $\hat{f}_i$ only acts on the ith particle. For example, for a system of N indistinguishable particles, the momentum operator of the system can be written as

$$\hat{\mathbf{p}}_{\text{tot}} = \sum_{i=1}^{N} \hat{\mathbf{p}}_i \, . \tag{19}$$

Single-particle operators are useful because it is unphysical to talk only about the momentum of the ith particle, since the particles are indistinguishable. We can therefore only talk about sums, such as that in the above expression.

In second quantization, single-particle operators can be written in the form

$$\hat{\Omega} = \sum_{\alpha,\beta} \langle \alpha | \hat{\omega} | \beta \rangle \, \hat{c}_\alpha^\dagger \hat{c}_\beta \, . \tag{20}$$

2 Tight-binding Hamiltonian

2.1 Position-space representation

Consider a system of free, non-interacting fermions given by the Hamiltonian

$$\hat{H}_{\text{free}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}}^{\text{free}} \hat{c}_{\mathbf{k}\sigma}^\dagger \hat{c}_{\mathbf{k}\sigma} \, , \tag{21}$$

where σ labels the spin states (for example, for spin-1/2 fermions, $\sigma \in \{\uparrow, \downarrow\}$) and

$$\epsilon_{\mathbf{k}}^{\text{free}} = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \tag{22}$$

is the energy dispersion relation of a free particle. We can express this Hamiltonian in position space (using Eqs. 14) as

$$\hat{H}_{\text{free}} = \frac{1}{N} \sum_{i,j,\sigma} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}^{\text{free}} e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} \, , \tag{23}$$

where N is the number of available $\mathbf{k}$ states (or equivalently, the number of positions the fermions can be in), $\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma}$ annihilates a fermion in the spin state σ at $\mathbf{r}_j$ and creates one in the spin state σ at $\mathbf{r}_i$, which we can physically interpret as a fermion in the spin state σ going from $\mathbf{r}_j$ to $\mathbf{r}_i$. Defining

$$\tilde{t}_{ij} \equiv \frac{1}{N} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}^{\text{free}} e^{i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \,, \tag{24}$$

the Hamiltonian then reads

$$\hat{H}_{\text{free}} = \sum_{i,j,\sigma} \tilde{t}_{ij} \hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} \,. \tag{25}$$

Let's now consider the case where these non-interacting fermions live on a Bravais[2] crystal lattice with a potential well located at each of the lattice sites. Note that these potential wells will change the energy dispersion relation of the fermions, so $\tilde{t}_{ij}$ will also change too; we will refer to this new parameter as the *hopping amplitude* t_{ij}. The fermions will now tend to become more localized to the lattice sites and it will be harder for a fermion to "hop" to sites that are far away (t_{ij} will be very small if $|\mathbf{r}_i - \mathbf{r}_j|$ is large). In the tight-binding approximation, we assume

$$t_{ij} = \begin{cases} -t \,, & i \text{ and } j \text{ are nearest neighbors} \\ 0 \,, & \text{otherwise} \end{cases} \,, \tag{26}$$

so we obtain the *tight-binding Hamiltonian*

$$\hat{H}_{\text{tb}} = -t \sum_{\langle ij \rangle, \sigma} (\hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^{\dagger} \hat{c}_{i\sigma}) \,. \qquad \text{(Bravais lattice)} \tag{27}$$

We can apply this position-space representation of the tight-binding Hamiltonian to non-Bravais lattices too if we are careful enough. For example, for a crystal with a bipartite lattice, such as graphene, we must distinguish fermions on the two sublattices by assigning them different fermionic operators, so the tight-binding Hamiltonian reads

$$\hat{H}_{\text{tb}} = -t \sum_{\langle ij \rangle, \sigma} (\hat{a}_{i\sigma}^{\dagger} \hat{b}_{j\sigma} + \hat{b}_{j\sigma}^{\dagger} \hat{a}_{i\sigma}) \,. \qquad \text{(bipartite lattice)} \tag{28}$$

2.2 Momentum-space representation

In order to obtain a momentum-space representation of the tight-binding model, we will first rewrite the sum over nearest neighbors as

$$\sum_{\langle ij \rangle, \sigma} (\hat{c}_{i\sigma}^{\dagger} \hat{c}_{j\sigma} + \hat{c}_{j\sigma}^{\dagger} \hat{c}_{i\sigma}) = \frac{1}{2} \sum_{i,\sigma} \sum_{\boldsymbol{\delta}} (\hat{c}_{i\sigma}^{\dagger} \hat{c}_{i+\boldsymbol{\delta},\sigma} + \hat{c}_{i+\boldsymbol{\delta},\sigma}^{\dagger} \hat{c}_{i\sigma}) \,, \tag{29}$$

where the sum over $\boldsymbol{\delta}$ is carried out over the nearest-neighbor vectors $\boldsymbol{\delta}_1, \boldsymbol{\delta}_2, \ldots, \boldsymbol{\delta}_q$, the operator $\hat{c}_{i+\boldsymbol{\delta},\sigma}$ annihilates a fermion in a spin state σ at the site whose position is $\mathbf{r}_i + \boldsymbol{\delta}$,

[2] A Bravais lattice is a lattice in which there is only one atom per unit cell, so all atoms in the lattice are equivalent.

and the factor of 1/2 is to avoid double counting. Then, rewriting the fermionic operators in momentum space using Eqs. 13 gives

$$\begin{aligned}\hat{H}_{\rm tb} &= -\frac{t}{2N}\sum_{i,\sigma}\sum_{\boldsymbol{\delta},\mathbf{k},\mathbf{k}'}(e^{-i\mathbf{k}\cdot\mathbf{r}_i}e^{i\mathbf{k}'\cdot(\mathbf{r}_i+\boldsymbol{\delta})}\hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}'\sigma} + e^{-i\mathbf{k}'\cdot(\mathbf{r}_i+\boldsymbol{\delta})}e^{i\mathbf{k}\cdot\mathbf{r}_i}\hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}'\sigma})\\ &= -\frac{t}{2}\sum_{\boldsymbol{\delta},\mathbf{k},\sigma}(e^{i\mathbf{k}\cdot\boldsymbol{\delta}} + e^{-i\mathbf{k}\cdot\boldsymbol{\delta}})\hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma}\\ &= -t\sum_{\boldsymbol{\delta},\mathbf{k},\sigma}\cos(\mathbf{k}\cdot\boldsymbol{\delta})\hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma}\,,\end{aligned}$$

where N is the number of sites on the lattice, and in the second line we have used Eq. 16. We therefore find that the momentum-space representation of the tight-binding Hamiltonian is

$$\hat{H}_{\rm tb} = \sum_{\mathbf{k},\sigma}\epsilon^{\rm tb}_{\mathbf{k}}\hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma}\,, \tag{30}$$

where

$$\epsilon^{\rm tb}_{\mathbf{k}} = -t\sum_{\boldsymbol{\delta}}\cos(\mathbf{k}\cdot\boldsymbol{\delta}) \tag{31}$$

is the system's energy dispersion relation.

2.3 Examples

2.3.1 1D chain

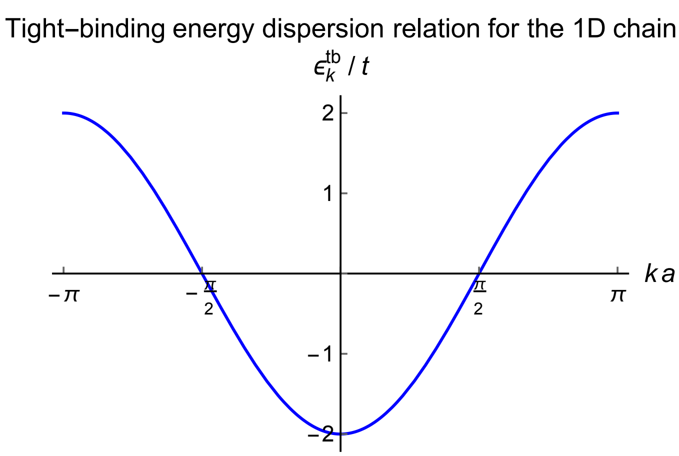
For the 1D chain, the nearest-neighbor vectors are

$$\delta_1 = a\,, \qquad \delta_2 = -a\,, \tag{32}$$

where a is the lattice constant, so the energy dispersion relation is

$$\begin{aligned}\epsilon^{\rm tb}_k &= -t[\cos(ka) + \cos(-ka)]\\ &= -2t\cos(ka)\,.\end{aligned} \tag{33}$$

A plot of this is shown below.



The tight-binding Hamiltonian thus reads

$$\hat{H}_{\text{tb}} = -2t \sum_{k,\sigma} \cos(ka) \hat{c}^\dagger_{k\sigma} \hat{c}_{k\sigma} \,. \tag{34}$$

2.3.2 2D square lattice

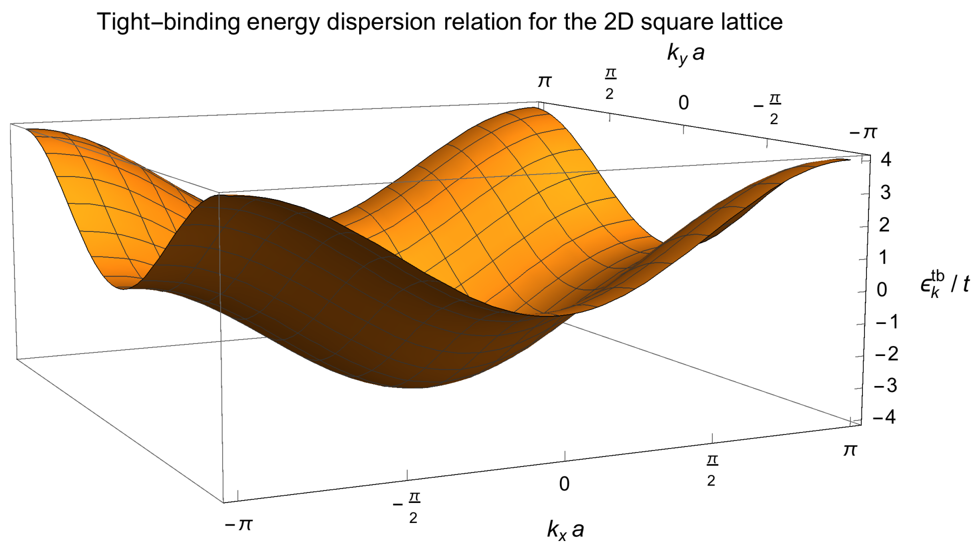
For the 2D square lattice, the nearest-neighbor vectors are

$$\delta_1 = a\hat{\mathbf{x}} \,, \qquad \delta_2 = -a\hat{\mathbf{x}} \,, \qquad \delta_3 = a\hat{\mathbf{y}} \,, \qquad \delta_4 = -a\hat{\mathbf{y}} \,, \tag{35}$$

where a is the lattice constant, so the energy dispersion relation is

$$\begin{aligned} \epsilon^{\text{tb}}_{\mathbf{k}} &= -t[\cos(k_x a) + \cos(-k_x a) + \cos(k_y a) + \cos(-k_y a)] \\ &= -2t[\cos(k_x a) + \cos(k_y a)] \,. \end{aligned} \tag{36}$$

A plot of this is shown below.



The tight-binding Hamiltonian thus reads

$$\hat{H}_{\text{tb}} = -2t \sum_{\mathbf{k},\sigma} [\cos(k_x a) + \cos(k_y a)] \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} \,. \tag{37}$$

References

[1] Christophe Mora. Introduction to Second Quantization. `http://www.phys.ens.fr/~mora/lecture-second-quanti.pdf`.

[2] Sandeep Pathak. An Introduction to Second Quantization. `http://www.phys.lsu.edu/~jarrell/COURSES/ADV_SOLID_HTML/Other_online_texts/Sandeep_Pathak/second_quantization_orig.pdf`, 2010.