

# Probability Current and Current Operators in Quantum Mechanics

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## Summary

A quantum particle such as an electron produces electric current because of its motion. That current is associated with the flow of its probability. The form of the wave function that describes the state of a particle determines these currents. At a more advanced level, one can find quantum operators that can act between states, or work together with a density matrix, to define the currents even in a situation such as the mixed states of thermal equilibrium. The ideas and equations used to apply these ideas are summarized here.

## 1 Quantum Particle Motion

One can consider quantum particles of charge  $e$ , mass  $m$ , momentum operator  $\hat{\mathbf{p}}$ , whose dynamics is determined by a nonrelativistic Hamiltonian,

$$\hat{H} = \frac{1}{2m} \left[ \hat{\mathbf{p}} - \frac{e}{c} \hat{\mathbf{A}}(\hat{\mathbf{r}}, t) \right]^2 + e\phi(\hat{\mathbf{r}}, t) + U(\hat{\mathbf{r}}) \quad (1)$$

$c$  is the speed of light,  $\hat{\mathbf{A}}$  is the vector potential,  $\phi$  is the scalar potential, and  $U$  is any other potential, such as that of a crystal lattice, that affects the particles. For this problem, including applied EM fields (which really are responsible for currents in many situations), it is convenient to see that the Hamiltonian depends on a "kinetic momentum" operator,  $\vec{\pi}$ , defined by

$$\vec{\pi} = \hat{\mathbf{p}} - \frac{e}{c} \hat{\mathbf{A}}. \quad (2)$$

In the real space representation of QM, the momentum operator is  $\hat{\mathbf{p}} = -i\hbar\vec{\nabla}$ , and the vector potential depends only on the space coordinates and time. The main topic of these notes is to find and describe the operations and operators that would be used to calculate the electric currents associated with the motion of these particles, assumed to be electrons<sup>1</sup>. That is a useful thing to have, because it will allow for determining their induced electric and magnetic dipole moments, which exhibit themselves in the optical properties of materials.

The main question to be addressed here is: What is the operator for the electric current density? Or, given a particular state of a quantum system, how does one find the distribution of electric current density? By the form of this question, mainly we are concerned with states described in real space, so the interest is primarily in their real space representations, or their real space wave functions.

Charge current is associated with the quantum motion of the charges. But motion in quantum mechanics is probabilistic, hence, the motion one talks about is how the probability for finding the particle moves around with time. So the main idea is that one needs to find a "probability current" that relates to how the probability for locating the electron might be changing with time, when a wave function satisfies a Schrodinger equation based on the above Hamiltonian.

In a semi-classical sense, we need to find the effective velocity operator  $\hat{\mathbf{v}}$  or current density operator  $\hat{\mathbf{j}}$  for one quantum particle. The electric charge density  $\rho_e$  for an individual electron needs

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<sup>1</sup>The charge will be written as  $e$ , although for real electrons that is a negative number,  $e = -4.8 \times 10^{-10}$  esu, in CGS units, or  $e = -1.602 \times 10^{-19}$  coulombs, in SI units. These notes use CGS.

to satisfy a continuity equation that ensures conservation of charge (these are QM expectation values),

$$\frac{\partial}{\partial t}\rho_e(\mathbf{r}) + \nabla \cdot \mathbf{j}(\mathbf{r}) = 0, \quad \text{or} \quad \nabla \cdot \mathbf{j} = -\dot{\rho}_e. \quad (3)$$

Note that these quantities are associated with a single electron (but assume they have the correct units). To get the physical charge and current densities, scale them by the number of electrons  $N$ ,

$$\rho_{Ne} = N\rho_e, \quad \mathbf{J} = N\mathbf{j}. \quad (4)$$

## 1.1 Current density in a wave function

First, consider the usual elementary approach, based on properties of a given arbitrary wave function  $\psi(\mathbf{r}, t)$ . This wave function could be an energy eigenstate of the Hamiltonian, or any mixture of those eigenstates, it really doesn't matter. The wave function evolves according to a Schrödinger equation,  $i\hbar\dot{\psi} = \hat{H}\psi$ , and its complex conjugate satisfies  $-i\hbar\dot{\psi}^* = \hat{H}^*\psi^*$ . The squared wave function gives the probability density, so the charge density is defined to be  $\rho_e = e|\psi|^2$ . One can get the current by looking at changes of  $\rho_e(\mathbf{r}, t)$  with time, which depend on changes in  $|\psi|^2$ :

$$\frac{\partial}{\partial t}|\psi|^2 = \frac{\partial}{\partial t}\psi^*\psi = \dot{\psi}^*\psi + \psi^*\dot{\psi} = \frac{1}{-i\hbar}(\hat{H}^*\psi^*)\psi + \frac{1}{i\hbar}\psi^*(\hat{H}\psi) \quad (5)$$

From the continuity equation, this can be connected to the current we are looking for, by

$$-\vec{\nabla} \cdot \mathbf{j} = e\frac{\partial}{\partial t}|\psi|^2. \quad (6)$$

The Hamiltonian has the nonrelativistic form (1), where the potential  $U(\mathbf{r})$  is assumed to be real. The EM potentials  $\mathbf{A}$  and  $\phi$  also technically must be real, because they describe the real electric and magnetic fields. At some points in calculations they may be taken as complex, but always, it is assumed that such expressions have an implied extra complex conjugate term, to make the total real. Using this Hamiltonian, the potentials cancel out, and only the kinetic energy terms remain,

$$e\frac{\partial}{\partial t}|\psi|^2 = \frac{e}{i\hbar}\frac{1}{2m} [\psi^*(\vec{\pi}^2\psi) - (\vec{\pi}^2\psi)^*\psi] \quad (7)$$

For simplicity of notation, and based on the momentum operator  $\hat{\mathbf{p}} = -i\hbar\vec{\nabla}$ , I introduce the definition,

$$\vec{\pi} = -i\hbar(\vec{\nabla} - i\vec{\alpha}), \quad \text{where} \quad \vec{\alpha} = \frac{e}{\hbar c}\hat{\mathbf{A}}. \quad (8)$$

This gives

$$e\frac{\partial}{\partial t}|\psi|^2 = \frac{e}{i\hbar}\frac{(-i\hbar)^2}{2m} \left\{ \psi^* [(\vec{\nabla} - i\vec{\alpha})^2\psi] - [(\vec{\nabla} + i\vec{\alpha})^2\psi^*] \psi \right\} \quad (9)$$

The scaled vector potential  $\vec{\alpha}$  also is a real function of space and time. When the kinetic momentum is inserted and squared out, the terms depending on  $\vec{\alpha}^2$  can be seen to cancel out. What remains gives two different contributions that produce currents. The first terms depending on  $\nabla^2$  will give the “momentum current”, so I place a subscript  $p$  to denote this part,

$$\left( \frac{\partial}{\partial t} e|\psi|^2 \right)_p = \frac{e}{i\hbar}\frac{(-i\hbar)^2}{2m} [\psi^*(\nabla^2\psi) - (\nabla^2\psi)^*\psi] = \vec{\nabla} \cdot \left\{ \frac{ie\hbar}{2m} [\psi^*(\vec{\nabla}\psi) - (\vec{\nabla}\psi^*)\psi] \right\} \quad (10)$$

Via the continuity equation as in (6), the momentum current contribution (expectation value) is

$$\mathbf{j}_p(\mathbf{r}) = \frac{-ie\hbar}{2m} [\psi^*(\vec{\nabla}\psi) - (\vec{\nabla}\psi^*)\psi] = \frac{e}{2m} [\psi^*(\hat{\mathbf{p}}\psi) + (\hat{\mathbf{p}}\psi)^*\psi] = \frac{e}{m}\text{Re}\{\psi^*(\hat{\mathbf{p}}\psi)\} \quad (11)$$

This is the action on a wave function  $\psi(\mathbf{r}) = \langle \mathbf{r} | \psi \rangle$ . One sees that this depends on an operator  $e\hat{\mathbf{p}}/m$ . However, to apply this formula, the indicated product must be formed, and then the real

part must be taken. There should be a slightly different (and more complicated) method to invent an individual operator whose effect between  $\psi^*$  and  $\psi$  does not require the real part operation. That is considered later in these notes.

The cross terms between  $\vec{\nabla}$  and  $\vec{\alpha}$  give a term which might be called the ‘‘gauge current’’ part,

$$\begin{aligned} \left( \frac{\partial}{\partial t} e|\psi|^2 \right)_A &= \frac{i\hbar e}{2m} \left\{ -i\psi^* \left[ (\vec{\nabla} \cdot \vec{\alpha} + \vec{\alpha} \cdot \vec{\nabla}) \psi \right] - i \left[ (\vec{\nabla} \cdot \vec{\alpha} + \vec{\alpha} \cdot \vec{\nabla}) \psi^* \right] \psi \right\} \\ &= \frac{e\hbar}{2m} \left\{ \psi^* \left[ \vec{\nabla} \cdot (\vec{\alpha}\psi) + \vec{\alpha} \cdot (\vec{\nabla}\psi) \right] + \left[ \vec{\nabla} \cdot (\vec{\alpha}\psi^*) + \vec{\alpha} \cdot (\vec{\nabla}\psi^*) \right] \psi \right\} \end{aligned} \quad (12)$$

Note that the second term is the complex conjugate of the first, so the result is absolutely real. If we assume the Coulomb gauge, then  $\vec{\nabla} \cdot \vec{\mathbf{A}} = 0$  and  $\vec{\nabla} \cdot \vec{\alpha} = 0$ . The relation  $\vec{\nabla} \cdot (\vec{\alpha}\psi) = \vec{\alpha} \cdot \vec{\nabla}\psi$  results, and this simplifies to

$$\left( \frac{\partial}{\partial t} e|\psi|^2 \right)_A = \frac{e\hbar}{2m} \left\{ 2\psi^* \vec{\alpha} \cdot \vec{\nabla}\psi + 2\psi \vec{\alpha} \cdot \vec{\nabla}\psi^* \right\} = \vec{\nabla} \cdot \left( \psi^* \frac{e^2}{mc} \vec{\mathbf{A}}\psi \right) \quad (13)$$

Since  $\vec{\mathbf{A}}$  is real, this object is automatically real and so there is no need for a real part operation in front of it. Thus the gauge current density (expectation value) is

$$\mathbf{j}_A = -\frac{e^2}{mc} \psi^* \vec{\mathbf{A}}\psi \quad (14)$$

and its operator is just  $-e^2 \vec{\mathbf{A}}/mc$ . Therefore the expectation value of the total current density at point  $\mathbf{r}$  in a wavefunction  $\psi(\mathbf{r})$  is

$$\mathbf{j}(\mathbf{r}) = \mathbf{j}_p + \mathbf{j}_A = \text{Re} \left\{ \frac{e}{m} \psi^* \hat{\mathbf{p}}\psi \right\} - \frac{e^2}{mc} \psi^2 \hat{\mathbf{A}}\psi = \text{Re} \left\{ \frac{e}{m} \psi^*(\mathbf{r}) \left( \hat{\mathbf{p}} - \frac{e}{c} \hat{\mathbf{A}} \right) \psi(\mathbf{r}) \right\}. \quad (15)$$

One can realize we can write this in terms of a velocity operator; this could make more physical sense:

$$\mathbf{j}(\mathbf{r}) = \text{Re} \{ e\psi^*(\hat{\mathbf{v}}\psi) \}, \quad \hat{\mathbf{v}} = \frac{\vec{\pi}}{m} = \frac{1}{m} \left( \hat{\mathbf{p}} - \frac{e}{c} \hat{\mathbf{A}} \right) \quad (16)$$

The general velocity operator depends on the total vector potential, that could be due to both AC optical fields and a DC magnetic field. We could have written this based on intuition but it is good to see the mathematical description works within the Schrödinger equation. Unfortunately, the result requires the application of *real* at the end of the calculation. This is OK but somewhat annoying, because it does not fit into the usual formalism for quantum expectation values. Note, however, this object is a density and not a matrix element. For a Hermitian operator like  $\hat{\mathbf{p}}$ , a matrix element, involving integrating over all space, will be real. But is it curious that the associated density could be complex.

### 1.1.1 Simple examples

Suppose there is no vector potential, and the wave function is a **plane wave**,

$$\psi = C_0 e^{i(kx - \omega t)} \quad (17)$$

traveling in one dimension with wave vector  $k$  and frequency  $\omega$ . The value of  $C_0$  is determined by the choice of volume of normalization. This would actually be stationary state of Hamiltonian (1) in the absence of applied fields and potentials (free qm particle). It describes a particle with precisely defined momentum  $p = \hbar k$  and kinetic energy  $E = (\hbar k)^2/2m$ . So it should have a nonzero current.

One has easily  $\hat{p}_x \psi = \hbar k \psi$ , and also then  $\psi^* \hat{p}_x \psi = \hbar k |\psi|^2$ . This is already a real number. Then the current density according to (15) is

$$j_x(\mathbf{r}) = \frac{e}{m} \psi^* \hat{p}_x \psi = \frac{e}{m} \hbar k |C_0|^2. \quad (18)$$

One could think of the velocity as  $v_x = p_x/m = \hbar k/m$ , then this result is the same as  $j_x = e|C_0|^2 v_x$ . This is the current *density*, which is seen to be independent of position. Everywhere the plane wave is, there is a uniform flow of charge (and probability), even though it is a stationary state! Note also that the charge density is  $\rho_e = \psi^* e \psi = e|C_0|^2$  is also a uniform constant in space. In fact, if the wave function is normalized to unity over some volume  $V$  (the volume available to each electron) then the normalization constant is  $C_0 = 1/\sqrt{V}$ . So really, the result is the same as

$$j_x(\mathbf{r}) = \rho_e \frac{\hbar k}{m} = \rho_e v_x. \quad (19)$$

This is a statement that the product of volume charge density and velocity gives the current density, which is totally the expected relationship.

Next, suppose the wave function is a **linear combination of real and imaginary parts**. Imagine we just have

$$\psi = \psi_1 + i\psi_2 \quad (20)$$

where each of the individual functions are real. Then also including the vector potential, one gets

$$\begin{aligned} \psi^* e \hat{\mathbf{v}} \psi &= (\psi_1 - i\psi_2) \frac{e}{m} \left[ -i\hbar \vec{\nabla} - \frac{e}{c} \hat{\mathbf{A}}(\mathbf{r}) \right] (\psi_1 + i\psi_2) \\ &= \frac{e\hbar}{m} (\psi_1 \vec{\nabla} \psi_2 - \psi_2 \vec{\nabla} \psi_1) - \frac{e^2}{mc} (\psi_1^2 + \psi_2^2) \mathbf{A}(\mathbf{r}) - \frac{i\hbar e}{m} (\psi_1 \vec{\nabla} \psi_1 + \psi_2 \vec{\nabla} \psi_2) \end{aligned} \quad (21)$$

That's a very interesting result. Of course, one needs to take the real part to actually get the physical current. So only the first two terms contribute to electric current:

$$\mathbf{j}(\mathbf{r}) = \text{Re}\{\psi^* e \mathbf{v} \psi\} = \frac{e\hbar}{m} (\psi_1 \vec{\nabla} \psi_2 - \psi_2 \vec{\nabla} \psi_1) - \frac{e^2 \mathbf{A}(\mathbf{r})}{mc} |\psi|^2 \quad (22)$$

The first term, the momentum current, results from the interference between the real and imaginary parts. It is zero in a wave function that is pure real or pure imaginary. This is usually the most important part in most problems. So if a wave function does not have an "i" in it somewhere, the momentum current is zero. The second term is caused by the vector potential, and just depends on the square of the wave function at the point of interest. In fact, it really depends on the electric charge density,  $\rho_e = e|\psi|^2$ . This is a curious term. The vector potential needed to describe some EM field is not unique. However, remember that this expression is derived for the Coulomb gauge where  $\vec{\nabla} \cdot \mathbf{A} = 0$ . This is indeed a strong constraint, on the other hand, it still leaves a lot of freedom in the choice of  $\mathbf{A}$ . Thus one sees a gauge dependence, but what is not as apparent, is that the momentum current could also have a gauge dependence. The solutions for  $\psi_1$  and  $\psi_2$  will depend on the choice of  $\mathbf{A}$ . In any specified physical situation, in the end, the physically measured results should come out independent of the choice of the EM gauge.

## 1.2 Doing quantum mechanics with the density matrix

Here before really discussing currents, some general ideas about quantum mechanics for statistical systems are expanded upon. This usually will mean any real system, where there is more than one particle and there is lack of knowledge about the preparation of the system.

When the state of a quantum system is specified by a single wave function, the system is said to be in a *pure state*. There are certain physical variables that could be measured and one will definitely know the probabilities for each possible outcome. (Unfortunately, in QM, this is the best that one can hope to achieve!) This makes the most sense, for example, if that state is an eigenstate of the Hamiltonian. It also applies to any superposition of eigenstates of  $\hat{H}$ , because we would be able to predict outcomes of experiments very precisely (in the sense of probabilities, however).

But in the real world, one can never really prepare a system exactly how we want it. Almost always, our system will be impossible to describe perfectly. We can say only that it is in a certain desired state with some probability. It is as if we want to write the state as a superposition, but, we

don't have a certain knowledge about the coefficients in the superposition. So one doesn't have the ability or knowledge to write out

$$\psi = \sum_i c_i \psi_i \quad (23)$$

because the coefficients  $c_i$  are not known, exactly. This sounds like the usual problem in QM, but it is worse.

When one has a situation where the wave function cannot be written directly out, the state is said to be a *mixed state*. It is not a linear super position. One can know the probabilities for being found in different states of the "mixture", instead of having the expansion coefficients.

Mixed states are important and necessary to describe a situation of thermal equilibrium, where the system of interest is continuously being modified by its surroundings. For example, the energy eigenstates are populated according to some thermal distribution (Fermi-Dirac, say, for electrons) for the given temperature, when the system is in equilibrium. A new operator called the *density operator*  $\hat{\rho}$  is a mathematical device to use in QM calculations for the properties of mixed states. An input to determine it, is a set of probabilities  $p_i$ , for each of a number of states  $\psi_i$  in the mixture. One also speaks of the *density matrix*, which is the matrix for this density operator, in some representation. The density operator is a way to introduce this population into the QM problem and provide for mixed states as opposed to pure states.

One can make a density operator even for a pure state whose wave function is  $\psi$ . In Dirac notation, it is

$$\hat{\rho} = |\psi\rangle\langle\psi| \quad (24)$$

It has the name "density operator" for various reasons. The most obvious is that its expectation value in an eigenstate of position,  $|x\rangle$ , for example, gives the probability density to find the particle at that position  $x$  (I take  $x$  to mean position in as many dimensions as is of interest):

$$\langle x|\hat{\rho}|x\rangle = \langle x||\psi\rangle\langle\psi||x\rangle = \psi(x)\psi^*(x) = |\psi(x)|^2. \quad (25)$$

The usual Dirac notation  $\psi(x) = \langle x|\psi\rangle$  is being used, as well as  $\psi(x)^* = \langle\psi|x\rangle$ . Of course, this object, which is really the particle density at position  $x$ , is just a diagonal matrix element of the operator  $\hat{\rho}$ . It can also have off-diagonal terms like

$$\langle x|\hat{\rho}|y\rangle = \langle x||\psi\rangle\langle\psi||y\rangle = \psi(x)\psi^*(y). \quad (26)$$

This, however, may not have such a simple interpretation, at this point.

Next one can make a density operator for a mixed state, that is composed from only two known wave functions (or eigenstates, say, of the Hamiltonian). For the two states, called "1" and "2", suppose there are probabilities  $p_1$  and  $p_2$  that the system is found in each state, respectively. Then the mixed state density operator is defined as

$$\hat{\rho} = p_1|\psi_1\rangle\langle\psi_1| + p_2|\psi_2\rangle\langle\psi_2| \quad (27)$$

The expectation value within eigenstates of position is simple,

$$\langle x|\hat{\rho}|x\rangle = p_1\langle x||\psi_1\rangle\langle\psi_1||x\rangle + p_2\langle x||\psi_2\rangle\langle\psi_2||x\rangle = p_1|\psi_1(x)|^2 + p_2|\psi_2(x)|^2. \quad (28)$$

In this simple case, the two parts don't interfere with each other. The expectation value is just a sum of that for each state in the mixture, weighted by their probabilities. But it wouldn't have to be that simple.

Consider the generalization to a situation of thermal equilibrium. The basic definition of the density operator in terms of the state probabilities  $p_i$  is

$$\hat{\rho} = \sum_i p_i|\psi_i\rangle\langle\psi_i| \quad (29)$$

This operator represents the state of the system. It is a different philosophy for doing QM. The time derivative follows from using the Schrödinger equation for each state:

$$\begin{aligned}\frac{\partial \hat{\rho}}{\partial t} &= \sum_i p_i \left\{ \left( \frac{\partial}{\partial t} |\psi_i\rangle \right) \langle \psi_i| + |\psi_i\rangle \left( \frac{\partial}{\partial t} \langle \psi_i| \right) \right\} \\ &= \sum_i p_i \left\{ \left( \frac{1}{i\hbar} \hat{H} |\psi_i\rangle \right) \langle \psi_i| + |\psi_i\rangle \left( \langle \psi_i| \hat{H} \frac{-1}{i\hbar} \right) \right\} = \frac{1}{i\hbar} [\hat{H}, \hat{\rho}]\end{aligned}\quad (30)$$

This simple result is known as the quantum Liouville equation. It is analogous to the Liouville equation for the evolution of probability density in classical statistical mechanics. Hence another explanation for the name, "density operator". Of course, notice that if  $\hat{\rho}$  is composed entirely from eigenstates of  $\hat{H}$ , then it is constant in time.

### 1.2.1 Expectation values using a density operator

Expectation values (besides real space densities) can be found using the density operator (for the defined system) combined with whatever operator whose average is desired. As a simplest case, say, for example, that the Hamiltonian is to be averaged for some arbitrary state of the system.

Before proceeding, it is good to realize that any operator can be expanded using some complete set of states. For example, the Hamiltonian can be expressed as a sum of projection operators for each of its (energy) eigenstates. This is done with the unity operator,

$$\hat{I} = \sum_n |n\rangle \langle n| \quad (31)$$

where the states could be the set of eigenstates, really, of any operator. For the Hamiltonian, inserting  $\hat{I}$  on each side,

$$\hat{H} = \hat{I} \hat{H} \hat{I} = \sum_n \sum_m |n\rangle \langle n| \hat{H} |m\rangle \langle m| = \sum_n \sum_m |n\rangle H_{nm} \langle m|, \quad H_{nm} \equiv \langle n| \hat{H} |m\rangle. \quad (32)$$

If the states being used really are the eigenstates of  $\hat{H}$ , then this becomes trivial, or really, diagonal, because the matrix elements are  $H_{nm} = \delta_{nm} E_n$ ,

$$\hat{H} = \sum_n \sum_m |n\rangle \delta_{nm} E_n \langle m| = \sum_n |n\rangle E_n \langle n| = \sum_n E_n |n\rangle \langle n| \quad (33)$$

Then to find the average of  $\hat{H}$  in some arbitrary state  $|\psi\rangle$ , we could do

$$\langle \hat{H} \rangle = \langle \psi | \hat{H} | \psi \rangle = \sum_n \langle \psi | n \rangle E_n \langle n | \psi \rangle = \sum_n \langle n | \psi \rangle E_n \langle \psi | n \rangle = \sum_n \langle n | E_n | \psi \rangle \langle \psi | n \rangle \quad (34)$$

This is a trivial case, but with a pure state density matrix,  $\hat{\rho} = |\psi\rangle \langle \psi|$  it is the same as

$$\langle \hat{H} \rangle = \sum_n \langle n | \hat{H} | \psi \rangle \langle \psi | n \rangle = \sum_n (\hat{H} \hat{\rho})_{nn} = \text{Tr}\{\hat{H} \hat{\rho}\} = \text{Tr}\{\hat{\rho} \hat{H}\} \quad (35)$$

The trace operation in the last parts is just the sum of the diagonal matrix elements. This was simple because eigenstates of  $\hat{H}$  were used. But they could have been eigenstates of any operator, and the result would come out the same.

If instead of  $\hat{H}$  one did the average of an arbitrary operator, call it  $\hat{A}$ , then this works as follows. The operator is expressed as was done for the Hamiltonian,

$$\hat{A} = \sum_n \sum_m |n\rangle A_{nm} \langle m|, \quad A_{nm} \equiv \langle n | \hat{A} | m \rangle. \quad (36)$$

Its expectation is

$$\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle = \sum_n \sum_m \langle \psi | n \rangle A_{nm} \langle m | \psi \rangle = \sum_n \sum_m \langle m | \psi \rangle \langle \psi | n \rangle A_{nm} \quad (37)$$

The first factor in the product is an element of the density *matrix*,  $\rho_{mn} \equiv \langle m|\hat{\rho}|n\rangle$ , for a pure state. Then the formula indicates matrix multiplication, followed by summing on the diagonal:

$$\langle \hat{A} \rangle = \sum_n \sum_m \rho_{mn} A_{nm} = \sum_m (\hat{\rho}\hat{A})_{mm} = \text{Tr}\{\hat{\rho}\hat{A}\} = \text{Tr}\{\hat{A}\hat{\rho}\}. \quad (38)$$

The order of the operators in the matrix product is irrelevant. Even if the density matrix is not diagonal, the trace operation still gives the correct expectation value.

### 1.2.2 Density operator in coordinate space

That was somewhat formal, what about starting from a real space wave function, how does it work? Say, for example, the average of an operator  $\hat{A}$  is desired (it could be anything macroscopic observable that is averaged over the whole system). Let's write this in the standard definition, starting from a wave function, and see that it can be written out using the density operator. Do this first for a pure state, to see how things work.

$$\langle \hat{A} \rangle = \int dx \psi^*(x) \hat{A}(x) \psi(x) = \int dx \langle \psi|x \rangle \hat{A}(x) \langle x|\psi \rangle \quad (39)$$

Now the  $\hat{A}(x)$  is like a diagonal matrix element, although it is meant to actually *operate* on the object to its right, which is  $\psi(x)$ . So it doesn't seem as simple as the matrix multiplication seen above. I want to see this really as a product of objects that obviously corresponds to matrix multiplication. How to do that? This is a confusion that appears strongly in the coordinate representation that everyone is familiar with. Suppose  $\hat{A}$  is the momentum operator. We don't usually think of the matrix elements of the momentum operator, but rather, think of it as the operation  $-i\hbar\vec{\nabla}$  onto the  $\psi$  to the right.

Really, the usual expectation has to come about using two identity operators  $\hat{I}$ . Instead of sums over states, the sums are integrals over positions, i.e., one is using the continuum of position eigenstates (still can think of it as summing). The expectation really starts out as

$$\langle \hat{A} \rangle = \int dx \int dy \langle \psi|x \rangle \langle x|\hat{A}|y \rangle \langle y|\psi \rangle = \int dx \int dy \psi^*(x) A(x,y) \psi(y) \quad (40)$$

In this way, the matrix element which I wrote as  $A(x,y)$  is clearly present. It does not have any operational effect on the  $\psi(y)$  to its right. Written this way,  $A(x,y)$  is just a numerical function, not any more an operator. It's great, but unfortunately, to get this extra simplicity, you pay for it by having an extra integration over an extra set of coordinates. (Note that "x" means all three position coordinates for 3D space, as does "y".)

From the formal perspective, however, this is also great. For the pure state being considered, the density matrix in coordinate representation was mentioned earlier. The operator  $\hat{\rho} = |\psi\rangle\langle\psi|$  has matrix elements,

$$\rho(x,y) \equiv \langle x|\hat{\rho}|y \rangle = \langle x|\psi\rangle\langle\psi|y \rangle = \psi(x)\psi^*(y). \quad (41)$$

So the expectation value desired is indeed a trace:

$$\langle \hat{A} \rangle = \int dx \int dy A(x,y) \rho(y,x) = \int dx [\hat{A}\hat{\rho}](x,x) = \text{Tr}\{\hat{A}\hat{\rho}\} = \text{Tr}\{\hat{\rho}\hat{A}\} \quad (42)$$

This involved using the product of two operators' matrices as

$$[\hat{A}\hat{\rho}](x,z) = \int dy \hat{A}(x,y) \hat{\rho}(y,z) \quad (43)$$

whereas, there only appeared the diagonal element of this object, hence, the trace.

### 1.2.3 Matrices for some common operators

A typical **local potential**  $U(x)$  in the Hamiltonian has a diagonal matrix. It means that really we would have had some original operator  $\hat{U}$ , whose space-space matrix elements are like

$$U(x, y) = \langle x | \hat{U} | y \rangle = U(x) \delta(x - y) \quad (44)$$

It is absolutely local. There is no effect if  $x$  and  $y$  are separated. The potential acts on the wave function at position  $y$  and the effect is felt at that same position. When its expectation value is found, it has the familiar look,

$$\langle U \rangle = \int dx \int dy \psi^*(x) U(x) \delta(x - y) \psi(y) = \int dx \psi^*(x) U(x) \psi(x) \quad (45)$$

It can also be expressed with the density matrix,

$$\langle U \rangle = \int dx \rho(x, x) U(x) = \text{Tr}\{\hat{\rho} \hat{U}\}. \quad (46)$$

A **nonlocal potential**  $\hat{U}$  cannot be written in terms of one coordinate  $x$ . This is not a typical physical potential. However, situations where there is a convolution integral might require this kind of potential. I could make up a simple one, whose matrix is as follows:

$$U(x, y) = \langle x | \hat{U} | y \rangle = U_0 e^{-(x-y)^2/2\sigma^2} \quad (47)$$

That is a potential whose nonlocality range is distance  $\sigma$ . But note that this range is not like the range, say, of a gravitational potential. If one studied a particle in a gravitational field, the potential it experiences is local.

Now the averaging of this potential gives

$$\langle U \rangle = \int dx \int dy \psi^*(x) U_0 e^{-(x-y)^2/2\sigma^2} \psi(y) \quad (48)$$

In such a fashion, it connects  $\psi^*$  and  $\psi$  at different points in space. One naturally has integrals over the two different coordinates. One could get it to be a convolution integral, in momentum space, by doing Fourier transforms. For the general case, suppose depends on the difference of the points,  $U(x, y) = U(x - y)$ . It could be written in terms of a Fourier transform pair for normalization volume  $V$ ,

$$U(x - y) = \frac{1}{\sqrt{V}} \int dk U(k) e^{ik \cdot (x-y)}, \quad U(k) = \frac{1}{\sqrt{V}} \int dx U(x) e^{-ik \cdot x}, \quad (49)$$

and there would be similar definitions for the FT of  $\psi$  (see the pages that follow). Then

$$\langle U \rangle = \int dx \int dy \psi^*(x) \left[ \frac{1}{\sqrt{V}} \int dk U(k) e^{ik \cdot (x-y)} \right] \psi(y) \quad (50)$$

Interchanging the order of integrations, the integrals over  $x$  and  $y$  can be done first, and also lead to FTs:

$$\langle U \rangle = \frac{1}{\sqrt{V}} \int dk U(k) [\sqrt{V} \psi(k)]^* [\sqrt{V} \psi(k)] = \sqrt{V} \int dk U(k) |\psi(k)|^2 \quad (51)$$

In fact, this is a local effect in the momentum space, because I chose  $U = U(x - y)$ . But one can see that the potential being nonlocal in real space does not necessarily mean the potential is unrealistic. If the potential did not satisfy this translational symmetry, one would have to do the FT as a double FT, with a  $1/\sqrt{V}$  normalization in each integration,

$$U(x, y) = \frac{1}{V} \int dk \int dq U(k, q) e^{ik \cdot x} e^{iq \cdot y}, \quad U(k, q) = \frac{1}{V} \int dx \int dy U(x, y) e^{-ik \cdot x} e^{-iq \cdot y}. \quad (52)$$



Then an expectation value is more interesting,

$$\langle U \rangle = \frac{1}{V} \int dx \int dy \psi^*(x) \int dk \int dq U(k, q) e^{ik \cdot x} e^{iq \cdot y} \psi(y) \quad (53)$$

After re-arranging the integrations, this becomes

$$\langle U \rangle = \int dk \int dq \psi^*(k) U(k, q) \psi(-q) \quad (54)$$

In this general case, the interaction is now still nonlocal even in momentum space, connecting the wave function at two different wave vectors or momenta. In some sense, the potential can be thought to exchange momentum with the QM particle.

#### 1.2.4 The momentum operator as a matrix

A momentum operator  $\mathbf{p}$  is usually thought of as a differential operator (in coordinate representation). What about its matrix? Indeed, in momentum space, it will be just a number, just as the position operator  $\mathbf{x}$  is just a number in real space. We can use this fact to find its matrix.

The reason for high interest in the momentum operator, is that it is part of the current density operator. Thus, one needs to have a clear understanding of it before proceeding to other analysis of the current density.

One can generate the momentum operator using its eigenstates, in some sense. A wave function with a well-defined momentum that is an eigenstate of the momentum operator  $\hat{p} = -i\hbar \vec{\nabla}$  is

$$u_p(x) = \frac{1}{\sqrt{V}} e^{ip \cdot x / \hbar} \equiv \langle x | p \rangle \quad (55)$$

That is what is meant by the Dirac bracket at the end: the x-representation of an eigenstate with momentum  $p$ . I am using a the wave function normalized to 1 over some system volume  $V$ . Now these provide the way to expand any wave function in coordinate representation,  $\psi(x) = \langle x | \psi \rangle$ . Use an expansion with the identity  $\hat{I}$  expressed in momentum states,

$$\psi(x) = \langle x | \left[ \int dp |p\rangle \langle p| \right] | \psi \rangle = \frac{1}{\sqrt{V}} \int dp \langle p | \psi \rangle \langle x | p \rangle = \frac{1}{\sqrt{V}} \int dp \psi(p) e^{ip \cdot x / \hbar}. \quad (56)$$

OK, I did this just to confirm how the basic Fourier transforms should be defined; this shows that the real space wave function is a FT of the momentum space wave function  $\psi(p) \equiv \langle p | \psi \rangle$ . One also has the complex conjugate,

$$u_p^*(x) = \frac{1}{\sqrt{V}} e^{-ip \cdot x / \hbar} = \langle p | x \rangle \quad (57)$$

One can use this to go back in the other direction of the FT, starting from  $\psi(p)$ ,

$$\psi(p) = \langle p | \left[ \int dx |x\rangle \langle x| \right] | \psi \rangle = \int dx \langle x | \psi \rangle \langle p | x \rangle = \frac{1}{\sqrt{V}} \int dx \psi(x) e^{-ip \cdot x / \hbar}. \quad (58)$$

We are interested in the matrix for  $\hat{p}$ , i.e., its elements like  $\langle x | \hat{p} | y \rangle$ . Towards that end, consider the action of the momentum operator on an eigenket of position  $|y\rangle$ . If we know that, we can figure out everything we need. To make it easy, expand again with an identity operator, using  $k$  to label its momentum states,

$$\hat{p} | \psi \rangle = \hat{p} \left[ \int dk |k\rangle \langle k| \right] | y \rangle = \int dk k |k\rangle \langle k | y \rangle = \int dk k |k\rangle \frac{1}{\sqrt{V}} e^{-ik \cdot y / \hbar}. \quad (59)$$

This expresses the effect in momentum space, where the action of  $\hat{p}$  is trivial. But we know  $\langle k | y \rangle$  from above, which was used in the last step. Now do a trick to get rid of that  $k$  in the integrand:

$$\hat{p} | y \rangle = i\hbar \frac{\partial}{\partial y} \left[ \int dk |k\rangle \frac{1}{\sqrt{V}} e^{-ik \cdot y / \hbar} \right] \quad (60)$$

Then recycle a bit,

$$\hat{p}|y\rangle = i\hbar \frac{\partial}{\partial y} \left[ \int dk |k\rangle \langle k|y\rangle \right] = i\hbar \frac{\partial}{\partial y} |y\rangle. \quad (61)$$

The sign is positive, curiously. But to see what happened to the expected negative sign, let's just test another operation, going to the left onto a bra instead of to the right onto a ket:

$$\langle x|\hat{p} = \langle x| \left[ \int dk |k\rangle \langle k| \right] \hat{p} = \int dk \langle x|k\rangle \langle k|k = \int dk \frac{1}{\sqrt{V}} e^{ik\cdot x/\hbar} \langle k|k \quad (62)$$

Do the same kind of trick to get rid of the  $k$  inside the integrand,

$$\langle x|\hat{p} = -i\hbar \frac{\partial}{\partial x} \left[ \int dk \frac{1}{\sqrt{V}} e^{ik\cdot x/\hbar} \langle k| \right] = -i\hbar \frac{\partial}{\partial x} \quad (63)$$

Then finally this does indeed have a derivative with a minus sign,

$$\langle x|\hat{p} = -i\hbar \frac{\partial}{\partial x} \left[ \int dk \langle x|k\rangle \langle k| \right] = -i\hbar \frac{\partial}{\partial x} \langle x|. \quad (64)$$

Now this last result is well-known, but in a different notation, because if there were a ket  $|\psi\rangle$  to the right, it would follow the same derivation, and  $|\psi\rangle$  just goes along for the ride. Then this well-known result is

$$\langle x|\hat{p}|\psi\rangle = -i\hbar \frac{\partial}{\partial x} \langle x|\psi\rangle = -i\hbar \frac{\partial}{\partial x} \psi(x). \quad (65)$$

That, in fact, is what is meant by the effect of the momentum operator in “elementary” QM. Similarly, the lesser known result (61), with a state bra vector on the left, is just the complex conjugate of this one,

$$\langle \psi|\hat{p}|y\rangle = i\hbar \frac{\partial}{\partial y} \langle \psi|y\rangle = i\hbar \frac{\partial}{\partial y} \psi^*(y). \quad (66)$$

I used  $x$  in one case and  $y$  in the other, but these are just arbitrary positions. When people say things like “the momentum operator is  $-i\hbar \vec{\nabla}$ ,” you have to understand that is the action it performs only on  $\psi(x)$ . It's action on the c.c. wave function has the opposite sign. Maybe this is all obvious if you understand QM well. But here for what I want, these things need to be completely clear.

Finally with this, it should be “simple” to get the actual matrix for the momentum operator in the coordinate representation. But because this will enter to define the current operator, make sure we get this correct. The desired typical matrix element that would be needed to apply the density matrix formalism is  $p_{xy} = \langle x|\hat{p}|y\rangle$ . (I'll use this shorter notation here instead of  $p(x,y)$ .) I can do an expansion again like above, or just think as follows. In expression (64), one wants to put  $\psi = y$ . That means to use  $\psi$  as the wave function for a particle that can only be found at position  $x$ , i.e., the eigenstate of position,  $|\psi\rangle = |x\rangle$ . But as a wave function, this has to be a delta function:

$$\langle x|\psi\rangle \rightarrow \langle x|y\rangle = \delta(x-y). \quad (67)$$

Then there results immediately from (64),

$$p_{xy} = \langle x|\hat{p}|y\rangle = -i\hbar \frac{\partial}{\partial x} \delta(x-y) = -i\hbar \partial_x \delta(x-y). \quad (68)$$

Try to verify this the other way, because perhaps the overall normalization is suspicious. If we applied some identity operators instead, we would follow this reasoning:

$$\langle x|\hat{p}|y\rangle = \int dk \int dq \langle x|k\rangle \langle k|\hat{p}|q\rangle \langle q|y\rangle = \int dk \int dq \left[ \frac{1}{\sqrt{V}} e^{ik\cdot x/\hbar} \right] \langle k|\hat{p}|q\rangle \left[ \frac{1}{\sqrt{V}} e^{-iq\cdot y/\hbar} \right] \quad (69)$$

where the interior momentum matrix element is diagonal:  $\langle k|\hat{p}|q\rangle = k\delta(k-q) = q\delta(k-q)$ . Now this either can have a  $k$  or a  $q$  within the integrand. One wants to get it out of there. The way is

as above, put a derivative on the outside that would produce the desired factor. Suppose we used  $\langle k|\hat{p}|q\rangle = k\delta(k-q)$ . Then the m.e. becomes

$$\langle x|\hat{p}|y\rangle = -i\hbar\partial_x \left[ \frac{1}{V} \int dk \int dq e^{i(k\cdot x - q\cdot y)/\hbar} \delta(k-q) \right] = -i\hbar\partial_x \left[ \frac{1}{V} \int dk e^{ik\cdot(x-y)/\hbar} \right] \quad (70)$$

For the normalization I am using, the integration gives volume times a delta function in  $(x-y)$ . So this **reproduces expression** (68). But what if one had used  $\langle k|\hat{p}|q\rangle = q\delta(k-q)$ ? Then there results

$$\langle x|\hat{p}|y\rangle = +i\hbar\partial_y \left[ \frac{1}{V} \int dk \int dq e^{i(k\cdot x - q\cdot y)/\hbar} \delta(k-q) \right] = +i\hbar\partial_y \left[ \frac{1}{V} \int dk e^{ik\cdot(x-y)/\hbar} \right] \quad (71)$$

Then this instead leads to

$$p_{xy} = \langle x|\hat{p}|y\rangle = +i\hbar \frac{\partial}{\partial y} \delta(x-y) = +i\hbar\partial_y \delta(x-y). \quad (72)$$

OK, so that is two equivalent expressions for one thing. They reflect the two relations (61) and (64). But these results seem to lack a certain symmetry and beauty. However, they do demonstrate that the matrix (and operator) for momentum is Hermitian, in that it satisfies the following symmetry,

$$p_{xy} = -i\hbar\partial_x \delta(y-x) = -i\hbar(-\partial_y)\delta(y-x) = i\hbar\partial_y \delta(y-x) = p_{yx}^* \quad (73)$$

That works out because  $\delta(x-y) = \delta(y-x)$ , and, the operators for observables such as momentum must be Hermitian so they will have real eigenvalues. Further,  $\partial_x f(x-y) = -\partial_y f(x-y)$  for any function. So both the expressions (68) and (72) give equivalent ways to write the (Hermitian) momentum matrix.

### 1.2.5 The current density operator $\hat{j}$

Now how to use the above results to get an operator (and its matrix) for the momentum current density? We know current density at some position  $r$  is given by the *real part* of the velocity sandwiched between  $\psi^*(r)$  and  $\psi(r)$ . But one might look for a new *operator*  $\hat{j}_1$  that is equivalent in the following sense, if possible:

$$\mathbf{j}(r) = \text{Re}\left\{e\psi^*(r)\frac{\hat{p}}{m}\psi(r)\right\} = \psi^*(r)\hat{j}_1(r)\psi(r). \quad (74)$$

For now I ignore the gauge current contribution, which is easy to include later. Also  $r$  is the point where the current will be measured, because  $x$  and  $y$  will be used as the integration and matrix element arguments. This transformation to this  $\hat{j}_1(r)$  could be useful so that the new operator can be used in the density matrix formalism. However, to really fit into the density matrix formalism, we need an operator and its matrix, which is not the format of  $\hat{j}_1(r)$ .

Instead, let me note some other interesting way to write  $\mathbf{j}(r)$ . The real part is equivalent to the following symmetrization (a number plus its c.c. divided by 2):

$$\mathbf{j}(r) = \frac{e}{2m} \left\{ \psi^*(r)[\hat{p}\psi(r)] + \psi(r)[\hat{p}\psi(r)]^* \right\} \quad (75)$$

In Dirac notation, this is

$$\mathbf{j}(r) = \frac{e}{2m} \left\{ \langle\psi|r\rangle\langle r|\hat{p}|\psi\rangle + \langle r|\psi\rangle [ \langle r|\hat{p}|\psi\rangle ]^* \right\} = \frac{e}{2m} \left\{ \langle\psi|r\rangle\langle r|\hat{p}|\psi\rangle + \langle\psi|\hat{p}^\dagger|r\rangle\langle r|\psi\rangle \right\} \quad (76)$$

Then this last result has the following operator within bra and kets for the state  $\psi$ :

$$\hat{j}(r) = \frac{e}{2m} [ |r\rangle\langle r|\hat{p} + \hat{p}^\dagger|r\rangle\langle r| ] \quad (77)$$

The combination in this order, with  $\hat{p}$  and its Hermitian conjugate (but actually  $\hat{p}^\dagger = \hat{p}$ ), construct not only a Hermitian operator, but a *real* operator. The operator will give the real current density

at the chosen position  $r$  for any state. But it is not exactly the same as  $\hat{j}_1$  being sought above, but it is on the right track. In fact, we'll see that it is even better.

I want to find now  $\mathbf{j}(r)$ , but by integration over positions  $x$  and  $y$  of an appropriate function. The expression for the current density in terms of operator  $\hat{j}(r)$  is

$$\mathbf{j}(r) = \langle \psi | \hat{j}(r) | \psi \rangle = \int dx \int dy \langle \psi | x \rangle \langle x | \hat{j}(r) | y \rangle \langle y | \psi \rangle = \int dx \int dy \psi^*(x) \hat{j}_{xy}(r) \psi(y) \quad (78)$$

That is the usual form desired for an interaction! This is what we were looking for, as long as we want the operators matrix and double integrations. So  $\hat{j}(r)$  in (77) is the operator that would be needed in the density matrix approach for finding expectation values. To completely specify what this means, also get the needed matrix elements.

$$\hat{j}_{xy}(r) = \langle x | \hat{j}(r) | y \rangle = \frac{e}{2m} [\langle x | r \rangle \langle r | \hat{p} | y \rangle + \langle x | \hat{p}^\dagger | r \rangle \langle r | y \rangle] \quad (79)$$

Due to the relations (68) and (72) there are various ways to express this. ( $\hat{p} = \hat{p}^\dagger$  can be used, too.) The expression can end up with derivatives w.r.t.  $r$  or w.r.t.  $x$  and  $y$ . Further, the bra-kets in different positions give delta functions. For example, one way to write this is

$$\hat{j}_{xy}(r) = \frac{e}{2m} \{ \delta(x-r) [-i\hbar \partial_r \delta(y-r)] + [i\hbar \partial_r \delta(x-r)] \delta(y-r) \} \quad (80)$$

Unfortunately it is a rather singular object, however, the deltas do help with the integration of it. Another way to express it, that may be more practice, is

$$\hat{j}_{xy}(r) = \frac{e}{2m} \{ \delta(x-r) [i\hbar \partial_y \delta(y-r)] + [-i\hbar \partial_x \delta(x-r)] \delta(y-r) \} \quad (81)$$

When this is used in (78), one delta can be used directly in each term, and there results

$$\mathbf{j}(r) = \frac{e}{2m} \left\{ \psi^*(r) \int dy [i\hbar \partial_y \delta(y-r)] \psi(y) + \psi(r) \int dx \psi^*(x) [-i\hbar \partial_x \delta(x-r)] \right\} \quad (82)$$

Integrations by parts on these last give

$$\mathbf{j}(r) = \frac{e}{2m} \{ \psi^*(r) [-i\hbar \partial_r \psi(r)] + \psi(r) [i\hbar \partial_r \psi^*(r)] \}, \quad (83)$$

and this was the original expression found for the current density, so this shows that the matrix elements are correct although they are very ugly.

The operator  $\hat{j}(r)$  given by (77) is really the operator needed for expectation values using the density operator formalism. It is what is needed to find the current density, indeed, by doing

$$\mathbf{j}(r) = \text{Tr} \{ \hat{j}(r) \hat{\rho} \} = \text{Tr} \{ \hat{\rho} \hat{j}(r) \} \quad (84)$$

This is what I set out to find. If one can manipulate the operator and matrix for  $\hat{j}(r)$  appropriately, one can do any required calculations and find expectation values.

Finally, to put the gauge current back in, just add it, this is trivial because in coordinate representation it commutes with position anyways.

$$\hat{j}(r) = \frac{e}{2m} [ |r\rangle \langle r | \vec{\pi} + \vec{\pi}^\dagger |r\rangle \langle r | ] \quad (85)$$

where  $\vec{\pi} = \hat{\mathbf{p}} - \frac{e}{c} \hat{\mathbf{A}}$ .

### 1.2.6 A diagonal current density operator?

This still leaves open the question, what is the operator  $\hat{j}_1(r)$ ? But that is not really so important, perhaps. This calculation does not give any answer. In fact, it tends to show that there isn't such

an operator. To have that form, the operator has to be diagonal, i.e., the only nonzero elements need to have  $x = y$ . The deltas make  $\hat{j}_{xy}(r)$  look that way, except that there are derivatives. The derivatives make the operator connect nearby portions of the wave function. That is a nonlocal or nondiagonal interaction, hence one cannot find a  $\hat{j}_1(r)$ .

Ignoring that for the moment, consider the following algebra. The m.e.s look like they are proportional to  $\delta(x - y)$  (i.e., diagonal) because of the two delta functions in each term. Suppose one simply tries to assume that the matrix elements are equivalent to this:

$$\hat{j}_{xy}(r) = \frac{e}{2m} \{ \delta(x - r) [i\hbar \partial_y \delta(x - y)] + [-i\hbar \partial_x \delta(x - y)] \delta(y - r) \} \quad (86)$$

When this is used in (78) to find  $\mathbf{j}(r)$ , one gets

$$\mathbf{j}(r) = \frac{e}{2m} \left\{ \psi^*(r) \int dy [i\hbar \partial_y \delta(r - y)] \psi(y) + \psi(r) \int dx \psi^*(x) [-i\hbar \partial_x \delta(x - r)] \right\} \quad (87)$$

Now do the obvious integrations by parts,

$$\mathbf{j}(r) = \frac{e}{2m} \{ \psi^*(r) [-i\hbar \partial_r \psi(r)] + \psi(r) [i\hbar \partial_r \psi^*(r)] \} \quad (88)$$

This is the correct current density. Even so, it does not point out what  $\hat{j}_1(r)$  should be. But it does give an alternative expression of the matrix for the current density operator. That can also be written as

$$\hat{j}_{xy}(r) = \frac{i\hbar e}{2m} [\delta(x - r) \partial_y - \delta(y - r) \partial_x] \delta(x - y) \quad (89)$$

Here the partial derivatives act on the last delta function. I thought I had a better derivation of this, but, cannot recover it at the moment. I don't need it anyway.

### 1.3 Averages of current density over a volume

In some problems one does not care so much about the current density at a particular point in space, but rather, the interest is in the average current density within some volume. In a real application, in fact, one wants to know the average current density due to many electrons,  $N$ , inside a volume  $V$ . Stated otherwise, what is the average current density when there are  $n = N/V$  electrons per unit volume? The volume of interest has to be similar in size to that that would be measured in some experiment.

This averaging can be done by integration over  $V$ , then dividing by  $V$ . I'll write a volume average (for the moment) with an overline like  $\bar{\mathbf{j}}$  or just the current density symbol with no position argument, like  $\mathbf{j}$  where the context is clear. The volume-averaged current density for one electron is

$$\bar{\mathbf{j}} = \frac{1}{V} \int d^3r \mathbf{j}(r) = \frac{1}{V} \int d^3r \text{Tr} \{ \hat{\rho} \hat{j}(r) \} = \frac{1}{V} \int d^3r \sum_{nm} \hat{\rho}_{nm} \hat{j}_{mn}(r) \quad (90)$$

The density matrix does not have an explicit dependence on the measurement position  $r$ . So the averaging over position involves only the dependence in the current operator. Its matrix elements between some arbitrary states are,

$$\hat{j}_{mn}(r) = \langle m | \hat{j}(r) | n \rangle = \frac{e}{2m} [\langle m | r \rangle \langle r | \vec{\pi} | n \rangle + \langle m | \vec{\pi} | r \rangle \langle r | n \rangle] \quad (91)$$

Using this explicit form, the averaging is

$$\frac{1}{V} \int d^3r \hat{j}_{mn}(r) = \frac{1}{V} \int d^3r \frac{e}{2m} [\langle m | r \rangle \langle r | \vec{\pi} | n \rangle + \langle m | \vec{\pi} | r \rangle \langle r | n \rangle] \quad (92)$$

But the integrations are identity operations,

$$\hat{I} = \int d^3r |r\rangle \langle r| \quad (93)$$

Then the volume-averaged current operator matrix elements are (with  $\vec{\pi} = m\hat{\mathbf{v}}$ ),

$$\frac{1}{V} \int d^3r \hat{j}_{mn}(r) = \frac{e}{2mV} [\langle m|\vec{\pi}|n\rangle + \langle m|\vec{\pi}|n\rangle] = \frac{e}{mV} \langle m|\vec{\pi}|n\rangle = \frac{e}{mV} \vec{\pi}_{mn} = \frac{e}{V} \hat{\mathbf{v}}_{mn}. \quad (94)$$

This gives a simple result for the volume-averaged current density,

$$\bar{\mathbf{j}} = \sum_{nm} \hat{\rho}_{nm} \frac{e}{V} \hat{\mathbf{v}}_{mn} = \text{Tr}\left\{\hat{\rho} \frac{e}{V} \hat{\mathbf{v}}\right\}. \quad (95)$$

It is a wonderful simple result. If one just averages the velocity operator, scaled by the charge per volume, it gives the volume-averaged current density! If there are  $N$  electrons in this volume then the result is multiplied by  $N$ ,

$$\bar{\mathbf{J}} = \sum_{nm} \hat{\rho}_{nm} ne\hat{\mathbf{v}}_{mn} = \text{Tr}\{\hat{\rho} ne\hat{\mathbf{v}}\}. \quad (96)$$

These suggest defining the one-electron current density operator  $\hat{\mathbf{j}} \equiv \frac{e}{V} \hat{\mathbf{v}}$  and the corresponding  $N$ -electron current density operator,  $\hat{\mathbf{J}} \equiv ne\hat{\mathbf{v}}$ , which appear in these trace operations. Their expectation values give the volume averages automatically and conveniently!

## 1.4 Using $\hat{j}(r)$ in problems

It is good to check that everything works in some simple examples. As a first case, suppose the system is 25% known to be in a plane wave of wave vector  $k_1$ , and 75% in a plane wave with  $k_2$ . Then the density matrix is

$$\hat{\rho} = \frac{1}{4} |k_1\rangle\langle k_1| + \frac{3}{4} |k_2\rangle\langle k_2| \quad (97)$$

These are, for all practical purposes, eigenstates of momentum  $\hbar k_1$  and  $\hbar k_2$ . The operator  $\hat{j}(r)$  for the current density (77) can be multiplied with this, and then the trace is to be taken. One has

$$\begin{aligned} \hat{j}(r)\hat{\rho} &= \frac{e}{2m} [|r\rangle\langle r|\hat{p} + \hat{p}|r\rangle\langle r|] \left[ \frac{1}{4} |k_1\rangle\langle k_1| + \frac{3}{4} |k_2\rangle\langle k_2| \right] \\ &= \frac{e}{2m} \left\{ \frac{1}{4} [|r\rangle\langle r|\hbar k_1|k_1\rangle\langle k_1| + \hat{p}|r\rangle\langle r|k_1\rangle\langle k_1|] + \frac{3}{4} [|r\rangle\langle r|\hbar k_2|k_2\rangle\langle k_2| + \hat{p}|r\rangle\langle r|k_2\rangle\langle k_2|] \right\} \\ &= \frac{e}{2m} \left\{ \frac{1}{4} \langle r|k_1\rangle (\hbar k_1 + \hat{p}) |r\rangle\langle k_1| + \frac{3}{4} \langle r|k_2\rangle (\hbar k_2 + \hat{p}) |r\rangle\langle k_2| \right\} \end{aligned} \quad (98)$$

Now imagine doing the trace using eigenstates of momentum, i.e.,  $\sum_k \langle k|\hat{j}(r)\hat{\rho}|k\rangle$ . The only terms that will survive will involve those where  $k$  matches  $k_1$  or  $k_2$ . Those terms will give, trivially,

$$\begin{aligned} \mathbf{j}(r) &= \frac{e}{2m} \left\{ \frac{1}{4} \langle r|k_1\rangle (2\hbar k_1) \langle k_1|r\rangle + \frac{3}{4} \langle r|k_2\rangle (2\hbar k_2) \langle k_2|r\rangle \right\} \\ &= \frac{e}{m} \left\{ \frac{1}{4} \hbar k_1 |\langle r|k_1\rangle|^2 + \frac{3}{4} \hbar k_2 |\langle r|k_2\rangle|^2 \right\} = \frac{e\hbar}{mV} \left( \frac{1}{4} \mathbf{k}_1 + \frac{3}{4} \mathbf{k}_2 \right) \end{aligned} \quad (99)$$

The factors  $|\langle r|k_1\rangle|^2$  and  $|\langle r|k_2\rangle|^2$  are normalization constants, which could be set to  $1/V$  where  $V$  is the normalization volume. So in the end, this is just the weighted average of the two momenta, scaled with the correct units. In this particular example, the current density is constant in space.

As the next example, consider the gauge current due to an applied electric field in some problem. Suppose the vector potential due a plane wave is as follows:

$$\mathbf{A}(r, t) = \mathbf{A}_{\mathbf{q}} e^{i(\mathbf{q}\cdot\mathbf{r} - \omega t)} + \mathbf{A}_{-\mathbf{q}} e^{-i(\mathbf{q}\cdot\mathbf{r} - \omega t)} \quad (100)$$

The two terms are necessary to make the field real, with the stipulation that  $\mathbf{A}_{-\mathbf{q}} = \mathbf{A}_{\mathbf{q}}^*$ . The electric field that corresponds to this potential is a time-dependent one, in the Coulomb gauge,

$$\mathbf{E}(r, t) = \frac{-1}{c} \frac{\partial \mathbf{A}}{\partial t} = \frac{i\omega}{c} \left\{ \mathbf{A}_{\mathbf{q}} e^{i(\mathbf{q}\cdot\mathbf{r} - \omega t)} - \mathbf{A}_{-\mathbf{q}} e^{-i(\mathbf{q}\cdot\mathbf{r} - \omega t)} \right\} \quad (101)$$

This is a real plane wave travelling along direction  $\mathbf{q}$ . Now the operator  $\hat{\mathbf{A}}$  forms part of the current operator. Here consider just its contribution to the current density at some position  $\mathbf{r}$ . The needed operator is, according to the formalism developed earlier,

$$\hat{j}_A(r, t) = \frac{-e^2}{2mc} \left[ |r\rangle\langle r| \hat{\mathbf{A}}(\hat{r}, t) + \hat{\mathbf{A}}(\hat{r}, t) |r\rangle\langle r| \right] = \frac{-e^2}{mc} |r\rangle\langle r| \hat{\mathbf{A}}(\hat{r}, t). \quad (102)$$

The last form holds because  $\hat{A}$  commutes with position operator  $\hat{r}$ . This is a function of both position and time, due to the dependence of  $\hat{A}$  on  $\hat{r}$  and  $t$ . If we simply had a pure state  $|\psi\rangle$  and directly took the expectation value in the simple way, it is

$$\langle \hat{j}_A(\hat{r}, t) \rangle = \langle \psi | \frac{-e^2}{mc} |r\rangle\langle r| \hat{\mathbf{A}}(\hat{r}, t) | \psi \rangle = \frac{-e^2}{mc} |\psi(r)|^2 \mathbf{A}(r, t) \quad (103)$$

This is completely identical to the current density obtained earlier by more elementary means. Note that the operator  $\hat{r}$  within  $\hat{A}$  extracted the eigenvalue of position  $r$ . But this is a very simple result, and depends explicitly on how the vector potential behaves, and also on the structure of the wave function. It indeed only gives the current density at some desired point where it is to be measured. This is clearly real, if  $\mathbf{A}$  is real. And, it is really the *expectation value* of the current density. If you think about that, it means that there are natural fluctuations of the current density about this value at the position  $r$ , associated with quantum uncertainty. Further, for the chosen example of vector potential, its spatial Fourier transform has intensity only at  $\mathbf{q}$  and  $-\mathbf{q}$ . If the wave function has amplitude only at particular wave vectors, then the Fourier space properties of the current density can be determined. Similarly, the frequency properties should be strongly dependent on the frequency  $\omega$  of the incident light field. The current density should primarily oscillate at frequencies  $\pm\omega$ . For instance, if  $\psi$  is a stationary state, then all of the time dependence comes from the vector potential, like

$$\mathbf{j}_A(r, t) = \langle \hat{j}_A(\hat{r}, t) \rangle = \frac{-e^2}{mc} |\psi(r)|^2 \left[ \mathbf{A}_{\mathbf{q}} e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)} + \mathbf{A}_{-\mathbf{q}} e^{-i(\mathbf{q}\cdot\mathbf{r}-\omega t)} \right] \quad (104)$$

Also, it is constructive to write this in terms of electric field intensity. The electric field could be expressed with two parts at frequencies  $\pm\omega$ :

$$\mathbf{E}(r, t) = \mathbf{E}_+ e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)} + \mathbf{E}_- e^{-i(\mathbf{q}\cdot\mathbf{r}-\omega t)}, \quad \mathbf{E}_+ = \frac{i\omega}{c} \mathbf{A}_{\mathbf{q}}, \quad \mathbf{E}_- = \frac{-i\omega}{c} \mathbf{A}_{\mathbf{q}}^* = \mathbf{E}_+^*. \quad (105)$$

Then the current density responses at "plus" and "minus" frequencies are separated, for instance,

$$\mathbf{j}_A = \mathbf{j}_{A+} e^{-i\omega t} + \mathbf{j}_{A-} e^{i\omega t}, \quad \mathbf{j}_{A\pm} = \frac{-e^2}{mc} |\psi(r)|^2 \frac{c}{i\omega} \mathbf{E}_{\pm} \quad (106)$$

The factor of  $\omega$  that comes into the denominator here ends up appearing in the theory for the plasmon frequency in the dielectric response for metals. [Another factor of  $\omega$  will appear in the denominator when the current density is used to get the dielectric function  $\epsilon(\omega)$ .]

Look also at the gauge current when there is a mixed state. In some thermally mixed state with occupation probabilities  $w_i$  for states labeled by their energies  $E_i$ , the density matrix to be used is

$$\hat{\rho} = \sum_i w_i |i\rangle\langle i|, \quad w_i = \frac{e^{-\beta E_i}}{Z} \quad (107)$$

This is stated using the probabilities in a canonical ensemble, as an example. The particular choice of probabilities isn't so important for the present discussion. If this is used to get the expectation value of the gauge current density, we have

$$\mathbf{j}_A(r, t) = \langle \hat{j}_A(\hat{r}, t) \rangle = \text{Tr} \left\{ \hat{\rho} \hat{j}_A \right\} = \sum_k \langle k | \sum_i w_i |i\rangle\langle i| \frac{-e^2}{mc} |r\rangle\langle r| \hat{\mathbf{A}}(\hat{r}, t) |k\rangle \quad (108)$$

The states  $|k\rangle$  can be eigenstates of any operator that is convenient. They may as well be energy eigenstates. Then only the terms with  $i = k$  survive. What results is

$$\mathbf{j}_A(r, t) = \frac{-e^2}{mc} \mathbf{A}(\mathbf{r}, t) \sum_k w_k |\langle r|k\rangle|^2 = \frac{-e^2}{mc} \mathbf{A}(\mathbf{r}, t) \sum_k w_k |\psi_k(r)|^2 \quad (109)$$

This is completely consistent with the current density obtained above, with the states weighted by their probabilities. From here, without knowing the structure of the energy wave functions, it is not possible to evaluate this further. However, it shows how the weighted wave function relates directly to the real space distribution of current density.

#### 1.4.1 Averaging over a volume, again

One thing that can be done, is to imagine averaging the current density over the whole system volume  $V$ . To do that, one should integrate over all the volume and divide by  $V$ . This gives

$$\bar{\mathbf{j}}_A(t) = \frac{1}{V} \int d^3r \frac{-e^2}{mc} \mathbf{A}(\mathbf{r}, t) \sum_k w_k |\psi_k(r)|^2 \quad (110)$$

This is again impossible to evaluate exactly, unless more is known about the state wave functions. However, suppose the volume of interest is something like an atomic wave function, or other atomic size, much smaller than the wavelength of the light. Then the vector potential can be considered a constant and taken outside the integration. The remaining integrals over the squared wave functions are all equal to 1, because they are assumed to be normalized. Finally, the sum over the probabilities gives a 1. This gives

$$\bar{\mathbf{j}}_A(t) = \frac{-e^2}{mcV} \mathbf{A}(\mathbf{r}_c, t) \quad (111)$$

where  $\mathbf{r}_c$  is the average position of the wave functions, which might need some better definition. This is approximate anyway. And, the volume should not have a diameter greater than the wavelength for the plane wave in  $\mathbf{A}$ . If the average is done over a very large volume, much larger than the quantum system, this average will tend towards zero. This is more meaningful for an average at microscopic length scales. One can check that the units are correct here (in CGS).

One point to keep in mind, however, is that this last result applies to a single electron. In a real system we need the response of  $N$  electrons. There will be a certain number of electrons per unit volume,  $n = N/V$ , then the result is that the current density is proportional to the number density of electrons:

$$\bar{\mathbf{J}}_A(t) = \frac{-ne^2}{mc} \mathbf{A}(\mathbf{r}_c, t) \quad (112)$$

If we had simply used expression (96), ignoring the contribution from the momentum, there would be

$$\bar{\mathbf{J}}_A(t) = \frac{-ne^2}{mc} \text{Tr}\{\hat{\rho} \hat{\mathbf{A}}(\hat{r}, t)\} \quad (113)$$

These two results are the same, as long as the averaged vector potential is the same as the potential at the “average position of the wave functions,  $\mathbf{r}_c$ ”. In the most general case where both the momentum and gauge currents are included, the net volume-averaged current density is

$$\bar{\mathbf{J}}(t) = \frac{ne}{m} \text{Tr}\left\{\hat{\rho} \left(\hat{\mathbf{p}} - \frac{e}{c} \hat{\mathbf{A}}(\hat{r}, t)\right)\right\} \quad (114)$$

Now suppose only the positive frequency response is studied. In electrodynamics, current density and electric field are related by the frequency-dependent conductivity  $\sigma(\omega)$ , which is itself related to the susceptibility  $\chi(\omega)$ . Supposing that  $\mathbf{E} = (i\omega/c)\mathbf{A}$ , there are these relations:

$$\mathbf{J} = \sigma\mathbf{E} = -i\omega \chi(\omega) \cdot \mathbf{E} = -i\omega \chi(\omega) \cdot \frac{i\omega}{c} \mathbf{A} = \frac{\omega^2}{c} \chi(\omega) \cdot \mathbf{A}. \quad (115)$$



Comparing with the result from the density matrix averaging, the susceptibility is found to be (symbolically for these tensor objects—this result is purely diagonal)

$$\chi(\omega) = \frac{c\mathbf{J}}{\omega^2\mathbf{A}} = \frac{-ne^2}{m\omega^2}. \quad (116)$$

Then the contribution of this to the dielectric function gives the plasmon term mentioned earlier,

$$\epsilon(\omega) = 1 + 4\pi\chi(\omega) = 1 - \frac{4\pi ne^2}{m\omega^2}. \quad (117)$$

It is interesting that this response comes directly from the gauge current term. It seems that the electrons respond almost instantaneously to the electric field oscillations—there is no delay or damping. This reproduces the well known result for the dielectric response of a free electron gas, showing the plasma oscillation term and plasma frequency, that can be read about in other notes!