\[ H_F = \int d\vec{r} \, U(\vec{r}) \psi^*(\vec{r}) \psi(\vec{r}) \] (1.43)

1.3.2. Kinetic energy

Momentum space

Total kinetic energy for a system with many particles is

\[ K.E. = \int \frac{d\vec{k}}{(2\pi)^d} \epsilon(\vec{k}) n(\vec{k}) \] (1.44)

Here, \( \epsilon(\vec{k}) \) is the dispersion relation of a single particle and \( n(\vec{k}) \) is the number of particles with momentum \( \vec{k} \). In the denominator, \( d \) is the spatial dimension of the system. In second quantization, the quantum operator for \( n(\vec{k}) \) is

\[ n(\vec{k}) = \psi^\dagger(\vec{k}) \psi(\vec{k}) \] (1.45)

Here, \( \psi^\dagger(\vec{k}) \) creates an electron at \( \vec{k} \) and \( \psi(\vec{k}) \) annihilate an electron at \( \vec{k} \). Therefore,

\[ H_K = \int \frac{d\vec{k}}{(2\pi)^d} \epsilon(\vec{k}) \psi^\dagger(\vec{k}) \psi(\vec{k}) \] (1.46)

If we consider nonrelativistic particles \( \epsilon(\vec{k}) = \frac{k^2}{2m} \),

\[ H_K = \int \frac{d\vec{k}}{(2\pi)^d} \frac{k^2}{2m} \psi^\dagger(\vec{k}) \psi(\vec{k}) \] (1.47)

Q: What shall we do for relativistic particles?

A: We cannot just set \( \epsilon(k) = ck \) or \( \epsilon(k) = \sqrt{c^2 k^2 + m_0^2 c^4} \). This is because \( ck \) or \( \sqrt{c^2 k^2 + m_0^2 c^4} \) are not analytic functions (they are singular at \( k = 0 \)). For fermions, it turns out that we need two species of fermions to have a relativistic dispersion. This topic will be discussed latter, when we study the Dirac theory.

Real space

The momentum space creation/annihilation operators and real space creation/annihilation operators are connected by the Fourier transformation. For the annihilation operator,

\[ \psi(\vec{k}) = \int d\vec{r} \, e^{-i\vec{k} \cdot \vec{r}} \psi(\vec{r}) \] (1.48)

The inverse transformation is

\[ \psi(\vec{r}) = \int \frac{d\vec{k}}{(2\pi)^d} \, e^{i\vec{k} \cdot \vec{r}} \psi(\vec{k}) \] (1.49)

The transformation for the creation operators can be obtained by taking the Hermitian conjugate

\[ \psi^\dagger(\vec{k}) = \int d\vec{r} \, e^{i\vec{k} \cdot \vec{r}} \psi^\dagger(\vec{r}) \] (1.50)

\[ \psi^\dagger(\vec{r}) = \int \frac{d\vec{k}}{(2\pi)^d} \, e^{-i\vec{k} \cdot \vec{r}} \psi^\dagger(\vec{k}) \] (1.51)

Therefore, it is easy to check that

\[ H_K = \int \frac{d\vec{k}}{(2\pi)^d} \frac{k^2}{2m} \psi^\dagger(\vec{k}) \psi(\vec{k}) = \int d\vec{r} \frac{\nabla \psi^\dagger(\vec{r}) \nabla \psi(\vec{r})}{2m} \] (1.52)

\[ H_K = \int d\vec{r} \frac{\nabla \psi^\dagger(\vec{r}) \nabla \psi(\vec{r})}{2m} = \int d\vec{r} \frac{1}{2m} \left[ \int \frac{d\vec{k}}{(2\pi)^d} e^{-i\vec{k} \cdot \vec{r}} \psi^\dagger(\vec{k}) \right] \nabla \left[ \int \frac{d\vec{k}}{(2\pi)^d} e^{i\vec{k} \cdot \vec{r}} \psi(\vec{k}) \right] \]
\[
\begin{align*}
&= \int \int d\vec{r} \left( \frac{\vec{k} \cdot \vec{k}}{2m} \right) \phi^\dagger(k) \phi(k) \exp\left( i (\vec{k}\cdot\vec{r}) - \frac{\vec{k} \cdot \vec{k}}{2} \right) \\
&= \int \int d\vec{k} \left( \frac{\vec{k} \cdot \vec{k}}{2m} \right) \phi^\dagger(k) \phi(k) \int d\vec{r} \exp\left( i (\vec{k}\cdot\vec{r}) - \frac{\vec{k} \cdot \vec{k}}{2} \right) \\
&= \int \int d\vec{k} \left( \frac{\vec{k} \cdot \vec{k}}{2m} \right) \phi^\dagger(k) \phi(k) (2\pi)^d \delta(\vec{k} - \vec{\tilde{k}}) = \int \frac{d\vec{k}}{(2\pi)^d} \left( \frac{\vec{k} \cdot \vec{k}}{2m} \right) \phi^\dagger(\vec{k}) \phi(\vec{k}) = \int \frac{d\vec{k}}{(2\pi)^d} \delta(\vec{k}) n(\vec{k})
\end{align*}
\]

1.3.3. Lattice systems

In a lattice, if we ignore the interactions between electrons, the Hamiltonian contains two terms.

\[
H = H_K + H_P = \int d\vec{r} \left[ \nabla \phi^\dagger(\vec{r}) \nabla \phi(\vec{r}) + U(\vec{r}) \phi^\dagger(\vec{r}) \phi(\vec{r}) \right]
\]

(1.54)

where the first term is the kinetic energy and the second term is the lattice potential, where \( U(\vec{r}) \) is a periodic potential. In principle, we could use this Hamiltonian. However, it is not the most convenient way to handle a lattice systems. A more convenient way utilizes Bloch waves and the band structure. In a lattice system, the kinetic energy of a single particle is described by the band structure \( \epsilon_n(\vec{k}) \). Here \( \vec{k} \) is the momentum point in the (reduced) Brillouin zone. Therefore, total energy of the system (if we ignore interactions is)

\[
E = \sum_n \int \frac{d\vec{k}}{(2\pi)^d} \epsilon_n(\vec{k}) n_n(\vec{k})
\]

(1.55)

Here, we sum over all bands \( (\sum_n) \) and the integral is over the first Brillouin zone \( (\frac{\pi}{a}) \). \( n_n(\vec{k}) \) is the occupation number for the quantum state in band \( n \) at momentum \( \vec{k} \). In second quantization, the quantum operator for \( n_n(\vec{k}) \) is

\[
n_n(\vec{k}) = \psi_n^\dagger(\vec{k}) \psi_n(\vec{k})
\]

(1.56)

where \( \psi_n(\vec{k}) \) creates a particles in band \( n \) with momentum \( \vec{k} \). In other words, it is the creation operator for a Bloch wave. \( \psi_n(\vec{k}) \) is the annihilation operator for a Bloch wave. Therefore, the Hamiltonian for non-interacting electrons is

\[
H_K = \sum_n \int \frac{d\vec{k}}{(2\pi)^d} \epsilon_n(\vec{k}) \psi_n^\dagger(\vec{k}) \psi_n(\vec{k})
\]

(1.57)

For simplicity, we will not consider lattices in this chapter. Instead, we will only consider particles moving in free space with dispersion \( \epsilon = \frac{\vec{k}^2}{2m} \). But please keep in mind that for a lattice system, we just need to substitute \( \epsilon = \frac{\vec{k}^2}{2m} \) into the corresponding dispersion for Bloch waves.

Both the kinetic energy part of the Hamiltonian and the potential energy part contain one creation and one annihilation operator. So they are both known as the quadratic terms, or two-fermion terms. If the Hamiltonian only contains these two terms, we call the system a non-interacting system, because there is no interaction between particles in this Hamiltonian.

1.3.4. Interactions

Let’s consider Coulomb interaction between electrons. The total Coulomb energy is

\[
E_{\text{int}} = \frac{1}{2} \int d\vec{r} d\vec{r}' V(\vec{r} - \vec{r}') \rho(\vec{r}) \rho(\vec{r}')
\]

(1.58)

where \( V(\vec{r}) = e^2/\vec{r} \) and \( \rho(\vec{r}) \) is the particle density. In second quantization, we know that particle density is \( \rho(\vec{r}) = \psi^\dagger(\vec{r}) \psi(\vec{r}) \)

Therefore, the interaction part of the Hamiltonian is

\[
H_I = \frac{1}{2} \int d\vec{r} d\vec{r}' V(\vec{r} - \vec{r}') \psi^\dagger(\vec{r}) \psi(\vec{r}) \psi^\dagger(\vec{r}') \psi(\vec{r}')
\]

(1.59)

The interaction term contains four creation/annihilation operators, and thus this term is called a quartic term or a four-Fermi term.

Typically, we reorder the operators using the anti-commutation relation between creation/annihilation operators.
\begin{align*}
H_I &= \frac{1}{2} \int d\vec{\tau} d\vec{\tau}' V(\vec{\tau} - \vec{\tau}') \psi(\vec{\tau}) \psi(\vec{\tau}') \\
&= \frac{1}{2} \int d\vec{\tau} d\vec{\tau}' V(\vec{\tau} - \vec{\tau}') \psi(\vec{\tau}) \psi(\vec{\tau}') \phi(\vec{\tau}) + \frac{1}{2} \int dr dr' V(\vec{\tau} - \vec{\tau}') \psi(\vec{\tau}) \phi(\vec{\tau}') \\
&= \frac{1}{2} \int d\vec{\tau} d\vec{\tau}' V(\vec{\tau} - \vec{\tau}') \psi(\vec{\tau}) \psi(\vec{\tau}') \phi(\vec{\tau}) + \frac{1}{2} \int dr V(0) \psi(\vec{\tau}) \phi(\vec{\tau}) \\
&= \frac{1}{2} \int d\vec{\tau} d\vec{\tau}' V(\vec{\tau} - \vec{\tau}') \psi(\vec{\tau}) \psi(\vec{\tau}') \phi(\vec{\tau}) + \frac{V(0)}{2} N
\end{align*}

where \( N \) is the total number of particles in the system. The last term may look problematic (it is singular), because for the Coulomb interaction, \( V(0) = 1/|0| = \infty \), but this term will not cause any trouble. We can simply drop it, because this term just shifts the total energy by a constant. In a solid state material, this term is canceled by the potential energy from the nucleons.

Very typically, when we write down the Hamiltonian, we put the operators in such an order that creation operators are put on the left and annihilation operators are on the right. This order is called normal order and the procedure to put operators in such an order is known as "normal ordering".

Typically, one use two colons to represent normal ordering. If we put the product of some creation and annihilation operators operator between two colons, it means that we reorder these operators into normal order. For bosons, we just reorder the operators. For fermions, we need an extra factor +1 or -1, depending on whether we have even or odd number of permutations to reorder the operators. For example,

\[ :\psi'(r)\psi(r') := \psi^\dagger(r)\psi(r') \]  (1.62)

\[ :\psi(r')\psi'(r) := -\psi^\dagger(r)\psi(r') \]  (1.63)

\[ :\psi(r')\phi(r) := \psi^\dagger(r)\phi(r') \]  (1.64)

For the interaction terms, instead of using the most straightforward formula,

\[ H_I = \frac{1}{2} \int d\vec{\tau} d\vec{\tau}' V(\vec{\tau} - \vec{\tau}') \psi(\vec{\tau}) \psi(\vec{\tau}') \phi(\vec{\tau}) \phi(\vec{\tau}') \]  (1.65)

we typically use the normal ordered interaction term

\[ H_I = \frac{1}{2} \int d\vec{\tau} d\vec{\tau}' V(\vec{\tau} - \vec{\tau}') \psi^\dagger(\vec{\tau}) \psi^\dagger(\vec{\tau}') \phi(\vec{\tau}) \phi(\vec{\tau}') \]  (1.66)

These two definitions differ by a constant, which doesn’t play any fundamental role. In other words, using normal order shifts the total energy by a constant. In fact, the reason we use normal ordering is because by doing so, the energy of the vacuum state is set to zero. In normal order, annihilation operator is put to the right side. By definition, the vacuum state is destroyed by any annihilation operator

\[ \psi |0\rangle = 0 \]  (1.67)

Therefore,

\[ : H : |0\rangle = \ldots \psi |0\rangle = 0 = 0 |0\rangle \]  (1.68)

So the vacuum state is an eigenstate of \( : H : \) with zero eigen energy.

### 1.3.5. Summary

In this chapter, we consider the simplest case

\[ H = \int d\vec{\tau} \frac{\nabla \psi^\dagger(\vec{\tau}) \nabla \psi(\vec{\tau})}{2m} + \frac{1}{2} \int d\vec{\tau} d\vec{\tau}' V(\vec{\tau} - \vec{\tau}') \psi^\dagger(\vec{\tau}) \psi^\dagger(\vec{\tau}') \phi(\vec{\tau}) \phi(\vec{\tau}') \]  (1.69)

The quadratic term: kinetic energy for non-relativistic particles \( \epsilon = k^2 / 2m \). The quartic term: normal ordered four-Fermi interactions. However, it is important to keep in mind that the conclusions and methods can be generalized easily to other more complicated cases.

### 1.4. Equation of motion for correlation functions

In the Heisenberg picture, the equation of motion of an operator \( X \) is

\[ i \frac{\partial X(t)}{\partial t} = [X(t), H(t)] \]  (1.70)