Lecture 1.1

Fermion operators and hopping bands

Most of our model Hamiltonians are naturally written in the language of creation and annihilation operators; and – in this text, at least – the particles usually move on lattices, not in the continuum. Therefore, we begin with fast tutorials on lattice hopping, Sec. 1.1 A, and on operator formalism, Sec. 1.1 B. To follow this text, you must know the creation/annihilation operator commutation relations; how they are used in algebraic manipulations of strings of operators; and how kinetic energy terms, single-particle potentials, and pair potentials are written in terms of creation/annihilation operators, which are all explained in Sec. 1.1 B.

Realistic Hamiltonians are local, meaning they connect sites within some bounded distance in direct space. Of course, locality in direct space is associated with nonlocality in Fourier space, and vice versa. This duality – localized versus extended – will be a recurring theme in the course. In particular, the kinetic energy term of the Hamiltonian is intrinsically diagonal in Fourier space, whereas the (single-particle) potential energy is diagonal in direct space. Depending on the situation, either term may dominate. Consequently, you must learn to switch between the real-space and the Fourier space version of any formula, as outlined in Sec. 1.1 C. When facing a new model (to build, solve, or just to grasp), you will ask: is this more easily (or naturally) handled in direct space, or in Fourier space?

The other key notion in this lecture, recurring in all the following ones, is “second-order off-diagonal perturbation theory” [Sec. 1.1 E]. The familiar second-order energy correction due to excited states, is, of course, diagonal in state space; this is the generalization to an off-diagonal second-order term. This technique is our basic tool for getting an effective Hamiltonian, after simplifying a model by restricting its state space to the (degenerate!) ground states of the zero-order term.

Many textbooks have an appendix about second quantization; I like the one in O. Madelung, Introduction to Solid State Theory (Springer, 1978), and also the one in G. Rickayzen, Greens Functions and Condensed Matter App. A and Table A.1; a few of the other texts are A. Auerbach, Interacting electrons and quantum magnetism; Appendix A L. P. Lévy, Magnetism and Superconductivity, App. B; J. R. Schrieffer, Theory of superconductivity, Appendix; W. A. Harrison, Solid State Theory, pp. 399-412.
1.1 A Hopping model: single-particle solution

Before tangling with many-fermion states and creation operators, let’s first face the lattice formulation of a single particle’s motion. Our basis is the $N$ states $|r_i\rangle$, meaning the particle is in the orbit on site $r_i$; and $\langle r'|r_i\rangle \equiv \delta_{r_i,r'}$. The general hopping Hamiltonian, with translational invariance, is

$$\hat{H}_{\text{hop}} \equiv - \sum_{rr'} t(r-r') |r'| \langle r| \quad (1.1.1)$$

In the particular case of a one-dimensional chain with nearest-neighbor hopping, this is

$$\hat{H}_{\text{hop}} |r\rangle = -t (|r+a\rangle + |r-a\rangle). \quad (1.1.2)$$

(We assume periodic boundary conditions, so $r \pm a$ is always understood modulo $L$.)

**About the hopping model**

Our “hopping Hamiltonian” is mathematically identical to the “tight-binding” approach to electron bands, which is described in every introductory solid-state course. However, our intent is significantly different here. When the tight-binding approximation is used to compute a real band structure, one relates the basis states $|r\rangle$ to specific atomic orbitals, and one sets $\varepsilon_0$ to the corresponding atomic level. Then one must overcome the fact that the atomic orbitals are *not* mutually orthogonal. Our adoption of the “hopping” model for non-interacting electrons is more akin to the use of the free-electron model in the theory of metals; we anticipate that every independent-electron model will yield similar qualitative behavior, so we might as well adopt the simplest one. Furthermore, the discreteness of the positions is reflected in the discrete number of parameters needed to specify a model; for example, when we admit interactions, we could limit them to those on the same site (one parameter, in e.g. the Hubbard model).

A convenience of the lattice hopping formulation is that we have just one band to deal with, whereas a continuum model would have an infinite number of bands. The one band of the lattice model corresponds, not necessarily to the lowest band of the continuum model, but the one “where the action is”. As you know, thanks to Fermi statistics the usual situation is that the lowest bands are completely filled, hence inert and (to the model builder) dispensable.

**Solving the hopping model**

In view of the lattice symmetry, we anticipate that the eigenstates have a well-defined crystal wavevector. Hence we’ll want to transform to the Fourier states

$$|k\rangle \equiv \frac{1}{\sqrt{N}} \sum_r e^{ik \cdot r} |r\rangle. \quad (1.1.3)$$

Inserting (1.1.3) into (1.1.1) we obtain

$$\hat{H}_{\text{hop}} |k\rangle = \frac{1}{\sqrt{N}} \sum_{rr'} t(r-r') e^{ik \cdot r} |r'\rangle. \quad (1.1.4)$$

$$= \frac{1}{\sqrt{N}} \left( \sum_R e^{i k \cdot R} \right) \left( \sum_{r'} e^{i k \cdot r'} |r'\rangle \right) = \epsilon(k) |k\rangle.$$
where the dispersion relation

$$\epsilon(k) = \sum_{\mathbf{R}} t(\mathbf{R}) e^{i \mathbf{k} \cdot \mathbf{R}}$$  \hspace{1cm} (1.1.5)$$
is the Fourier transform of the hopping. In the one-dimensional chain (1.1.2),

$$\epsilon(k) = -2t \cos ka$$  \hspace{1cm} (1.1.6)$$
as shown in Fig. 1.1.1. The “band width” $\epsilon_B$ – an important parameter – is defined as the difference of the maximum and minimum values of $\epsilon(k)$. For the dispersion in (1.1.6), $\epsilon_B = 4t$.

![Dispersion relation (1.1.6) (with $\epsilon_0 = 0$) for hopping on a 1D chain, plotted in the 1D Brillouin zone. Hatching shows states occupied by fermions, at half filling.](image)

Figure 1.1.1:

Small-$k$ limit: hopping operator as a kinetic energy

One way to connect the familiar Schrödinger equation to the hopping model is to view the latter as a discretization of a free continuum electron. So for the chain

$$|\psi\rangle \equiv \sum_r \psi(r)|r\rangle.$$  \hspace{1cm} (1.1.7)$$

Acting with the Hamiltonian (1.1.2) gives

$$\hat{\mathcal{H}}_{\text{hop}}|\psi\rangle = -2t|\psi\rangle + (-t) \sum_r \psi(r) \left[ |r-a\rangle + |r+a\rangle - 2|r\rangle \right]$$

$$= -2t|\psi\rangle + (-t) \sum_r \left[ \psi(r+a) + \psi(r-a) - 2\psi(a) \right]|r\rangle$$  \hspace{1cm} (1.1.8)$$

Taylor expanding $\psi(r \pm a)$ to second order, you can see second difference of $\psi(r)$ in brackets approximates $a^2 d^2 \psi(r)/dr^2$ (provided $\psi(r)$ varies slowly compared to $a$.) In other words, (1.1.8) reduces to the continuum time-independent Schrödinger equation:

$$\hat{\mathcal{H}}_{\text{hop}}|\psi\rangle \approx \left\{ -2t - \frac{\hbar^2}{2m_\ast} \frac{d^2}{dr^2} \right\} \psi(r) = E\psi(r).$$  \hspace{1cm} (1.1.9)$$

The effective mass $m_\ast$ can be read off, namely

$$\frac{\hbar^2}{2m_\ast a^2} = t.$$  \hspace{1cm} (1.1.10)$$
Indeed, for our lattice model, $\hat{H}_{\text{hop}}$ plays exactly the role that the kinetic-energy operator $-i\hbar^2 \nabla^2 / 2m_e$ does in a continuum. For example, if you confine a particle in a potential well, the $\hat{H}_{\text{hop}}$ part of the energy grows as the well dimensions shrink. And in the “semiclassical” approximation (developed in basic solid-state texts) $\hat{H}_{\text{hop}}$ acting on a wavepacket with crystal momentum $\mathbf{k}$ propagates it at the group velocity given by $\hbar v_g(\mathbf{k}) \equiv \nabla_\mathbf{k} \epsilon(\mathbf{k})$. Therefore, I will sometimes call $\hat{H}_{\text{hop}}$ the “kinetic energy term”. It is the kinetic energy in exactly the same sense that the band effective mass is a real mass. (But if you view $\hat{H}_{\text{hop}}$ as a tight-binding approximation of electronic band structure, then $t$ is the amplitude to tunnel from one orbital to the next: at that more microscopic level, $t$ incorporates both kinetic and potential energy contributions.)

**Bloch theorem and translation symmetry**

A remark on the Bloch theorem: in quantum mechanics it is a general law that a symmetry implies a conservation law; in the case of continuous symmetry it is called Noether’s theorem. In the present case the system has a discrete symmetry of translation by lattice vectors; corresponding to this is the conservation (modulo reciprocal lattice vectors) of crystal momentum.

**Particle-hole symmetry**

Observe that the band (1.1.6) has “particle-hole symmetry”: in general, that means $\epsilon(\mathbf{k}) = -\epsilon(\mathbf{k} + \mathbf{Q})$ for some offset $\mathbf{Q}$ (in this case $Q = \pi/a$). If the band is half-filled, too – as is often the case – the entire Fermi sea ground state has particle-hole symmetry. One physical consequence: there are just as many thermally excited holes as excited electrons, hence the Fermi level does not shift with $T$; thermoelectric effects cancel, too (see (Ex. 1.1.3).

Watch out: realistic bands usually don’t have particle-hole symmetry, nor does the free-electron dispersion. In simplifying a model, the model builder may unintentionally introduce a non-generic symmetry, throwing out a key factor for its qualitative behavior. (As Einstein put it, “as simple as possible but not simpler”)

### 1.1 B Second quantization: fermion operators

Here begins a brief tutorial on creation/annihilation operators and the occupation-number representation. This is quantum mechanics in the spirit of the lattice-gas of statistical physics. We set up a discrete Hilbert space for spinless fermions $^3$ on a Bravais lattice in $d$ dimensions with periodic boundary conditions, having one orbital on each of the $N = L^d$ sites. Then by the Pauli exclusion principle the occupation $\rho(\mathbf{r})$ of site $\mathbf{r}$ is either 0 or 1, which gives $M = 2^N$ distinct states (orthogonal by definition) forming the (finite) basis for the Hilbert space.

We postulate that (modulo the phase factor) there is a one-to-one correspondence between independent basis states of the Hilbert space, and the list of site occupations $\{\rho(\mathbf{r})\}$. Compare this to the more elementary representation of a the $N_f$-fermion wavefunction as $\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_f})$. A given configuration of occupations appears as $N_f!$ amplitudes, differing only by permutations of the $\{\mathbf{r}_i\}$ (and constrained to be equal,

$^3$In the real world, the spin-statistics theorem of quantum mechanics ensures that fermions always have spin 1/2 (or any half-odd-integer). But – until we get to magnetic effects! – the sole effects of this is that we must write additional indices on all fermion operators, and we must remember the resulting factors of 2 in our answers.
modulo the sign of the of the permutation which is ±1). The occupation-number language wipes out this awkward redundancy: \( N_f! \) terms in the wavefunction become just one term written \(|0110\ldots\).

The creation operator \( c^\dagger(r) \) is defined to act on the basis states such that if site \( r \) is vacant in \(|\psi\rangle\), then \( c^\dagger(r)|\psi\rangle \) has the same occupations as \(|\psi\rangle\), except that site \( r \) is occupied too. Whereas if site \( r \) is occupied in state \(|\psi\rangle\), then \( c^\dagger(r)|\psi\rangle = 0 \).

The real-space occupation (or density) operator at \( r \) is

\[
\hat{\rho}(r) = c^\dagger(r)c(r).
\]  

(1.1.11)

Define the “vacuum” \(|0\rangle\) as the state with zero occupation. Then all basis states are given by

\[
|\rho_1\rho_2\ldots\rangle = \prod_{i=1}^{N} (c^\dagger(r_i))^{\rho_i}|0\rangle
\]  

(1.1.12)

Each factor makes just one fermion and the product runs over \( N \) sites, and every basis state by construction, is an eigenstate of (1.1.11): \( \hat{\rho}(r_i)|\alpha\rangle = \rho_i|\alpha\rangle \).

\textbf{Anticommutation}

Fermion operators have standard anticommutation relations

\[
\{c(r), c^\dagger(r')\} \equiv c(r)c^\dagger(r') + c^\dagger(r')c(r) = \delta_{rr'}.
\]  

(1.1.13a)

For consistency, we also need

\[c(r)|0\rangle = 0
\]  

(1.1.13b)

for any site \( r \). These questions are the basic tools for simplifying an arbitrary operator (i.e. a polynomial in \( c \)'s and \( c^\dagger \)'s) acting on an arbitrary basis state (i.e. a string of \( c^\dagger \)'s acting on \(|0\rangle\).) One first uses (1.1.13a) to move annihilation operators towards the right and creation operators towards the left. Whenever an annihilation operator reaches \(|0\rangle\), by (1.1.13b) that term is zero and can be dropped.

Eq. (1.1.12) is not trivial, in the case of fermions. Merely listing the occupation numbers does specify a unique state, but only up to an overall sign factor. For example, the commutation relations (1.1.13a) imply \( c^\dagger_i c^\dagger_j|0\rangle = -c^\dagger_j c^\dagger_i|0\rangle \). To define the many-fermion state \(|\rho_1\rho_2\rho_3\ldots\rangle\) properly, you must adopt a conventional ordering of the sites \( \{r_1, r_2, \ldots\} \) then always write the creation operator in that order.  

The wavefunction of our system (or any discrete basis system) is just a vector of \( M \) complex numbers, \( \{\Psi_{\rho_1\rho_2\ldots\rho_N}\} \) where \( M \) is the (very large) number of basis states; for spinless fermions in one orbital per site, \( M = 2^N \), since each site may be empty or full. I will write \( \Psi_\alpha \) where \( \alpha \) is short for the string of occupations that serves as a label for each basis state. The system state is then written \( \sum \Psi_\alpha|\alpha\rangle \). Then the Schrödinger equation is just the matrix equation,

\[
\frac{-\hbar}{i} \frac{d}{dt} \Psi_\alpha = \sum_\beta H_{\alpha\beta} \Psi_\beta.
\]  

(1.1.14)

In other words, the Hamiltonian is the matrix \( (H_{\alpha\beta}) \).

\footnote{The sign change upon switching operators is equivalent to the minus sign for exchange of two fermions’s coordinates in a Schrödinger wavefunction.}

\footnote{For fermions with spin, we need a convention too, e.g. write the up-spin creation operator to the left of the down-spin one on the same site.}
**Hopping Hamiltonian in operators**

In second-quantized form, the “hopping Hamiltonian” reads

$$\hat{H}_{\text{hop}} = - \sum_{r, r'} t(r, r') \left( c^\dagger(r) c(r') + h.c. \right)$$  \hspace{1cm} (1.1.15)

Here $h_{ij}$ means we sum (just once) over each nearest-neighbor pair $(i, j)$, and the “$h.c.$” ("Hermitian conjugate") in this case is just the reverse hopping $c_j^\dagger c_i$. One action of $\hat{H}_{\text{hop}}$ moves just one fermion, which "hops" from one site to a neighbor (hence the name of this model). Thus, when acting on the one-particle subspace, (1.1.15) is completely equivalent to (1.1.1).

But (1.1.15) goes much further, in that it also specifies the evolution of states with any numbers of particles. So on a chain $d = 1$ the term $c_1^\dagger c_2$ annihilates a fermion on site 2 and creates one on site 1, i.e. the states differ by the hopping of a fermion from 2 to 1. Note the economy of the second-quantized notation, in situations where there can be more than one fermion: it encodes $2^{N-2}$ distinct matrix elements, from $|010\ldots0\rangle \rightarrow |100\ldots0\rangle$, up to $|011\ldots1\rangle \rightarrow |101\ldots1\rangle$. (See the example in Fig. 1.1.2.)

Note also – an example of locality (see below) – that if a configuration has well-separated particles, each of them hops in the same fashion it would do if it were the only particle, as our physics common sense would demand.

**Why the number of fermion operators is always even**

Given a Hamiltonian (or other operator), how do we inspect if it is well-posed – whether it could possibly be a physical observable in some system? Of course, the number of real electrons is conserved – so every term should have an equal number of creation and annihilation operators – but this is not absolute: in the most economical description of a superconducting state (Part 7), the Hamiltonian has operators which create or annihilate two electrons. But it is remains true that all terms have an even number of fermion operators: why? We can’t invoke the spin-statistics theorem, which can only be derived in relativistic quantum mechanics.

This is a fairly subtle point which comes down to the locality of physics: if our physical system does not have an interaction with faraway degrees of freedom, then its evolution ought to be independent of them.  \footnote{In the quantized Hall effect (Part 9), the “anion” excitation states do pick up nontrivial phases depending on the motions of faraway anions. But the eigenvalues of local operators aren’t affected by those motions.}

Consider spinless fermions on long a chain of $N$ sites, described by the Hamiltonian

$$\hat{H} = u \left[ c(1) + c^\dagger(1) \right].$$ \hspace{1cm} (1.1.16)

(As an aside, the operator in [...] is its own conjugate, which makes it a “Majorana fermion”). Let $|\Psi\rangle = \left( |0\rangle - c^\dagger(1)|0\rangle \right) / \sqrt{2}$. This clearly has eigenvalue $-u$; it’s one of
1.1 C. SECOND QUANTIZATION AND FOURIER SPACE

the ground states of (1.1.16). But what if we stick another fermion into site $N$, letting $|\Psi'\rangle = c^\dagger(N)|\Psi\rangle$? It is easy to evaluate $\mathcal{H}|\Psi'\rangle$ by anticommuting, and when the dust settles we find $|\Psi'\rangle$ has a different eigenvalue $+u$. This contradicts the locality condition, hence $\mathcal{H}$ is no good. (Locality can rule out other bad kinds of Hamiltonian, too.)

Why second quantization: yet more on locality

A brief philosophical digression: the handiness of the creation/annihilation operator formalism is a consequence of the nature of physics. If we had, say, a random Hamiltonian, with comparable matrix elements between any pair of states, this would look no simpler in second-quantized form: one might as well simply list all $2^N \times 2^N$ matrix elements. The formalism is adapted to the physical laws. But real Hamiltonians are local: that is, a typical term involves only a few sites within a bounded range. (That term might e.g. be the hop of a single particle from one site to a nearby one, or it might be a potential interaction between two particles on nearby sites.) This is why a physical operator, which in principal has very many possible matrix elements, reduces to one or two terms when written using creation/annihilation operators, as in the “hopping Hamiltonian” (1.1.15).

1.1 C Second quantization and Fourier space

Solid state physics traditionally deals with crystals – its central dogma is periodicity. The translational symmetry of the crystal lattice (or of free space) permits us to vastly simplify the problem by Fourier transforming.

In particular, a non-interacting (electron or phonon) Hamiltonian separates (in Fourier space) into disjoint blocks, each labeled by a crystal wavevector $\mathbf{k}$. The eigenenergies were given by a dispersion relation, a continuous function $\omega_\nu(\mathbf{k})$ or $\epsilon_\nu(\mathbf{k})$ [where $\nu$ is a band index.] Not surprisingly, we will Fourier transform the creation/annihilation operators and several other mathematical objects as well.

Creation/annihilation operators in Fourier space

Our models will be written in a lattice form wherever possible; hence “momentum” means “crystal momentum” unless otherwise noted. Our Fourier transforms are then discrete, which has the great convenience (in checking equations) that the transformed quantity has the same dimensions. Following Ashcroft and Mermin, I normalize Fourier transforms of particle states with a $1/\sqrt{N}$ factor, so the inverse transform, conveniently, has a $1/\sqrt{N}$ factor too. As usual, there are $N$ discrete values of $\mathbf{k}$ permitted by the periodic boundary conditions. Our Fourier-space creation operator $\tilde{c}^\dagger$ is

$$\tilde{c}^\dagger_{\mathbf{k}} \equiv \frac{1}{\sqrt{N}} \sum_\mathbf{r} e^{-i\mathbf{k} \cdot \mathbf{r}} c^\dagger(\mathbf{r}) \tag{1.1.17}$$

The state $\tilde{c}^\dagger_{\mathbf{k}}|0\rangle$ created by this operator is simply the Bloch state $|\mathbf{k}\rangle$ defined in (1.1.3). You can check ([(Ex. 1.1.4)]) that $\{\tilde{c}^\dagger_{\mathbf{k}}, \tilde{c}^\dagger_{\mathbf{k}'}\} = \delta_{\mathbf{k}=\mathbf{k}'}$. [I will define “\textit{\textbf{Condition}}” to be unity

7To avoid confusing the Fourier and direct space operators, many books write the latter using $\psi^\dagger$ and $\psi$ rather than $c^\dagger$ and $c$; I prefer to reserve the letter $\psi$ for wavefunctions. In one dimensional case, I’ll place a tilde “$\tilde{\psi}^\dagger$” on the Fourier operator to reduce the notational confusion with $c^\dagger_i$.}
(zero) when Condition is true (false). Correspondingly,
\[ c^\dagger(r) \equiv \frac{1}{\sqrt{N}} \sum_k e^{+i\mathbf{k} \cdot \mathbf{r}} \tilde{c}_k \] (1.1.18)

The hopping Hamiltonian was off-diagonal in the real-space basis, but \((\text{Ex. 1.1.4})\) it becomes diagonal in the Fourier basis, just like its single-particle analog (1.1.4):
\[ \hat{H}_{\text{hop}} = \sum_k c(k) \tilde{c}_k^\dagger \tilde{c}_k \] (1.1.19)

**Many-electron eigenstates in Fourier space**

Just what is the many-fermion eigenstate corresponding to a given set of occupations? In elementary quantum mechanics, it would appear as a massive \((\sqrt{N_f} \times \sqrt{N_f})\) determinant designed to ensure proper antisymmetrization, since the particles are identical fermions. But using creation/annihilation operators, the state with occupations \(n_k\) in the Bloch basis has a streamlined form:
\[ \prod_k (\tilde{c}_k^\dagger)^{n_k} |0\rangle. \] (1.1.20)

The \(k\)-space occupation number operator is defined as
\[ \hat{n}_k \equiv \tilde{c}_k^\dagger \tilde{c}_k \] (1.1.21)

Obviously this has eigenvalue \(n_k = 0\) or \(1\) when it acts on the Fourier basis states, but just as obviously the real-space basis states are not eigenstates of this operator!

Then the usual Fermi ground state is
\[ |\Psi_{\text{Fermi}}\rangle = \prod_{k \in S_F} \tilde{c}_k^\dagger |0\rangle \] (1.1.22)

where \(S_F \equiv \{k : \epsilon(k) < E_F\}\). In particular, in the 1D hopping model (in which \(\epsilon(k)\) is monotonic with \(k\) up to the zone boundary) or for a free-electron \(\epsilon(k)\), we can simply write the Fermi sea wavefunction \(|\Psi_{\text{Fermi}}\rangle = \prod_{|k| < k_F} \tilde{c}_k^\dagger |0\rangle\). The real-space correlations of this wavefunction are nontrivial and will be studied in Lec. 1.2.

**Duality of direct space and Fourier space**

There is an obvious similarity between (1.1.11) and (1.1.21) the real-space density operator \(\hat{\rho}(\mathbf{r})\) and the Bloch state occupation \(n_k\). But these operators are not related by a Fourier transform; the actual Fourier transform of the density is \(^8\)
\[ \hat{\rho}_q = \sum_{\mathbf{R}} e^{-i\mathbf{q} \cdot \mathbf{r}} \hat{\rho}(\mathbf{r}) \sum_{\mathbf{p}} \tilde{c}_p^\dagger \tilde{c}_p \] (1.1.23)

since
\[ \hat{\rho}(\mathbf{r}) = \frac{1}{N} \sum_{\mathbf{q}} e^{-i\mathbf{q} \cdot \mathbf{r}} \hat{\rho}_q. \] (1.1.24)

\(^8\)For particle states (1.1.3) and creation/annihilation operators (1.1.19), the discrete Fourier transforms are normalized with \(1/\sqrt{N}\); otherwise, it makes sense to define one Fourier transform with a \(1/N\) normalization, as here, and its inverse with no prefactor.
1.1 D. POTENTIAL ENERGY TERMS

In fact, $\hat{\rho}_n$ and $n_\mathbf{q}$ are completely different operators. The density operator is local in direct space but not in momentum space (it mixes different wavevectors); the Bloch occupation operator is local in Fourier space, but nonlocal in real space.

Hamiltonian terms have the same two behaviors. Hopping (or kinetic energy) terms are local in momentum space, not in direct space; on the other hand, (external or interaction) potential terms are local in direct space but not in momentum space. Depending whether hopping dominates (“weak coupling limit”, nearly free electrons) or interactions (“strong coupling limit”), the model will best be written in momentum space or in direct space. Nontrivial models, of course, include both kinds of terms.

1.1 D Potential energy terms

With the formulas of Sec. 1.1 C we’re now equipped to convert any Hamiltonian into second-quantized form, in either the real space or Fourier space basis. This has already been done with the hopping terms, (1.1.15) and (1.1.19). The other common terms are one-body or two-body potential terms.

In the Schrödinger language, a one-body potential energy operator is written

$$\hat{V} \equiv \sum_j V(r_j),$$

(1.1.25)

where the sum is over electrons (not sites). What is the second-quantized form in real space? Fortunately, Eq. (1.1.25) doesn’t care matter which electron is on which site, and in any state of our basis set, each site has definite occupation number $\rho(r)$. Hence,

$$\hat{\mathcal{H}}_V = \sum_r V(r) \hat{\rho}(r) = \sum_r V(r) c^\dagger(r)c(r)$$

(1.1.26)

Converting to Fourier space, we obtain

$$\hat{\mathcal{H}}_V = \frac{1}{N} \sum_{\mathbf{k},\mathbf{k}'} \hat{V}(\mathbf{k} - \mathbf{k}') \hat{c}^\dagger_{\mathbf{k}'} \hat{c}_\mathbf{k} = \frac{1}{N} \sum_\mathbf{q} \rho_\mathbf{q}$$

(1.1.27)

where $\hat{V}(\mathbf{q})$ and $V(r)$ are related by a Fourier transform. [This should be shown] just like the coefficients in (1.1.15) and (1.1.19). The interaction is diagonal in real space, but off-diagonal in Fourier space. [Note $\hat{V}(-\mathbf{q}) = \hat{V}(\mathbf{q})$, since $V(r)$ is real.]

Particle-particle interactions

It is nearly as easy to transcribe a two-body fermion-fermion potential into second-quantized form as it was for the one-body potential (1.1.26). We start with a sum over electrons $\mathcal{H}_U = \frac{1}{2} \sum_{i,j} U(r_i - r_j)$, with the $\frac{1}{2}$ compensating the double-counting of each $(i,j)$ pair; of course, $U(\mathbf{R}) = U(-\mathbf{R})$. This is very easy to convert into real-space number operators since $\rho(r)$ is either 0 or 1: we get

$$\mathcal{H}_U = \frac{1}{2} \sum_{r,r'} U(r - r') \hat{\rho}(r) \hat{\rho}(r') = \frac{1}{2} \sum_{r,r'} U(r - r') c^\dagger(r)c(r)c^\dagger(r')c(r')$$

(1.1.28)

\[9\text{As we're considering interactions more in advanced than in introductory solid state, we're working more in direct space.}\]
To convert (1.1.28) to Fourier space, simply insert (1.1.24):

$$\mathcal{H}_U = \frac{1}{2} \sum_{\mathbf{q}} \tilde{U}(\mathbf{q}) \hat{\rho}_\mathbf{q} \hat{\rho}_{-\mathbf{q}}$$  \hspace{1cm} (1.1.29)

where

$$\tilde{U}(\mathbf{q}) = \frac{1}{N} \sum_{\mathbf{R}} U(\mathbf{R}) e^{-i\mathbf{q} \cdot \mathbf{R}}$$  \hspace{1cm} (1.1.30)

The dual relationship of different Hamiltonian terms is summarized in Table 1.1.1.

<table>
<thead>
<tr>
<th>hopping term</th>
<th>Direct space</th>
<th>Fourier space</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\sum_{r,r'} t(r-r')c^\dagger(r)c(r')$ (nondiagonal)</td>
<td>$\sum_k \epsilon(k)c^\dagger_k \hat{c}_k$ (diagonal, $n_k$)</td>
</tr>
<tr>
<td>potential term</td>
<td>$\sum_r V(r)c^\dagger(r)c(r)$ (diagonal, $\hat{\rho}(r)$)</td>
<td>$\sum_{kk'} \tilde{V}(k-k')c^\dagger_k \hat{c}_{k'}$ (nondiagonal)</td>
</tr>
<tr>
<td>2-body potential</td>
<td>$\sum_{r,r'} U(r-r')\hat{\rho}(r)\hat{\rho}(r')$</td>
<td>$\sum_k \tilde{U}(k)\hat{\rho}<em>k \hat{\rho}</em>{-k}$</td>
</tr>
</tbody>
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Table 1.1.1: Duality of direct and Fourier space.

### 1.1 Effective Hamiltonians via canonical transformation

The second big idea in this lecture is a bit of elementary quantum mechanics that will be used over and over in later lectures. Say that our Hamiltonian is $\mathcal{H} + \mathcal{H}_0$ where $\mathcal{H}_0$ is a perturbation. Further assume that $\mathcal{H}$ has a degenerate ground state; that’s very common, due to rotational symmetry (e.g. $d$ orbitals in magnetic ions) or the translational symmetry of a lattice. (Indeed, when the physics is interesting, the system is always close to a degeneracy of some sort.) We’re after the low-energy states, which (let’s assume) are built from the ground states of $\mathcal{H}$. Therefore, we want to replace $\mathcal{H} + \mathcal{H}_0$ by an effective Hamiltonian $\tilde{\mathcal{H}}$ (read it “check $\mathcal{H}$”) which acts on a sub Hilbert space, the ground states of $\mathcal{H}$.

When $\langle \alpha | \mathcal{H}_0 | \beta \rangle \neq 0$, we have degenerate first order perturbation theory, and $\tilde{\mathcal{H}}$ splits the states by a (comparatively) large energy. If so, we don’t need to go on, unless there’s a remaining degeneracy; in that case, we press on, using states which also diagonalize $\tilde{\mathcal{H}}$ within the degenerate eigenstates of $\mathcal{H}$.

#### Degenerate second-order perturbation theory

There are two cases. If $\tilde{\mathcal{H}}$ has matrix elements in the smaller subspace, we are done: $\tilde{H}_{\alpha \beta} = \langle \alpha | \mathcal{H}_0 | \beta \rangle$. which is simply degenerate first-order perturbation theory. The second case is that $\langle \alpha | \mathcal{H}_0 | \beta \rangle = 0$ for all $\alpha, \beta$ among the degenerate states;\(^{10}\) this occurs frequently too, and the correct answer is

$$\tilde{H}_{\alpha \beta} = -\sum_n \frac{\mathcal{H}_{\alpha n}' \mathcal{H}_{n\beta}'}{E_n - E_0}$$  \hspace{1cm} (1.1.31)

---

\(^{10}\)This is derived in Landau and Lifshitz, *Quantum Mechanics: Non-relativistic theory* (Pergamon, 1977), eq. (39.4).
where the prime means \( n \) runs over states not in the degenerate manifold, and \( E_0 \equiv E_\alpha = E_\beta \).

I’ll call (1.1.31) “degenerate second-order perturbation theory”; in the familiar non-degenerate case, only a diagonal term appears in (1.1.31) i.e. a correction to the eigenenergy. In many cases, \( \hat{H} \) is itself a quite nontrivial Hamiltonian.

**Off-diagonal second-order perturbation theory**

I will use this name for an extension of (1.1.31) in which the states \( \alpha \) and \( \beta \) in the effective Hamiltonian are *not* exactly degenerate. (Now the reduced Hilbert space must be specified in some fashion other than exact degeneracy.)

We apply the method of canonical transformation. Imagine a unitary transformation \( U \), so the Hamiltonian gets converted into \( \hat{\mathcal{H}} \):

\[
\hat{\mathcal{H}} = U(\mathcal{H} + \hat{\mathcal{H}}')U^\dagger. \tag{1.1.32}
\]

Now choose \( U \) so that \( \hat{\mathcal{H}} \) has no terms first order in \( \hat{\mathcal{H}}' \): to lowest order, it is noninteracting! You simply write \( U = e^{iS} \) with a certain operator \( S \), first order in \( \hat{\mathcal{H}}' \).

To get an explicit formula for \( S \), assume you know the eigenstates \( |\alpha\rangle \) and eigenenergies \( E_\alpha \) of \( \mathcal{H} \). We can assume \( \langle \alpha|\hat{\mathcal{H}}'|\beta\rangle \neq 0 \).

Expand \( \hat{\mathcal{H}} \) given in (1.1.32) to first order in \( \hat{\mathcal{H}}' \) (remembering that \( S \) is first order in \( \hat{\mathcal{H}}' \)). It can be shown that, to ensure \( \hat{\mathcal{H}} \) has no first-order terms, we need

\[
i[S, \hat{\mathcal{H}}] = \hat{\mathcal{H}}'
\]

(1.1.33)

to first order in \( \hat{\mathcal{H}}' \). The unique \( S \) solving this equation is

\[
iS = \sum_{ab} \langle a| \frac{V_{ab}}{E_\alpha - E_\beta} |b\rangle \tag{1.1.34}
\]

(Note that \( a, b \) refer to *any* state, whether or not it is in the submanifold.) Next, expanding to *second* order, we get

\[
\hat{\mathcal{H}} = \mathcal{H} + \frac{1}{2}[iS, \hat{\mathcal{H}}']. \tag{1.1.35}
\]

When this is substituted back, we obtain

\[
\hat{H}_{\alpha\beta} = -\sum_n \frac{1}{2} \left( \frac{1}{E_n - E_\alpha} + \frac{1}{E_n - E_\beta} \right) \mathcal{H}_{\alpha n} \mathcal{H}_{\beta n}. \tag{1.1.36}
\]

Now we have reduced our Hilbert space, at the price of complicating our Hamiltonian with \( \hat{\mathcal{H}} \). We often find this new Hamiltonian is still degenerate, so we need another round of elimination; in this fashion, we may go through several levels of description, and successive degeneracy breakings with smaller and smaller energy scales.

Canonical transformation is how the state \( |\hat{a}\rangle \) (acted on by \( \hat{\mathcal{H}} \)) gets “dressed” compared to the “bare” state \( |\alpha\rangle \) (acted on by \( \mathcal{H} \) or \( \mathcal{H}' \)). After reduction we are working with dressed states \( \{|\hat{a}\rangle\} \). Normally we will leave off the check mark, and for all practical purposes we can manipulate these states as if they were merely \( \{|\alpha\rangle\} \). But if we examine what they are in terms of the original (unreduced) Hilbert space, they in fact contain not only \( |\alpha\rangle \) but admixtures of higher states. The admixture matters since actual experiments (e.g. tunneling) usually involve interaction with free electrons or photons outside your system, which didn’t undergo the same canonical transformation.

\footnote{In the case there was a first-order matrix element, we just work among the subset which were degenerate according to \( \mathcal{H}' \); within that subset, the matrix element of \( \hat{H}' \) is a constant that can be absorbed into the unperturbed Hamiltonian.}
1.1 Examples: hopping models in band structure

Graphene included mainly so we can subsequently refer to this band structure; the other two examples are applications of degenerate second-order perturbation theory.

1. Graphene dispersion relation

Standard “tight-binding” bandstructure formulations may be considered as one example of hopping models. If our single-electron Hilbert space is built from linear combinations of atomic orbitals $|\phi_r\rangle$, we must take into account the nonzero overlap of adjacent orbitals, $\langle \phi_r | \phi_{r'} \rangle \equiv \omega(r - r')$. The translational symmetry makes this easy to handle: the Fourier combinations are orthogonal and need only be normalized, namely $|k\rangle = \tilde{\omega}(k)^{-1/2} \sum_r e^{ik \cdot r} |\phi_r\rangle$, where $\tilde{\omega}(k)$ is just the Fourier transform of $\omega(R)$.

For future use, let’s work out the bandstructure of graphene, a single layer of graphite. Since 2004 these have been isolated and studied experimentally; when rolled up (i.e. with periodic boundary conditions) it forms a carbon nanotube. The sites are a (non-Bravais) honeycomb lattice \textit{SHOULD MAKE A FIGURE} which is bipartite. The nearest neighbors to the even sites are separated by vectors $(a = \sqrt{3})u_m$, for $m = 1; 2; 3$, where $u^{(m)} = [\cos(2\pi m/3), \sin(2\pi m/3)]$ are unit vectors. We take one orbital on each site, which physically is the carbon $p_z$ orbital, and assume a hopping $t$ between these orbitals. (The $p_x$ and $p_y$ orbitals’ larger hopping produces four bands with a large bandgap; two bands are always filled and the other two are empty, so they are inert and omittable.)

A useful trick is to define the Fourier basis states for the even sites (similarly for the odd sites) as \textsuperscript{12}

$$|k_E\rangle \equiv \frac{1}{\sqrt{N}} \sum_{r \text{ even}} e^{ik \cdot r} |r\rangle.$$  \hspace{1cm} (1.1.37)

The result is two bands with dispersions $\epsilon_{\pm}(k) = \pm t|f(k)|$, where

$$f(k) = \sum_{m=1}^{3} e^{i(a/\sqrt{3})k \cdot u^{(m)}}.$$  \hspace{1cm} (1.1.38)

When $k = Q$, where $Q$ is one of the Brillouin zone corners, it happens that

$$e^{i(a/\sqrt{3})Q \cdot u^{(m)}} = e^{2\pi im/3},$$  \hspace{1cm} (1.1.39)

so $\epsilon_{\pm}(Q) = f(Q) = 0$. (This zero is the same as the “extinction” which is seen in diffraction from anything with the same space group; indeed, the unusual band structure is forced by the symmetry and does not depend on being in a tight-binding regime.) The zone has six corners, but modulo reciprocal lattice vectors there are just two inequivalent corners $Q$. Since we have half-filling plus electron-hole symmetry, the Fermi energy must be exactly zero, and the $Q$’s are the two Fermi points of this semi-metal system.

Further, when you Taylor expand the exponentials in (1.1.38), you find $f(Q + \delta k) = (3/2)(\delta k_x + i\delta k_y)$. Thus, near the two Fermi points, the dispersion is

$$\epsilon(Q + \delta k) = \pm \frac{3}{2}t|\delta k|;$$  \hspace{1cm} (1.1.40)

the graph of this function looks like a cone. Near a Fermi point, this function looks like the dispersion of an relativistic electron according to Dirac’s theory of negative-energy

\textsuperscript{12}Defining the phase factors by the actual site positions, rather than the Bravais lattice points, makes the symmetries much clearer.
1.1 X. EXAMPLES: HOPPING MODELS IN BAND STRUCTURE

states, if its rest mass were zero; consequently, such a dispersion is called a “Dirac spectrum” by field theorists. Electrons in graphene and Bogoliubov quasiparticles in cuprate superconductors (Lec. 8.4).

2. Diatomic chain

Let’s apply the off-diagonal second-order perturbation theory to the hopping problem on a diatomic chain,

$$\mathcal{H}_{\text{diat}} = \mathcal{H}_{\text{hop}} + \mathcal{V}$$

(1.1.41)

with a potential $V(r)$ that alternates $\mp W$ on even and odd sites (Fig. 1.1.3).

Figure 1.1.3: Discrete (diatomic) chain with alternating potentials. Large and small circles indicate even and odd sites. (a). Original model (b). Effective model, with odd sites eliminated. (c) and (d), chains of $d_{xy}$ and $p_y$, or of $d_{x^2-y^2}$ and $p_x$ orbitals respectively, which may be approximated by these models.

This problem is easy to solve exactly by the standard techniques found in introductory solid-state texts ((Ex. 1.1.6)) obtaining the two bands

$$\epsilon_{\pm}(k) = \pm \sqrt{W^2 + (2t \cos ka)^2}.$$  

(1.1.42)

if the unit cell had more than two orbitals; its validity encompasses both limits, $W \ll t$ to $W \gg t$. But to understand it yourself – or for a technique that still gives an answer in a complex geometry – approach it from those limits. The $W \ll t$ (weak potential) limit can be handled in strict analogy to the nearly-free-electron (NFE) approach developed in most introductory texts; the only differences are that the free electron dispersion in the NFE approach gets replaced here by a $W = 0$ hopping band (1.1.6), and the potential only mixes two wavevectors ($q$ and $q + \pi/a$, modulo $2\pi/a$). I will focus on the $W \gg t$ case for this example.

Our zero-order Hamiltonian $\mathcal{H}$ is $V(r)$ here, which has a degenerate ground state, with energy $-W$ in any even site. The perturbation $\mathcal{H}' = \mathcal{H}_{\text{hop}}$ has no first-order matrix elements, so degenerate second-order perturbation theory is in order. Then application of (1.1.31) yields a corrected well energy $\epsilon_{\text{well}}$ and the effective hopping

$$-\tilde{t} \approx -t^2/2W$$  

(1.1.43)
which is basically the amplitude to tunnel from any even site to an adjacent even site via the intervening site with an energy barrier. (Notice our $\mathcal{H}$ acts on a Hilbert space with half the original size, since the odd site states were thrown away.) See (Ex. 1.1.6)

Finally, in light of (1.1.6) the dispersion of the lower band is

$$\epsilon_-(k) \approx \epsilon_{\text{well}} - 2t \cos ka. \quad (1.1.44)$$

You can check (1.1.44) by expanding the exact result (1.1.42) as a Taylor series in $1/W$. (You'll also get a value $\epsilon_{\text{well}}$; it agrees with the formula of ordinary second-order perturbation theory for the amount the energy is reduced from $-W$.) The perturbative approach has an advantage over the exact solution that it doesn't depend on periodicity: an exercise in a later part (see Sec. 3.1 X and Ex. 3.1.3) applying the above “off-diagonal” second-order perturbation theory to hopping on a non periodic (Fibonacci quasiperiodic) chain.

Fig. 1.1.3(c,d) are a one-dimensional cartoon of the alternating Cu $d$ orbitals and O $p$ orbitals found in the CuO$_2$ plane of a high-temperature superconductor, as a real-world system with this sort of band structure. (Of course, in reality both the (c) and (d) orbitals are found on the same chain, giving rise to two bands which differ by their sign under $y$ mirror reflection.) In the usual treatment of that system (see Lec. 8.3 and Lec. 8.4 ), the oxygen $p$ orbitals are eliminated in favor of the copper $d$ orbitals.

3. Hopping in an organic conductor

An interesting set of conducting crystals is based on the big, flat organic molecule BEDT-TTF, which is short for “bis-(ethylenedithia-tetrathiafulvalene)” ; the BEDT-TTF’s are arranged in layers, so the materials are two-dimensional to first approximation.

![Diagram of organic conductor](image)

Figure 1.1.4: Hopping model for organic conductor $\kappa$-(BEDT-TTF)$_2$X. (a). The molecules are schematically represented by dashed ovals with one orbital per molecule and hoppings $t_D$, $t_b$, $t_p$, and $t_q$. [Amusingly, these hoppings have the topology of a triangular lattice.] (b). The effective hopping model each dimer is replaced by one effective site, producing a rectangularly distorted triangular lattice with two kinds of hopping $\tilde{t}_1$ and $\tilde{t}_2$.

Fig. 1.1.4(a) schematically represents the $\kappa$-(BEDT-TTF)$_2$X layer, which has a rectangular Bravais lattice with a glide plane. The BEDT-TTF molecules pair up in dimer, and each dimer donates one electron to the X$^-$ anion, where X could be e.g. Cu(SCN)$_2$. 
So only the “highest occupied molecular orbital” on each BEDT-TTF matters, since the holes will be distributed among these. In the case that $X=I_3$, the hoppings between these orbitals take the values $t_D = 247\text{meV}$, $t_b = 88\text{meV}$, $t_p = 119\text{meV}$, and $t_q = 33\text{meV}$. This is tunneling, sensitive to the intermolecular separations hence to pressure (and substitution of various anions $X$ has the same effects as a change in pressure).

Since $t_D$ (intra-dimer) is clearly the biggest hopping, let’s work in the limit $t_D \gg t_b, t_p, t_q$, rather than solve for the somewhat ungainly band structure. The zero-order Hamiltonian is just the $t_D$ part, which has a binding (antisymmetric) and an antibinding (symmetric) state on every dimer. Thus, we have two $N$-fold degenerate levels with energy $\pm t_D$, each of which broadens into a band when other hoppings are included. The effective Hamiltonian is obtained from degenerate first-order perturbation theory. Fig. 1.1.4(b) shows the result: each dimer gets replaced by one effective site, and we have only two effective hoppings $\tilde{t}_1$ and $\tilde{t}_2$. This gives a simple band structure roughly like the hopping on a triangular lattice. (It turns out $\tilde{t}_1/\tilde{t}_2 = 0.58$ in the case $X=I_3$).

It turns out the Coulomb repulsion is big compared to the kinetic energy, so these materials are a playground of strong correlation physics, with antiferromagnetic and exotic superconducting phases, as well as a metal-insulator transition.\(^\text{13}\)

**Exercises**

**Ex. 1.1.1 Hopping bands**

(a). What would (1.1.6) become on a simple cubic lattice in 3D? By expanding $\epsilon(\mathbf{k})$ to $O(\mathbf{k}^2)$, explicitly verify that the effective mass tensor is isotropic at the bottom of the band and find the effective mass.

(b). Does the hopping dispersion on the simple cubic lattice have particle-hole symmetry? How about on the triangular lattice in 2D?

(c). Show that if a band has particle-hole symmetry and is half-filled, then the chemical potential sticks exactly at zero for all $T$.

**Ex. 1.1.2 (T) Relating one-particle hopping to continuum Schrödinger equation**

(a). How do you change (1.1.8) to get the lattice version of the *time-dependent* Schrödinger equation? (b). One might instead make the connection through the dispersion relation, e.g. (1.1.5): can write it $\epsilon(k) \approx \epsilon_0 + \hbar^2 k^2 / 2m_*$ for $k \ll 2\pi/a$? (What would this give for $m^*$?)

**Ex. 1.1.3 Particle-hole symmetry (T)**

If you have a thermal gradient in a half-filled metal with particle-hole symmetric band, must the charge current cancel? What about the heat current? (Hint: draw the electron and hole currents separately, and consider their contributions.)

**Ex. 1.1.4 Operators in direct and Fourier space**

Whenever a Fourier-space result is required, the recipe is just to substitute (1.1.18) into the real-space Hamiltonian. Then, exchange the order of summation so the sums

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over sites are on they inside; those can always be collapsed, using \( \sum_{\mathbf{r}} e^{i \mathbf{k} \cdot \mathbf{r}} = N \delta_{\mathbf{k}=0} \), until the final result is purely sums over wavevectors.

(a). Verify that the operators defined in (1.1.17) actually do have the proper commutation relations.

(b). Write the inverse Fourier transform (giving \( \hat{c}^\dagger (\mathbf{r}) \) in terms of \( \hat{c}_{\mathbf{k}}^\dagger \)). Verify that this, substituted into (1.1.15), does give (1.1.19). The moral here is that solving a noninteracting particle Hamiltonian is diagonalizing an \( N \times N \) quadratic form (quadratic in creation/annihilation operators).

(c) Confirm the second-quantized hopping Hamiltonian in Fourier space, (1.1.19), deriving the formula for \( \epsilon (\mathbf{k}) \).

(d) Derive (1.1.24) and (1.1.23), the Fourier transform of the density operator.

(e) Derive (1.1.29), the two-body interaction.

(f) What is the commutator \( \left[ \hat{\rho} (\mathbf{r}), \hat{\rho} (\mathbf{r}') \right] \)?

**Ex. 1.1.5 Exact diagonalization with two particles**

Consider a ring of \( L \) sites (\( L \) even) with two spinless fermions hopping as in the Hamiltonian (1.1.15). (Since there is just one spin flavor and one orbital per site, this means the two fermions can never pass each other.) Exact diagonalization is an important computational technique for understanding interacting models; this example is easily done by hand.

Our approach is to build an appropriate basis of two-particle states, which we will represent for short by \( |m,n\rangle \equiv c_m^\dagger c_n^\dagger |0\rangle \). Note that \( |m,n\rangle = -|n,m\rangle \) (!).

Now, since the Hamiltonian is translationally invariant, it conserves total (crystal) wavevector \( \mathbf{K} \). That means that, given a basis state, we can add up translations of the same state with the appropriate phase factors to make a “Bloch state” with the desired \( \mathbf{K} \), e.g.

\[
|1,3\rangle \rightarrow N^{-1/2} \left( |1,3\rangle + e^{i K a} |2,4\rangle + e^{i 2 K a} |3,5\rangle + \ldots + e^{i K (L-3) a} |L-2,L\rangle + e^{i K (L-2) a} |L-1,1\rangle + |L,2\rangle \right)
\]  

(a). Limit yourself to \( \mathbf{K} = 0 \) for simplicity, and let

\[
|\phi_r\rangle \equiv N^{-1/2} \left( |1,1+r\rangle + |2,2+r\rangle + |3,3+r\rangle + \ldots + |L,r\rangle \right)
\]  

These \( |\phi_r\rangle \) constitute a complete basis for the \( \mathbf{K} = 0 \) sector. Here \( 1 \leq r < L/2 \); why does (1.1.46) give zero in the case \( r = L/2 \)?

(b). Work out the action of \( \hat{\mathcal{H}}_{\text{hop}} \) on \( |1,1+r\rangle \) explicitly, by substituting the definition of \( |1,1+r\rangle \) and using the anticommutation relations (plus the vacuum’s properties).

(c). Hence show that \( \hat{\mathcal{H}}_{\text{hop}} |\phi_r\rangle = -2t (|\phi_{r-1}\rangle + |\phi_{r+1}\rangle) \), except when one of the latter two states would be \( |\phi_0\rangle \) or \( |\phi_{L/2}\rangle \). What is \( \hat{\mathcal{H}}_{\text{hop}} |\phi_r\rangle \) in that case?

(d). Within the \( \mathbf{K} = 0 \) subspace, spanned by the \( |\phi_r\rangle \) states as noted above, your Hamiltonian now has the appearance of a single “particle” hopping on a chain, like (1.1.1), but of length \( L/2 \) and with open rather than periodic boundary conditions: a particle in a box! What is the ground state wavefunction and energy?

(e). As a check on your answer in (d), re-construct the eigenfunctions as antisymmetrized products (Slater determinants) of single-particle wavefunctions. The single-particle energies are the same as a chain (but the wavevectors are limited to \( q_l = 2\pi l / L \)).
Let the electrons have wavevectors $q_A$ and $q_B$, and write the product wavefunction $\sum_{m,n} \psi_A(m) \psi_B(n|m,n)$. Then antisymmetrize the result with respect to exchanging the two fermions, and convert to the $|\phi_r\rangle$ basis. Does it match the result of (d)?

(f) (T) (Optional) What changes when $L$ is odd? And how would (c) be modified if $K$ was nonzero?

Ex. 1.1.6 Diatomic chain I: hopping dispersion

(a). Derive the exact result (1.1.42). (Hint: the arithmetic is very much like the diatomic-chain phonon problem, found in most of the introductory texts.)

(b). Expand (1.1.42) in powers of $t/W$, verifying (1.1.44). Show that your value for $\epsilon_{\text{well}}$ is just what ordinary second-order perturbation theory would have told you for the energy in a well.

Ex. 1.1.7 Diatomic chain II: operator change of variables

Consider the diatomic chain hopping model, with $W \neq 0$. Let $\gamma^\dagger_k$ be the creation operator for the lower band.

(a). Write $\gamma^\dagger_k$ as a linear combination

$$\gamma^\dagger_k = \alpha_k \tilde{c}^\dagger_k + \beta_k \tilde{c}^\dagger_{k+\pi/a}. \tag{1.1.47}$$

(b). (T) Why must $\alpha_k$ and $\beta_k$ depend on $W$ only through the ratio $W/t$? Why are there no terms in $\tilde{c}^\dagger_{k'}$ for any $k'$ other than $k$ and $k + \pi/a$?

(c) In the ground state of a half-filled band, what is the difference between $\langle \hat{\rho}_r \rangle$ for even and odd $r$? (Hint: use the result of (b) to write $\langle \hat{\rho}_r \rangle$ in terms of $\gamma^\dagger_k$ and $\gamma_k$.)

Ex. 1.1.8 Canonical transformation

Start assuming a Hamiltonian $\mathcal{H} + \tilde{\mathcal{H}}$.

(a). Verify (1.1.33).

(b). Show that the solution of (1.1.33) is indeed (1.1.34). Set to zero the undefined terms $(0/0)$ in (1.1.34); by our assumptions, none of them is $1/0$. It should be clear that apart from the choice of those undefined terms, (1.1.34) is the unique solution.

(c). Now expand $\mathcal{H}$ to second order to confirm (1.1.35), and substitute this back to confirm (1.1.36).

Ex. 1.1.9 Organic conductor

Refer to Sec. 1.1 X(3) and Fig. 1.1.4.

(a) Starting from Fig. 1.1.4, sketch the lattice representing the original hopping model: place a dot for each “lattice site” (one BEDT molecule) and an edge for all hoppings $t_D, t_b, t_p, t_q$.

(b) Show that $\tilde{t}_1 = t_b/2$ and $\tilde{t}_2 = (t_p + t_q)/2$ for the upper (valence) band, centered at $+t_D$. What would $\tilde{t}_1$ and $\tilde{t}_2$ be for the other band (centered around energy $-t_D$)?

(c) The conventional “setting” of the crystal axes makes Fig. 1.1.4 be the $xz$ plane, with lattice constants $a, c$. The effective lattice is centered rectangular. Obtain the dispersion (for the upper band) $\epsilon(k_x, k_z) = t_D + A \cos(k_x c) + B \cos(k_z a/2) \cos(k_z c/2)$, giving $A$ and $B$ in terms of $\tilde{t}_1$ and $\tilde{t}_2$. 
Figure 1.1.5: Model chains with 3- or 4-site cells. (a) 3-site cell for (Ex. 1.1.10): dimers (intra-dimer hopping $-t_D$) alternate with single sites that have hopping $-t$ to the adjacent sites of the dimers. (b) Effective single-site model with hopping $t$, approximating the 3-site chain; each large disk represents a dimer. (c) Figure for (Ex. 1.1.11): another model chain with EEOO pattern of hoppings

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**Ex. 1.1.10 (T) Chain with dimers and monomers**

Consider the chain shown in Fig. 1.1.5(a,b): this combines ideas from Secs. 1.1 X(2) and 1.1 X(3). Standard tight-binding theory will yield a simple $3 \times 3$ determinant, but don’t even think of anything that complicated or exact. Instead, let your zero Hamiltonian be $t_D$ only, and aim at the lowest band which is built from the bonding orbital on each dimer. What is the effective hopping $t$ and the corresponding dispersion?

**Ex. 1.1.11 (T) Chain with two hoppings $t_E$ and $t_O$**

Imagine a chain [see Fig. 1.1.5(c)] with Hamiltonian

$$\sum_i \left[ (-t_i)(c_i^\dagger c_{i+1} + c.c.) + U_i c_i^\dagger c_i \right] \quad (1.1.48)$$

The unit cell has 4 sites. The potential alternates; we want first to eliminate the high-energy sites. But the sites to be kept are not symmetry equivalent; the even sites have hopping $t_E$ to the high-energy sites, while the odd ones have hopping $t_O$.

Assuming $t_E, t_O \ll U$, what is the effective hopping Hamiltonian for the reduced model (with high energy sites eliminated)?

**Ex. 1.1.12 (T) Bands of $d = 3$ lattice with two-atom basis**

Consider the unusual band structure of graphene. The hexagonal-close-packed and diamond lattices, each with a two-atom basis, are (in some ways) 3D analogs of the honeycomb lattice. Do you think they (can) have a Dirac dispersion, too?

(Hints for organizing your thinking: (i) the diffraction of both cases exhibits extinctions (ii) In graphene the Dirac point happens in the band of $p_z$ orbitals – what orbital would be analogous in these cases?)