ICFP Master Program
Condensed Matter Theory (B. Douçot, B. Estienne, L. Messio)
Homework for the fall vacation, 2018

This homework will count for 25% of the total note.

1 Particle current operator on a 1D tight-binding chain

We consider a one-dimensional tight-binding model, with single site orthonormal orbitals denoted by $|n\rangle$, where n runs over integers. Plane-wave states, denoted by $|k\rangle$, are defined as: $|k\rangle = \sqrt{a}\sum_n e^{ikan}|n\rangle$, where a is the lattice spacing. This leads to the following expression for overlaps: $\langle k|k'\rangle = 2\pi \sum_{m\in\mathbb{Z}} \delta(k - k' - \frac{2\pi}{a}m) \equiv 2\pi\delta_{\text{per}}(k - k')$. Because the sum defining $|k\rangle$ runs over integers, we have the periodicity $|k\rangle = |k + \frac{2\pi}{a}\rangle$, so we will often restrict k to the first Brillouin zone (BZ) $|k| \leq \frac{\pi}{a}$. The local orbitals can be expressed in the plane-wave basis as: $|n\rangle = \sqrt{a}\int_{\text{BZ}} \frac{dk}{2\pi}\, e^{-ikan}|k\rangle$. The tight binding orbitals generate an energy band characterized by the dispersion relation $\epsilon(k)$ between energy and wave-vector. This leads to the band Hamiltonian $H_0 = \int_{\text{BZ}} \frac{dk}{2\pi}\epsilon(k)|k\rangle\langle k|$. We will study the effect of a spatially uniform and constant in time electric field E, which will be taken into account by the additional term $-eEa\hat{n}$ in the single particle Hamiltonian, where $\hat{n}$ is the dimensionless position operator $\hat{n} = \sum_{n\in\mathbb{Z}} n|n\rangle\langle n|$, and e is the electron charge.

We will be interested in filling this band with a finite density of spinless fermions. To describe them, we associate to single particle orbitals $|n\rangle$ fermionic creation and annihilation operators $\psi^\dagger(n)$ and $\psi(n)$. Likewise, we also associate to plane-wave states $|k\rangle$ the corresponding fermionic operators $c^\dagger(k)$ and $c(k)$. In the lectures, we have encountered many examples of *single particle operators*, i.e. $A_1 = \sum_{mn} A_{mn}|m\rangle\langle n|$, being extended to operators acting on *fermionic Fock space* by the rule $A_{\text{Fock}} = \sum_{mn} A_{mn}\psi^\dagger(m)\psi(n)$. We will need to adapt this idea to *unitary operators*, which can be obtained by *exponentiating* single particle operators. If $U_1 = e^{-iA_1}$, it induces an operator U_{Fock} on Fock space whose action can be described as follows: starting from an antisymmetrized N-particle state built from single particle states $|\psi_1\rangle$,...,$|\psi_N\rangle$, U_{Fock} returns the antisymmetrized N-particle state built from $U_1|\psi_1\rangle$,...,$U_1|\psi_N\rangle$. Note that it is natural to assume that the vacuum state $|0\rangle$ ($N = 0$) is invariant under the action of U_{Fock}. Exemples of such unitary operators in the present problem are the evolution operator and also the lattice translation operator $\mathcal{T}$. To simplify notations, we will denote operators acting on the single particle Hilbert space, such as A_1 or U_1 and their extension to Fock space A_{Fock} or U_{Fock}, by the *same* symbol A or U. With this explanation, we hope that this will not cause any confusion.

1) Translate all previous definitions related to single particle states and operators in second quantization language. In particular, write down canonical commutation relations compatible with the above normalizations for single particle states. Express $\psi^\dagger(n)$ and $\psi(n)$ in terms of $c^\dagger(k)$ and $c(k)$, and vice-versa. Finally, give the second quantization expression corresponding to the single-particle Hamiltonian $H = H_0 - eE\hat{n}$.

2) Express the local particle density $\rho(n) = \psi^\dagger(n)\psi(n)$ in terms of $c^\dagger(k)$ and $c(k')$ operators.

3) Evaluate $[H_0, c^\dagger(k)c(k')]$, and use this to compute $[H, \rho(n)]$.

4) Recall the definition of Heisenberg operators $A_H(t) = e^{iHt/\hbar}Ae^{-iHt/\hbar}$. We recall that $\frac{dA_H}{dt} = \frac{i}{\hbar}[H, A]_H$. We want to define the particle current operator $J(n)$. For continuous models, one usually starts from the continuity equation $\frac{\partial \rho(x)_H}{\partial t} + \frac{\partial J(x)_H}{\partial x} = 0$, but on a lattice, x is an integer multiple of a, so defining the derivative with respect to x could lead to some ambiguities. To avoid them, we propose to consider two current operators, $J_L(n)$ and $J_R(n)$ defined by:

$$\begin{aligned}
\frac{d}{dt}\left(\sum_{m=n}^{\infty} \rho(m)_H(t) e^{-\eta(m-n)}\right) &= J_L(n)_H(t) \\
\frac{d}{dt}\left(\sum_{m=-\infty}^{n} \rho(m)_H(t) e^{\eta(m-n)}\right) &= -J_R(n)_H(t)
\end{aligned}$$

where η is a small and positive dimensionless number. How do you interpret these definitions? What is the role of η?

5) We define the lattice current operator $J(n)$ by $J(n) = \frac{1}{2}\lim_{\eta\to 0^+}(J_L(n)+J_R(n))$. Show that:

$$J(n) = \int_{\mathrm{BZ}} \frac{dk}{2\pi} \int_{\mathrm{BZ}} \frac{dk'}{2\pi}\, e^{i(k'-k)an}\, \frac{\epsilon(k)-\epsilon(k')}{\hbar}\, \frac{a\cos\left((k-k')a/2\right)}{2\sin\left((k-k')a/2\right)}\, c^\dagger(k)c(k').$$

What do you think of this expression?

6) In the sequel, an important role will be played by the lattice translation operator $\mathcal{T}$ defined by $\mathcal{T}|n\rangle = |n+1\rangle$. Show that $\mathcal{T}|k\rangle = e^{-ika}|k\rangle$, and that the second quantized version of $\mathcal{T}$ obeys $\mathcal{T}\psi^\dagger(n)\mathcal{T}^{-1} = \psi^\dagger(n+1)$, $\mathcal{T}\psi(n)\mathcal{T}^{-1} = \psi(n+1)$, $\mathcal{T}c^\dagger(k)\mathcal{T}^{-1} = e^{-ika}c^\dagger(k)$, and $\mathcal{T}c(k)\mathcal{T}^{-1} = e^{ika}c(k)$.

7) In the following, we shall be mostly interested in many particle states $|\Psi\rangle$ which are translationally invariant, i.e. they are eigenvectors for the lattice translation operator $\mathcal{T}$. Show that, for such states, we have: $\langle\Psi|c^\dagger(k)c(k')|\Psi\rangle = 2\pi n(k)\delta_{\mathrm{per}}(k-k')$ and $\langle\Psi|c(k')c^\dagger(k)|\Psi\rangle = 2\pi(1-n(k))\delta_{\mathrm{per}}(k-k')$, with $0 \le n(k) \le 1$.

8) Use this to simplify the expectation value of $J(n)$ in a translationally invariant state $|\Psi\rangle$. Does the result sound consistent with physical intuition?

2 Dynamics under a constant and uniform electric field

Because we consider a non-interacting problem, with Hamiltonian $H = H_0 - eEa\hat{n}$, it is useful to study first the single particle dynamics.

9) For a single particle system, compute $[\hat{n}, \mathcal{T}]$. Deduce from this that $\mathcal{T}_H(t) = e^{-ieEat/\hbar}\mathcal{T}$.

10) Denoting par $U(t) = e^{-iHt/\hbar}$ the single particle evolution operator, show that we have: $U(t)|k\rangle = e^{i\theta_k(t)}|k+eEt/\hbar\rangle$, for some phase $\theta_k(t)$ which will not play a role in the following discussion. What do you think of this result?

11) We now translate this for the second quantized fermionic system. Show that we get: $U(t)c^\dagger(k)U(t)^{-1} = e^{i\theta_k(t)}c^\dagger(k+eEt/\hbar)$ and $U(t)c(k)U(t)^{-1} = e^{-i\theta_k(t)}c(k+eEt/\hbar)$.

12) Show that, *extended to Fock space*, the result in question **9)** becomes $\mathcal{T}_H(t)|\Psi\rangle = e^{-iNeEat/\hbar}\mathcal{T}|\Psi\rangle$, where $|\Psi\rangle$ is a state with N particles.

13) Let $|\Psi\rangle$ be a translationally invariant many-particle state with a distribution function $n_0(k)$. Show that $|\Psi(t)\rangle = U(t)|\Psi\rangle$ is also a translationally invariant many-particle state with a distribution function $n(k,t) = n_0(k - eEt/\hbar)$. Show that $n(k,t)$ obeys a very simple form of kinetic equation. How do you interpret it?

14) Denote by $J(t)$ the expectation value of the lattice current operator in state $|\Psi(t)\rangle$, in the particular case where $n_0(k)$ is a Fermi-Dirac distribution at zero temperature, i.e. $n_0(k) = 1$ for $|k| \leq k_{\mathrm{F}} \leq \pi/a$ and else $n_0(k) = 0$. What can you say in general for $J(t)$ as a function of t? What do you think of such behavior?

15) Apply this to the particular case of nearest-neighbor hopping, so that $\epsilon(k) = -2W\cos(ka)$. Comment in particular the dependence of the current versus the Fermi momentum k_{F}.

16) Specialize the result in the case of a Galilean invariant free particle dispersion relation $\epsilon(k) = \frac{\hbar^2 k^2}{2m}$, after expressing k_{F} in terms of the particle density n. How do you interpret the qualitative difference with the previous result?

17) Coming back to the situation of question **14)**, give the *linear response* limit for $J(t)$, and compare it to the *exact* response. Are you surprised by such qualitative difference? What kind of physical processes, absent in the present model, could contribute to make the full response closer to its linear approximation?

3 Simple model for relaxation processes

In an attempt to make a slightly more realistic model, we assume that the time evolution of the distribution function $n(k,t)$ is given by a Boltzmann type equation:

$$\frac{\partial n}{\partial t}(k,t) + \frac{eE}{\hbar}\frac{\partial n}{\partial k}(k,t) = \int_{\mathrm{BZ}} \frac{dk'}{2\pi} \left(\gamma_{kk'}(1-n(k))n(k') - \gamma_{k'k}(1-n(k'))n(k) \right)$$

where $n(k,t)$ has been abbreviated as $n(k)$ on the right-hand site to lighten the notation.

18) What kind of physical processes can be modelled by such equation? Which processes are either missing, or are only taken into account approximately?

19) Write down an evolution equation for the kinetic energy density $\langle H_0\rangle(t) = \int_{\mathrm{BZ}} \frac{dk}{2\pi}\epsilon(k)n(k,t)$, and interpret the two terms that contribute to its time derivative.

20) We first take a model where $\gamma_{kk'} = 2\pi\gamma_e\delta(k+k')$. What could be its physical justification?

21) Show that, in this case, the Boltzmann equation becomes linear, and identify its eigenmodes and eigenfrequencies. Indication: use Fourier modes of $n(k,t)$.

22) Show that, for any initial distribution $n_0(k)$, $n(k,t)$ converges at large time t towards a unique stationary distribution, which depends only on the total particle number in the system. What is the average value of the current in this stationary state? What do you think of this result?

23) Now, we consider the Boltzmann equation in which $\gamma_{kk'} = \gamma_{in}$ if $\epsilon(k) \leq \epsilon(k')$ and $\gamma_{kk'} = 0$ if $\epsilon(k) > \epsilon(k')$. What is the physical motivation for such choice?

24) Finding explicitely the stationary state is more difficult in this case, because the Boltzmann equation is non-linear in the distribution function. As an approximation, we consider a shifted Fermi-Dirac distribution $n(k) = 1$ if $-k_\mathrm{F} + q \leq k \leq k_\mathrm{F} + q$ and $n(k) = 0$ elsewhere. Determine q so as to satisfy energy conservation on average, i.e. to enforce that the time derivative of $\langle H_0 \rangle$ is zero. For this, you may assume that E and thus q are small, so that you can linearize the dispersion relation near the Fermi wave vectors: $\epsilon(k) \simeq \epsilon_\mathrm{F} + v_\mathrm{F}(k - k_\mathrm{F})$ for k close to k_F and $\epsilon(k) \simeq \epsilon_\mathrm{F} - v_\mathrm{F}(k + k_\mathrm{F})$ for k close to $-k_\mathrm{F}$.

25) Express the average current in this shifted Fermi-Dirac distribution for this particular value of q. Is Ohm's law satisfied? How to you interpret this?

26) Do you think of possible experimental systems to observe some of the phenomena discussed in this problem?