# Equation of continuity for $\psi^*\psi$

QM is characterized via the Schrödinger equation

$$-\frac{\hbar}{i}\frac{\partial\psi}{\partial t} = H\psi$$

where $H = -\frac{\hbar^2}{2m}\nabla^2 + V(\underline{r})$ "Hamiltonian"

and we work in the coordinate representation,

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \qquad V = V(x,y,z) \qquad \psi = \psi(x,y,z,t)$$

where $x, y, z$ are the coordinates of the particle we are considering.

We will postulate/"derive" this later. But, it is probably familiar to you from a previous course. (After all, $ma = F$, $F = -dV/dx$ is also a postulate) $a = d^2x/dt^2$)

The probability interpretation of QM says that $(dx\,dy\,dz)\,\psi^*\psi$ is the probability of observing the particle in the volume $dx\,dy\,dz$ at time $t$.

$\psi$ is a complex function, in general. $\psi^*$ is its complex conjugate (c.c.): $\psi = \psi_{re} + i\psi_{im}$; ($\psi_{re}$, $\psi_{im}$ reals) $\psi^*\psi = (\psi_{re} - i\psi_{im})$ $\times(\psi_{re} + i\psi_{im})$ $= \psi_{re}^2 + -i\psi_{im}\psi_{re} + i\psi_{re}\psi_{im} + \psi_{im}^2$ $= \psi_{re}^2 + \psi_{im}^2 \geq 0$

Since a function $\otimes$ complex conjugate function is real, $\psi^*\psi$ is real and can be a probability.

Probabilities can be normalized, so we require

$$\int dx\,dy\,dz\ \psi^*\psi = 1$$

The particle, at time $t$, must be somewhere, so we get the "whole" particle by integrating over all space

define term
gradient $\nabla f$
divergence $\nabla \cdot \underline{V}$
Lap. $\nabla^2 f$



We can take the c.c. of the Schrödinger eq.

$$H \psi^* = \frac{\hbar}{i} \frac{\partial \psi^*}{\partial t}$$

note that $i \equiv \sqrt{-1}$ and $i^* = -i$

self-adjoint

note that $H^* = H$ a so-called Hermitian operator – we will discuss this in more detail later.

The first thing we will do is get a conservation of probability law. It will be useful for discussing how a quantum particle behaves in a potential. Also for connection to classical mechanics.

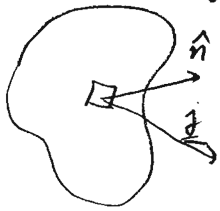
A conservation of probability equation has the general form (notation $\underline{a} \cdot \underline{b} \equiv a_x b_x + a_y b_y + a_z b_z = \sum_{\alpha=1}^{3} a_\alpha b_\alpha$ $(\alpha \in x, y, z)$)

$$\frac{\partial \rho}{\partial t} + \underline{\nabla} \cdot \underline{j} \equiv 0$$

(See e.g. Arfken for mathematics of $\underline{\nabla}$ and for conservation eq.)

$\rho = \psi^* \psi$ $\quad \underline{j}$ is "flux" (probability current density)

Consider a surface (in x, y, z – space) The flux vector $\underline{j}$ is drawn, along with the normal vector (unit vector) $\hat{n}$ to the surface at that "point" (differential area)




$\underline{j} \cdot \hat{n}$ gives amount (of probability) / cm$^2$-sec that exits/enters, at time $t$, per unit time.

Note $\underline{\nabla} \cdot \underline{j} \equiv \operatorname{div} \underline{j} \equiv \frac{\partial}{\partial x} j_x + \frac{\partial}{\partial y} j_y + \frac{\partial}{\partial z} j_z$

Note $\nabla f(x,y,z) \equiv \hat{\imath} \frac{\partial f}{\partial x} + \hat{\jmath} \frac{\partial f}{\partial y} + \hat{k} \frac{\partial f}{\partial z}$


$$\nabla \cdot \nabla f = \left(\hat{\imath} \frac{\partial}{\partial x} + \hat{\jmath} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z}\right)\left(\hat{\imath} \frac{\partial f}{\partial x} + \hat{\jmath} \frac{\partial f}{\partial y} + \hat{k} \frac{\partial f}{\partial z}\right) = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

Lets get $\frac{\partial}{\partial t}(\psi^* \psi)$.

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}(\psi^*\psi) = -\frac{\hbar}{i}\left[\psi^* \frac{\partial \psi}{\partial t} + \psi\frac{\partial \psi^*}{\partial t}\right] = -\frac{\hbar}{i}\left[\psi^*\left(\frac{-i}{\hbar}H\psi\right) + \psi\left(\frac{i}{\hbar}H\psi^*\right)\right]$$

$$= \psi^* H \psi - \psi H \psi^*$$

Sub. in $H = -\frac{\hbar^2}{2m}\nabla^2 + V$

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}(\psi^*\psi) = -\frac{\hbar^2}{2m}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right), \quad \text{(V part cancels)}$$

Want to write rhs as a divergence.
It is

$$\underline{\nabla}\cdot(\psi^*\underline{\nabla}\psi - \psi\underline{\nabla}\psi^*) = \cancel{\nabla\psi^*\nabla\psi} + \psi^*\nabla^2\psi - \cancel{\nabla\psi\nabla\psi^*} - \psi\nabla^2\psi^*$$
$$= \underline{\psi^*\nabla^2\psi - \psi\nabla^2\psi^*} \quad \checkmark$$

So

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\rho = -\frac{\hbar^2}{2m}\underline{\nabla}\cdot(\psi^*\underline{\nabla}\psi - \psi\underline{\nabla}\psi^*) = +\frac{\hbar}{i}\frac{\hbar}{2mi}\underline{\nabla}\cdot(\psi^*\underline{\nabla}\psi - \psi\underline{\nabla}\psi^*)$$

or $$\boxed{\frac{\partial\rho}{\partial t} + \underline{\nabla}\cdot\underline{j} = 0 \quad \text{with} \quad \underline{j} = \frac{\hbar}{2mi}(\psi^*\underline{\nabla}\psi - \psi\underline{\nabla}\psi^*)}$$

If we multiply by $m$, the particle mass we get a mass density $\rho_m = m\rho$

and momentum density $\underline{g} = m\underline{j}$ $\left(\underline{g}\,(m/cm^2 \cdot sec) \times \overset{\text{volume}}{cm^3} \sim \frac{m \cdot cm}{sec} = \text{moment}\right)$

So continuity eq. is that of mass conservation

Multiply by $e$, particle charge, get conservation of charge

Say: in hydrodynamics $\vec{j} = \rho\cdot\vec{v}$

The total momentum of the Schrödinger "field" is

$$\underline{p} = \int dx\,dy\,dz\ \underline{g} = \frac{\hbar}{2i}\int dx\,dy\,dz\left(\Psi^* \underline{\nabla}\,\Psi - \Psi\underline{\nabla}\,\Psi^*\right)$$

Integrate the second term by parts. Let $d\tau = dx\,dy\,dz$

$$\int d\tau\ \Psi\nabla\Psi^* = \int d\tau\ \nabla(\Psi\Psi^*) - \int d\tau\,\Psi^*\nabla\Psi$$

But $\int d\tau\ \nabla(\Psi\Psi^*) = (\Psi\Psi^*)\Big|_{\text{evaluate on boundary} \to \infty}$

Assume $\Psi \to 0$ as boundary $\to \infty$ so this term vanishes.
(Note that we assumed $\Psi$ is normalizable from the outset)

Therefore, $\underline{p} = \frac{\hbar}{2i}\left(\int dx\,dy\,dz\ \Psi^*\nabla\Psi + \int d\tau\ \Psi^*\nabla\Psi\right) = \frac{\hbar}{i}\int d\tau\ \Psi^*\nabla\Psi$ , $\hat{A}$ operator

Since expectation values in QM are defined as $A = \langle\hat{A}\rangle = \int d\tau\ \Psi^*\hat{A}\Psi$,
this motivates <u>definition</u> of <u>momentum operator</u>

$$\hat{\underline{p}} = \frac{\hbar}{i}\underline{\nabla}$$

with two arbitrary functions $u$ and $v$, both complex and only chosen so that the integrals exist. With $\Omega$ the operator (7.3) and $\alpha$ real, this yields

$$\frac{\hbar}{i}\int d^3x\,u^*\left[(1-\alpha)x\frac{\partial v}{\partial x}+\alpha\frac{\partial(xv)}{\partial x}\right]=-\frac{\hbar}{i}\int d^3x\left[(1-\alpha)x\frac{\partial u^*}{\partial x}+\alpha\frac{\partial(xu^*)}{\partial x}\right]v$$

or

$$\int d^3x\,u^*\left[x\frac{\partial v}{\partial x}+\alpha v\right]=-\int d^3x\left[x\frac{\partial u^*}{\partial x}+\alpha u^*\right]v\,.$$

Reordering leads on to

$$\int d^3x\,x\frac{\partial}{\partial x}(u^*v)=-2\alpha\int d^3x\,u^*v$$

or, by partial integration on the left-hand side, to

$$-\int d^3x\,u^*v=-2\alpha\int d^3x\,u^*v$$

which, of course, yields the result of $\alpha=\frac{1}{2}$, Eq. (7.5), again.

## Problem 8. Derivatives of an operator

Let $f(p,x)$ be an integer function of the operators $p_k, x_k$. Then the general relations

$$\frac{\partial f}{\partial x_k}=-[f,p_k] \tag{8.1}$$

and

$$\frac{\partial f}{\partial p_k}=[f,x_k] \tag{8.2}$$

with the abbreviation

$$[f,g]=\frac{i}{\hbar}(fg-gf)$$

shall be derived from the commutation rules.

**Solution.** The commutation rules are

$$[p_k,p_l]=0;\qquad [x_k,x_l]=0;\qquad [p_k,x_l]=\delta_{kl}\,. \tag{8.3}$$

From these we construct (8.1) and (8.2) in four consecutive steps:

1. Let $f=p_l$, then we have $\partial f/\partial x_k=0$ and $\partial f/\partial p_k=\delta_{kl}$. Hence, Eqs. (8.1) and (8.2) become $[p_k,p_l]=0$ and $[p_l,x_k]=\delta_{kl}$; i.e. they are satisfied according to (8.3). In the same way, for $f=x_l$, $\partial f/\partial x_k=\delta_{kl}$, $\partial f/\partial p_k=0$, they may be proved to hold.

2. Let (8.1) and (8.2) hold for two functions $f$ and $g$. Then they hold as well for any linear combination $c_1 f + c_2 g$ with complex numbers $c_1$ and $c_2$, in consequence of their linearity.

3. With $f$ and $g$, they hold for the product $fg$. For (8.1) this is easily checked by direct computation:

$$\frac{\partial}{\partial x_k}(fg) = f\frac{\partial g}{\partial x_k} + \frac{\partial f}{\partial x_k}g = -\{f[g,p_k]+[f,p_k]g\}$$
$$= -\frac{i}{\hbar}\{fgp_k - fp_kg + fp_kg - p_kfg\} = -[fg,p_k]$$

with the two central terms cancelling. An analogous computation is easily performed to prove (8.2).

4. It then follows that the relations hold for any linear combination of products consisting of an arbitrary number of $p_k$'s and $x_k$'s, i.e. for any integer function in these variables, as had to be proved.

## Problem 9. Time rate of an expectation value

Let $\langle A\rangle$ be the expectation value of an operator not explicitly dependent upon time in a time dependent state $\psi$. How does $\langle A\rangle$ change with time? What follows for $\langle x_k\rangle$ and $\langle p_k\rangle$?

**Solution.** The expectation value

$$\langle A\rangle = \langle\psi|A|\psi\rangle = \int d\tau\, \psi^*(t) A\, \psi(t) \tag{9.1}$$

has the time rate

$$\frac{d}{dt}\langle A\rangle = \int d\tau \{\dot\psi^* A\psi + \psi^* A\dot\psi\}. \tag{9.2}$$

The time derivatives of the two wave functions $\psi$ and $\psi^*$ satisfy the Schrödinger equations

$$-\frac{\hbar}{i}\dot\psi = H\psi; \qquad \frac{\hbar}{i}\dot\psi^* = H^\dagger\psi^* \tag{9.3}$$

with the hamiltonian operator $H$ being hermitian: $H = H^\dagger$. Putting (9.3) into (9.2), we find

$$\frac{d}{dt}\langle A\rangle = \frac{i}{\hbar}\int d\tau \{(H^\dagger\psi^*)A\psi - \psi^* A H\psi\}$$

or, in Hilbert space notation,

$$\frac{d}{dt}\langle A\rangle = \frac{i}{\hbar}\{\langle H\psi|A\psi\rangle - \langle\psi|AH\psi\rangle\}. \tag{9.4}$$

LECTURE 1.

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Read Merz Chp. 2, 3. Study 4.
I will assume some familiarity with Q.M., but always go back eventually to state assumptions formally.



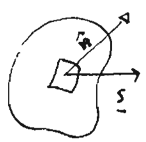
# I. General Concepts

### Problem 1. Law of probability conservation

If the normalization relation

$$\int d^3x\,\psi^*\psi = 1 \tag{1.1}$$

is interpreted in the sense of probability theory, so that $d^3x\psi^*\psi$ is the probability of finding the particle under consideration in the volume element $d^3x$, then there must be a conservation law. This is to be derived. How may it be interpreted classically?




$\underset{\sim}{s} \sim \#/cm^2 \cdot sec$

**Solution.** The conservation law sought must have the form of an equation of continuity,

$$\operatorname{div} s + \frac{\partial \rho}{\partial t} = 0 \tag{1.2}$$

with

$$\rho = \psi^*\psi \tag{1.3}$$

the probability density, and $s$ the probability current density. As $\rho$ is a bilinear form of $\psi$ and its complex conjugate, Eq. (1.2) can be constructed only by a combination of the two Schrödinger equations

$$H\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t}; \qquad H\psi^* = \frac{\hbar}{i}\frac{\partial\psi^*}{\partial t} \tag{1.4}$$

with the hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(r) \tag{1.5}$$

the same for both equations. Thus we find

$$\psi^* H\psi - \psi H\psi^* = -\frac{\hbar}{i}\frac{\partial\rho}{\partial t}.$$

According to (1.2) it ought to be possible to write the left-hand side in the form of a divergence. Indeed we have use explicit $S$, eg.

$$\psi^* H\psi - \psi H\psi^* = -\frac{\hbar^2}{2m}(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*) = -\frac{\hbar^2}{2m}\operatorname{div}(\psi^*\nabla\psi - \psi\nabla\psi^*)$$

so that we may identify

$$s = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*). \tag{1.6}$$

Classical interpretations may be arrived at as follows. If the quantities $\rho$ and $s$ are both multiplied by $m$, the mass of the particle, we obtain mass density $\rho_m$ and momentum density $g$:

$\rho$ : cm$^3$ $g \sim \underline{\underline{mv}}$

$$\rho_m = m\rho; \quad g = ms, \tag{1.7}$$

$g \sim m/\mathrm{cm}^2 \cdot \sec$

and the equation of continuity may be interpreted as the law of mass conservation. In the same way, multiplication by the particle charge, $e$, yields charge density $\rho_e$ and electric current density $j$:

$$\rho_e = e\rho; \quad j = es, \tag{1.8}$$

and (1.2) becomes the law of charge conservation.

It is remarkable that the conservation laws of both mass and charge are essentially identical. This derives from the fact that one particle by its convection current causes both.

The expression for the total momentum of the Schrödinger field, derived from (1.6) and (1.7),

$$p = \int d^3x\, g = \frac{\hbar}{2i}\int d^3x(\psi^*\nabla\psi - \psi\nabla\psi^*),$$

may by partial integration in the second term be reduced to

$$p = \int d^3x\,\psi^*\left(\frac{\hbar}{i}\nabla\right)\psi \tag{1.9}$$

corresponding to its explanation as the expectation value of the momentum operator $(\hbar/i)\,\nabla$ in the quantum state $\psi$ (cf. Problem 3). $= \hat{p} = \frac{\hbar}{i}\nabla$

**Problem 2. Variational principle of Schrödinger**

To replace the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\psi = E\psi \tag{2.1}$$

by a variational principle for the energy.

**Solution.** Since the constraint

$$\int d^3x\,\psi^*\psi = 1 \tag{2.2}$$

holds for any solution $\psi$ of the differential equation (2.1), the energy will be found by multiplying (2.1) with $\psi^*$ and integrating over the whole space:

$$E = \int d^3x\,\psi^* \left\{ -\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\psi \right\}. \tag{2.3}$$

A partial integration in the first term yields, according to Green's law,

$$\int d^3x\,\psi^*\nabla^2\psi = \oint df\cdot\psi^*\nabla\psi - \int d^3x\,\nabla\psi^*\cdot\nabla\psi\,. \tag{2.4}$$

Now, the normalization integral (2.2) exists only if, at large distances $r$, the solution $\psi$ vanishes at least as

$$\psi \propto r^{-\frac{3}{2}-\varepsilon}; \qquad \varepsilon > 0\,.$$

Under this condition, however, the surface integral in (2.4) vanishes when taken over an infinitely remote sphere so that (2.3) may be written

$$E = \int d^3x \left\{ \frac{\hbar^2}{2m}\nabla\psi^*\cdot\nabla\psi + \psi^* V(r)\psi \right\}. \tag{2.5}$$

This equation is completely symmetrical in the functions $\psi$ and $\psi^*$, as is the normalization (2.2), so that it might equally well have been derived from the complex conjugate of Eq. (2.1),

$$-\frac{\hbar^2}{2m}\nabla^2\psi^* + V(r)\psi^* = E\psi^*\,. \tag{2.1*}$$

It would not be difficult to show that (2.1) and (2.1*) are the Euler equations of the variational problem to extremize the integral (2.5) with the constraint (2.2). We shall, however, make no use of the apparatus of variational theory and prefer a direct proof, instead.

Let $\psi_\lambda$ be a solution of (2.1) that belongs to its eigenvalue $E_\lambda$. It will give the integral (2.5) the value $E_\lambda$. Let us then replace $\psi_\lambda$ by a neighbouring function $\psi_\lambda + \delta\psi$ with $|\delta\psi|$ being small but arbitrary, except for (2.2) still to hold for $\psi_\lambda + \delta\psi$ as well as for $\psi_\lambda$:

$$\int d^3x(\psi_\lambda^* + \delta\psi^*)(\psi_\lambda + \delta\psi) = 1$$

and therefore

$$\int d^3x(\psi_\lambda\delta\psi^* + \psi_\lambda^*\delta\psi) + \int d^3x\,\delta\psi^*\delta\psi = 0\,. \tag{2.6}$$

Setting $\psi_\lambda + \delta\psi$ into the energy integral (2.5), the energy becomes $E_\lambda + \delta E_\lambda$ with

$$\delta E_\lambda = \int d^3x \left\{ \frac{\hbar^2}{2m} (\nabla\psi_\lambda^* \cdot \nabla\delta\psi + \nabla\psi_\lambda \cdot \nabla\delta\psi^*) + V(\psi_\lambda \delta\psi^* + \psi_\lambda^* \delta\psi) \right\}$$
$$+ \int d^3x \left\{ \frac{\hbar^2}{2m} \nabla\delta\psi^* \cdot \nabla\delta\psi + V\,\delta\psi^*\,\delta\psi \right\}. \tag{2.7}$$

Here the first-order changes stand in the first, and the second-order changes in the second line. By partial integration in the sense opposite to the one above we fall back, in the first line, on $\delta\psi\,\nabla^2\psi_\lambda^*$ and $\delta\psi^*\,\nabla^2\psi_\lambda$ where (2.1) and (2.1*) may be used to eliminate the derivatives. E.g. we then have

$$\int d^3x \left\{ \frac{\hbar^2}{2m} \nabla\psi_\lambda^* \cdot \nabla\delta\psi + V\psi_\lambda^*\,\delta\psi \right\} = E_\lambda \int d^3x\,\delta\psi\,\psi_\lambda^*,$$

so that with the help of Eq. (2.6), the first line of (2.7) may finally be reduced to second-order contributions only:

$$\delta E_\lambda = \int d^3x \left\{ \frac{\hbar^2}{2m} |\nabla\delta\psi|^2 + (V - E_\lambda)|\delta\psi|^2 \right\}. \tag{2.8}$$

Since no linear contribution in $\delta\psi$ or $\delta\psi^*$ remains, $E_\lambda$ clearly is a maximum or a minimum for $\delta\psi = 0$, i.e. for $\psi_\lambda$ being a solution of the Schrödinger equation. Whether we get a maximum or a minimum will be decided by the sign of (2.8).

To get some insight into this last question we make use of the set $\{\psi_\nu\}$ of solutions to (2.1) to form a complete orthogonal system of functions,

$$\int d^3x\,\psi_\mu^*\,\psi_\nu = \delta_{\mu\nu}. \tag{2.9}$$

We then expand $\delta\psi$ with respect to this system:

$$\delta\psi = \sum_\nu c_\nu \psi_\nu. \tag{2.10}$$

Eq. (2.8) then renders

$$\delta E_\lambda = \sum_\mu \sum_\nu c_\mu^* c_\nu \int d^3x \left\{ \frac{\hbar^2}{2m} \nabla\psi_\mu^* \cdot \nabla\psi_\nu + (V - E_\lambda)\psi_\mu^* \psi_\nu \right\}$$
$$= \sum_\mu \sum_\nu c_\mu^* c_\nu \int d^3x\,\psi_\mu^* \left\{ -\frac{\hbar^2}{2m} \nabla^2\psi_\nu + (V - E_\lambda)\psi_\nu \right\}$$

or, using (2.1) and (2.9):

$$\delta E_\lambda = \sum_\mu |c_\mu|^2 (E_\mu - E_\lambda). \tag{2.11}$$

If $E_\lambda$ is the ground state, we have $E_\mu \geqslant E_\lambda$ for all states $\mu$, so that the sum (2.11) is positive. The variational principle therefore makes $E_\lambda$ a minimum. No such general rule can be established for excited states where the sum (2.11) consists of positive and negative terms.

## Problem 3. Classical mechanics for space averages

To show that Newton's fundamental equation of classical dynamics,

$$\frac{d\boldsymbol{p}}{dt} = \boldsymbol{F}\,, \tag{3.1}$$

with $\boldsymbol{p}$ the momentum of, and $\boldsymbol{F}$ the force acting upon the particle, still holds for the space averages (expectation values) of the corresponding operators in quantum mechanics.

**Solution.** If the force $\boldsymbol{F}$ derives from a potential, $\boldsymbol{F} = -\nabla V$, and momentum is replaced by the operator $(\hbar/i)\nabla$, then the two space averages in Eq. (3.1) are defined by

$$\boldsymbol{p} = \frac{\hbar}{i}\int d^3x\, \psi^* \nabla \psi\,; \tag{3.2}$$

$$\boldsymbol{F} = -\int d^3x\, \psi^* (\nabla V)\psi\,. \tag{3.3}$$

Our task then is to prove that (3.1) is valid for the integrals (3.2) and (3.3) if $\psi$ and $\psi^*$ satisfy the Schrödinger equations

$$\left.\begin{aligned} -\frac{\hbar}{i}\frac{\partial \psi}{\partial t} &= -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi\,;\\ +\frac{\hbar}{i}\frac{\partial \psi^*}{\partial t} &= -\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^*\,. \end{aligned}\right\} \tag{3.4}$$

We start our proof with the time derivative of Eq. (3.2):

$$\dot{\boldsymbol{p}} = \frac{\hbar}{i}\int d^3x(\dot\psi^*\nabla\psi + \psi^*\nabla\dot\psi) = \frac{\hbar}{i}\int d^3x(\dot\psi^*\nabla\psi - \dot\psi\nabla\psi^*)$$

where the surface contribution of the space partial integration in the last term vanishes and has been omitted. Replacing $\dot\psi^*$ and $\dot\psi$ according to (3.4), we may proceed to

Homework 1.7 does these steps, so go from here to 3.6

$$\dot{p} = -\frac{\hbar^2}{2m}\int d^3x(\nabla^2\psi^*\nabla\psi + \nabla^2\psi\nabla\psi^*)$$
$$+\int d^3x(\psi^* V\nabla\psi + V\psi\nabla\psi^*)\,. \tag{3.5}$$

A partial integration,

$$\int d^3x\,\nabla^2\psi^*\nabla\psi = -\int d^3x\,\nabla\psi^*\nabla^2\psi$$

shows that the two terms of the first integral cancel each other out. In the other integral of Eq. (3.5) we perform a partial integration in the last term,

$$\dot{p} = \int d^3x\,\psi^*\{V\nabla\psi - \nabla(V\psi)\}\,. \qquad 3.6$$

Making use of

$$\nabla(V\psi) = V\nabla\psi + \psi\nabla V,$$

we finally arrive at

$$\dot{p} = -\int d^3x\,\psi^*(\nabla V)\psi = F\,,$$

as was to be proved.

N.B. This is not classical relation. Classical is $\dot{p} = -F(\langle r\rangle)$ where $\langle F\rangle \equiv \int d^3x\,\rho(x)(-\nabla V(x)) := F(\langle x\rangle) = F(\int d^3x\,\rho(x)x)$. True for $\rho(x)$ versus $F(x)$

## Problem 4. Classical laws for angular motion

To show that the classical relation between angular momentum $L = r\times p$ and torque $T = r\times F$ (where $p$ stands for linear momentum and $F$ for force),

mention this
$$\frac{dL}{dt} = T\,, \tag{4.1}$$

still holds for the space averages in quantum mechanics.

**Solution.** As in the preceding problem, we start by constructing the space averages

$$L = \frac{\hbar}{i}\int d^3x\,\psi^*(r\times\nabla)\psi \tag{4.2}$$

and

$$T = -\int d^3x\,\psi^*(r\times\nabla V)\psi\,. \tag{4.3}$$

The wave functions, $\psi$ and $\psi^*$, are again supposed to satisfy the Schrödinger equations (3.4).

We begin the proof of Eq. (4.1) by differentiating $\boldsymbol{L}$, Eq. (4.2):

$$\dot{\boldsymbol{L}} = \frac{\hbar}{i} \int d^3x \, \{\dot{\psi}^*(\boldsymbol{r} \times \nabla\psi) + \psi^*(\boldsymbol{r} \times \nabla\dot{\psi})\}.$$

In the second term we use the identity

$$\psi^* \nabla\dot{\psi} = \nabla(\psi^* \dot{\psi}) - \dot{\psi} \nabla\psi^*,$$

to the first term of which we apply the general vector rule

$$\int d^3x \, \boldsymbol{r} \times \nabla f = 0 \tag{4.4}$$

with $f = \psi^* \dot{\psi}$. Thus we arrive at

$$\dot{\boldsymbol{L}} = \frac{\hbar}{i} \int d^3x \, \boldsymbol{r} \times (\dot{\psi}^* \nabla\psi - \dot{\psi} \nabla\psi^*)$$

where we replace the time derivatives $\dot{\psi}^*$ and $\dot{\psi}$ according to (3.4):

$$\begin{aligned} \dot{\boldsymbol{L}} = & -\frac{\hbar^2}{2m} \int d^3x \, \boldsymbol{r} \times (\nabla^2\psi^* \nabla\psi + \nabla^2\psi \nabla\psi^*) \\ & + \int d^3x \, V \boldsymbol{r} \times (\psi^* \nabla\psi + \psi \nabla\psi^*). \end{aligned} \tag{4.5}$$

Now, in the first integral, the bracket

$$\nabla^2\psi^* \nabla\psi + \nabla^2\psi \nabla\psi^* = \nabla(\nabla\psi^* \cdot \nabla\psi)$$

is the gradient of the scalar function $f = \nabla\psi^* \cdot \nabla\psi$ so that, according to (4.4), this integral vanishes. In the second integral, the bracket is equal to $\nabla(\psi^* \psi)$. We then use the identity

$$V \nabla(\psi^* \psi) = \nabla(V \psi^* \psi) - \psi^* \psi \nabla V$$

and for $f = V\psi^*\psi$ again the vector rule (4.4). Then the integral becomes finally

$$\int d^3x \, \boldsymbol{r} \times [V \nabla(\psi^* \psi)] = -\int d^3x \, \boldsymbol{r} \times (\psi^* \psi \nabla V),$$

i.e. it becomes identical with the torque average (4.3), as was to be proved.

Show that Newton's equation of classical dynamics

$$d\underline{p}/dt = \underline{F}$$

hold for <u>expectation</u> values of the corresponding operators of momentum $\hat{p}$ and force $\hat{F}$ in QM,

Assume: $\underline{F}$ arises from a potential $V$

$$\underline{F} = -\underline{\nabla} V$$

Assume momentum is replaced by the momentum operator $\frac{\hbar}{i}\underline{\nabla}$.

The two expectation values are defined by

$$\langle \underline{p} \rangle = \frac{\hbar}{i}\int d\tau \; \psi^* \underline{\nabla} \psi \qquad d\tau = dx\,dy\,dz$$

$$\langle \underline{F} \rangle = -\int d\tau \; \psi^* \underline{\nabla} V \psi$$

Once again consider the Schrödinger equation and its c.c.

$$-\frac{\hbar}{i}\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi \, ; \qquad +\frac{\hbar}{i}\frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^*$$

Lets look at time derivative of $\underline{p}$ equation $\quad \frac{dA}{dt} \equiv \dot{A}$

$$\langle \dot{\underline{p}} \rangle = \frac{\hbar}{i}\int d\tau \left( \dot{\psi}^* \nabla \psi + \psi^* \nabla \dot{\psi} \right)$$

In last term, integrate by parts (in space derivatives of course) and drop boundary term once again assuming normalizable wavefunction.

Then $\langle \dot{\underline{p}} \rangle = \frac{\hbar}{i} \int d\tau \left( \dot{\psi}^* \nabla \psi - \dot{\psi} \nabla \psi^* \right)$

In homework 1.7 you will substitute in $\dot{\psi}$ in terms of $H$, write out as KE + PE parts and do integration by parts on both the KE + PE parts to get

$$\langle \dot{\underline{p}} \rangle = - \int d\tau \; \psi^* \{ V \nabla \psi - \nabla (V \psi) \}$$

Then use $\underline{\nabla}(V\psi) = V\underline{\nabla}\psi + \psi \underline{\nabla} V$ so

$$\langle \dot{p} \rangle = - \int d\tau \; \psi^* \{ V \nabla \psi - V \nabla \psi + \psi \underline{\nabla} V \}$$

$$\langle \dot{\underline{p}} \rangle = - \int d\tau \; \psi^* (\nabla V) \psi = \langle \underline{F} \rangle$$

which is Newton-like in that it has the form of Newton but is for the expectation values

NOTE: This is not classical equation of motion

Classical is $\dot{p} = - F(\langle \underline{r} \rangle)$

~~where $\langle E \rangle = - \int d\tau \; \psi^* (\underline{\nabla} V) \psi = F(\int d\tau \; \psi^*$~~

meaning when $\rho$, prob density is very concentrated in space we can replace expectation value of some function of $\underline{r}$ by the function of the expectation value of $\underline{r}$.

Similar to usual averages.

$\langle x^n \rangle \simeq \langle x \rangle^n$ if $p(x)$ is very concentrated,

## Problem 5. Energy conservation law

If the energy content of a Schrödinger wave field is described by the space integral (2.5) of problem 2, the law of energy conservation should be of the form

$$\frac{\partial W}{\partial t} + \operatorname{div} S = 0 \tag{5.1}$$

with $W$ the energy density and $S$ the energy flux vector. This law shall by derived by constructing the flux vector $S$.

**Solution.** We have found in (2.5) that

$$E = \int d^3x\, W \tag{5.2}$$

with

$$W = \frac{\hbar^2}{2m} \nabla\psi^* \cdot \nabla\psi + \psi^* V \psi\,, \tag{5.3}$$

where the first term is the kinetic, the second the potential energy density. According to Eq. (5.1) we need the derivative

$$\dot{W} = \frac{\hbar^2}{2m} (\nabla\dot{\psi}^* \cdot \nabla\psi + \nabla\psi^* \cdot \nabla\dot{\psi}) + V(\dot{\psi}^* \psi + \psi^* \dot{\psi})\,. \tag{5.4}$$

Since

$$\nabla\dot{\psi}^* \nabla\psi = \nabla(\dot{\psi}^* \nabla\psi) - \dot{\psi}^* \nabla^2 \psi$$

and

$$\nabla\psi^* \nabla\dot{\psi} = \nabla(\dot{\psi} \nabla\psi^*) - \dot{\psi} \nabla^2 \psi^*$$

we can reshape the kinetic energy part of (5.4) and write

$$\begin{aligned} \dot{W} = \nabla \left\{ \frac{\hbar^2}{2m} (\dot{\psi}^* \nabla\psi + \dot{\psi} \nabla\psi^*) \right\} - \frac{\hbar^2}{2m} \dot{\psi}^* \nabla^2 \psi - \frac{\hbar^2}{2m} \dot{\psi} \nabla^2 \psi^* \\ + \dot{\psi}^* V \psi \qquad + \dot{\psi} V \psi^*\,. \end{aligned} \tag{5.5}$$

In the last terms, use of the Schrödinger equations (3.4) permits us to replace space derivatives and potential by time derivatives. The resulting terms

$$\dot{\psi}^* \left( -\frac{\hbar}{i} \dot{\psi} \right) + \dot{\psi} \left( \frac{\hbar}{i} \dot{\psi}^* \right) = 0$$

exactly cancel so that Eq. (5.5) indeed is of the form (5.1) to be proved with

$$S = -\frac{\hbar^2}{2m} (\dot{\psi}^* \nabla\psi + \dot{\psi} \nabla\psi^*) \tag{5.6}$$

the energy flux vector.

## Problem 6. Hermitian conjugate

The hermitian conjugate $\Omega^\dagger$ of an operator $\Omega$ is defined by

$$\int d\tau (\Omega\psi)^* \varphi = \int d\tau\, \psi^* \Omega^\dagger \varphi \tag{6.1a}$$

or, in Hilbert space notation,

$$\langle \Omega\psi | \varphi \rangle = \langle \psi | \Omega^\dagger \varphi \rangle \tag{6.1b}$$

with $\psi$ and $\varphi$ any two functions normalized according to

$$\langle \psi | \psi \rangle = 1; \qquad \langle \varphi | \varphi \rangle = 1\,. \tag{6.2}$$

This definition shall be translated into a matrix relation. What follows for the eigenvalues of a hermitian operator defined by $\Omega = \Omega^\dagger$?

**Solution.** The matrix of an operator is defined with respect to a complete set of orthonormal functions, $\{u_\nu\}$:

$$\langle u_\nu | u_\mu \rangle = \delta_{\mu\nu}\,. \tag{6.3}$$

The arbitrary, but normalized functions $\psi$ and $\varphi$ then may be expanded,

$$\psi = \sum_\nu a_\nu u_\nu\,, \qquad \varphi = \sum_\mu b_\mu u_\mu\,. \tag{6.4}$$

Putting (6.4) into (6.1), we get

$$\sum_\mu \sum_\nu a_\nu^* b_\mu \langle \Omega u_\nu | u_\mu \rangle = \sum_\mu \sum_\nu a_\nu^* b_\mu \langle u_\nu | \Omega^\dagger u_\mu \rangle$$

and, since this is supposed to hold for any pair $\psi$, $\varphi$, it must hold for each term separately,

$$\langle \Omega u_\nu | u_\mu \rangle = \langle u_\nu | \Omega^\dagger u_\mu \rangle\,. \tag{6.5}$$

We now use the set $\{u_\nu\}$ for matrix definition, writing the right-hand side of (6.5)

$$\langle u_\nu | \Omega^\dagger | u_\mu \rangle = (\Omega^\dagger)_{\mu\nu}\,.$$

The left-hand side may be reshaped as follows

$$\langle \Omega u_\nu | u_\mu \rangle = \int d\tau (\Omega u_\nu)^* u_\mu = \left\{ \int d\tau\, u_\mu^* (\Omega u_\nu) \right\}^* = \langle u_\mu | \Omega u_\nu \rangle^* = \Omega_{\nu\mu}^*\,.$$

Hence, it follows from (6.5) for the matrix elements of $\Omega$ and $\Omega^\dagger$ that

$$(\Omega^\dagger)_{\mu\nu} = \Omega_{\nu\mu}^*\,, \tag{6.6}$$

i.e. the elements of the hermitian conjugate (or adjoint) matrix are obtained by transposing ($\mu \rightleftharpoons \nu$), and taking the complex conjugate of, the elements of $\Omega$.

It may be noted that from (6.6) we get immediately $\Omega^{\dagger\dagger} = \Omega$.

## Problem 16. Force-free case: Basic solutions

The one-dimensional wave equation shall be solved in the case $V=0$ and the physical significance of the solutions shall be discussed.

**Solution**[1]. The wave equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t} \tag{16.1}$$

permits factorization,

$$\psi(x,t) = u(x)g(t), \tag{16.2}$$

because by putting (16.2) in (16.1) one arrives at

$$-\frac{\hbar^2}{2m}\frac{u''}{u} = -\frac{\hbar}{i}\frac{\dot{g}}{g} = \hbar\omega, \tag{16.3}$$

where $\hbar\omega$ stands as abbreviation for the separation parameter. Splitting (16.3) into two separate equations we obtain

$$\dot{g} = -i\omega g, \quad \text{i.e.} \quad g(t) = e^{-i\omega t} \tag{16.4}$$

$\hat{T}u = \hbar\omega u$. $\hbar\omega = E$

and

$$u'' + \frac{2m\omega}{\hbar}u = 0. \tag{16.5}$$

$-\frac{\hbar^2}{2m}u'' = \hbar\omega u$

With real $\omega$, the wave function is periodic in, and $|\psi|^2$ independent of, time *(stationary state)*; with $\omega$ positive, the constant

$$\frac{2m\omega}{\hbar} = k^2 \tag{16.6}$$

becomes positive too, and the solutions of (16.5) are as well periodic in space.

It is an essential feature of quantum mechanics that time dependence is of the complex form (16.4); the real functions $\sin\omega t$ and $\cos\omega t$ are not solutions of the differential equation (16.4). This behaviour, so different from classical physics, is a consequence of the Schrödinger equation being of the *first* order in time.

The physical meaning of the parameter $\omega$ may be further interpreted by considering the operator on the left-hand side of (16.1) to be the hamiltonian, consisting only of the kinetic energy operator in our case. It follows that $E=\hbar\omega$ is the kinetic energy of a particle and must hence be positive real. Our solution therefore is an eigenstate of the hamiltonian.

recall $p = \frac{\hbar}{i}\frac{\partial}{\partial x}$, $\frac{p^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

[1] In the following we shall write $\psi$ again for the one-dimensional part of the wave function satisfying Eq. (A.4), and $u$ for its space part.

Since $k^2$ is a positive constant, the complete solution of (16.5) or

$$u'' + k^2 u = 0 \tag{16.7}$$

is

$$u(x) = A\,e^{ikx} + B\,e^{-ikx} \tag{16.8a}$$

so that the one-dimensional wave function $u(x)g(t)$

$$\psi(x,t) = A\,e^{i(kx-\omega t)} + B\,e^{-i(kx+\omega t)} \tag{16.8b}$$

$$= A\,e^{ik(x - v_{ph} t)} + B\,e^{-ik(x + v_{ph} t)}$$

consists of two waves running in opposite directions, both with phase velocity $v_{ph} = \omega/k$.

The physical significance of the space part (16.8a) of the wave function becomes clear when we derive density

$$\rho = \psi^* \psi \tag{16.9}$$

and flux

$$s = \frac{\hbar}{2im}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right) \tag{16.10}$$

from (16.8b). We find problem 1.8

$$\rho = |A|^2 + |B|^2 + \underbrace{(A B^* e^{2ikx} + A^* B e^{-2ikx})}_{\text{interference of waves}};$$

$$s = \frac{\hbar k}{m}(|A|^2 - |B|^2).$$

The two waves, of amplitudes $A$ and $B$, apparently correspond to two opposite currents, whose intensity is given by their respective normalization constants and is proportional to $k$. The density shows interference of the two (coherent) waves causing a space periodicity.

As long as no special reason (like boundary conditions) is given to achieve coherence, it will be reasonable to take either of the two waves, putting $B = 0$ and obtaining $s > 0$, or $A = 0$ giving $s < 0$. The result then corresponds to the linear motion of particles in one or the other direction. Admitting both signs of $k$, we may therefore summarize the final result as follows:

need this (C) form for wavepackets

$$\left.\begin{aligned} &\psi(x,t) = C\,e^{i(kx-\omega t)}; \\ &E = \hbar\omega; \quad k^2 = \frac{2m\omega}{\hbar}; \\ &\rho = |C|^2; \quad s = \frac{\hbar k}{m}|C|^2. \end{aligned}\right\} \tag{16.11}$$

Elimination of $\omega$ yields

$$E = \frac{\hbar^2 k^2}{2m} \tag{16.12}$$

so that

$$p = \hbar k \tag{16.13}$$

is the momentum, and

$$v = \frac{\hbar k}{m} \tag{16.14}$$

the classical velocity of the particle. The latter is by no means identical with the phase velocity of the wave, $p^2/2m$

$$v_{\text{ph}} = \frac{\omega}{k} = \frac{E}{p} = \frac{1}{2} v;$$

it is, however, identical with the group velocity

$$v_{\text{gr}} = \frac{\hbar\, d\omega}{\hbar\, dk} = \frac{dE}{dp} = v.$$

This makes sense for wavepackets - so consider now wavepackets

**NB.** The fundamental differential equation (16.1) may be interpreted as a *diffusion equation* with an imaginary constant of diffusion, $D$:

$$D \frac{\partial^2 \psi}{\partial x^2} = \frac{\partial \psi}{\partial t}; \qquad D = i \frac{\hbar}{2m}.$$

Whereas factorization plays rather an important role in quantum theory but not in diffusion problems, the typical source-type solutions of (real) diffusion theory,

$$\psi(x,t) = \frac{1}{\sqrt{t}} \int_{-\infty}^{+\infty} d\xi\, f(\xi)\, e^{i \frac{m}{2\hbar} \frac{(x-\xi)^2}{t}},$$

are of no importance in quantum theory.

*Time reversal* in (16.1) changes $\psi$ in $\psi^*$.

## Problem 17. Force-free case: Wave packet

A wave packet shall be constructed and its development as a function of time be investigated.

**Solution.** We start from the special solution of the wave equation found in (16.11):

$$\psi(k; x, t) = C(k)\, e^{i(kx - \omega t)} \tag{17.1}$$

with

$$\omega = \frac{\hbar}{2m} k^2 \tag{17.2}$$

S eq is linear (in $\psi$) eq. So linear superposit. is also a solution



and $C(k)$ an arbitrary amplitude constant. Here, $k$ still is a free parameter so that the complete solution of the wave equation is obtained as any convergent integral of (17.1) over $k$:

$$\psi(x,t)=\int_{-\infty}^{+\infty} dk\,\psi(k;x,t). \tag{17.3}$$

Eq. (17.3) describes the most general form of an one-dimensional wave packet. The amplitude function $C(k)$ must, in order to make the integral converge, tend to zero at least as $1/k$ with $|k|\to\infty$. Every suitable choice of $C(k)$ yields a special solution.

Let us now construct the wave packet so that, for an initial time $t=0$, the probability of finding the particle it describes differs appreciably from zero only inside a small region around $x=0$, and that the particle moves with momentum $p_0=\hbar k_0$. This can be accomplished if we choose $\Rightarrow$ real $\psi$ no momentum

gaussian w width 'a'

$$\psi(x,0)=A\exp\left[-\frac{x^2}{2a^2}+ik_0x\right], \tag{17.4}$$

$A \sim a$

because then the density

$$\rho(x,0)=|\psi(x,0)|^2=|A|^2\exp\left[-\frac{x^2}{a^2}\right]$$

localizes the particle within $|x|\lesssim a$, and the flux (16.10) becomes

$$s(x,0)=\frac{\hbar}{2mi}2ik_0|A|^2\exp\left[-\frac{x^2}{a^2}\right]=\rho\frac{\hbar}{m}k_0$$

so that the particle velocity is $v_0=\frac{\hbar}{m}k_0$ and $p_0=mv_0=\hbar k_0$ the momentum of the packet. Since the wave function represents one particle, the normalization condition

$$\int_{-\infty}^{+\infty} dx\,\rho=1$$

holds, i. e.

$$|A|^2=\frac{1}{a\sqrt{\pi}}. \tag{17.5}$$

The expression (17.4) may be decomposed into plane waves using (17.3) and (17.1):

$$\psi(x,0)=\int_{-\infty}^{+\infty} dk\,C(k)e^{ikx}. \tag{17.6}$$

$W=\frac{\hbar^2}{2m}\nabla\psi^*\nabla\psi=\frac{\hbar^2}{2m}\left(\frac{x^2}{a^4}+k_0^2\right)\rho$ $\quad E=\int dx\,W(x)=\frac{\hbar^2}{2ma^2}\int\frac{dx}{a}e^{-x^2/a^2}\left(\frac{x^2}{a^2}\right)$ $+\hbar^2k_0^2/2m$, 1st term is Loc. en. $\sim 1/a^2$ $\quad F_L\sim-\partial E/\partial a\sim\frac{1}{a^3}$ versus conf.

$$j = \frac{\hbar}{2im}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right)$$

$$\psi(x,0) = A\, e^{-\frac{x^2}{2a^2}}\, e^{ik_0 x} \qquad \psi^* = \text{c.c.}$$

$$\psi' = \left(-\frac{x}{a^2} + ik_0\right)\psi \qquad \psi'^* = \left(-\frac{x}{a^2} - ik_0\right)\psi$$

$$j = \frac{\hbar}{2im}\left[\psi^*\psi\left(-\frac{x}{a^2} + ik_0\right) - \psi\psi^*\left(-\frac{x}{a^2} - ik_0\right)\right]$$

$$j = \frac{\hbar}{2im}\, 2ik_0\, \rho = \frac{\hbar k_0}{m}\rho$$

remember $mj$ = momentum density

so $\hbar k_0 \equiv p_0$ $\quad v_0 = \hbar k_0/m$ this defines "group velocity".

This is a Fourier integral whose inversion is

$$C(k)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} dx\,\psi(x,0)\,e^{-ikx}$$

$$=\frac{A}{2\pi}\int_{-\infty}^{+\infty} dx\exp\left[-\frac{x^2}{2a^2}+i(k_0-k)x\right].$$

This integral may be evaluated using the well-known formula

$$\int_{-\infty}^{+\infty} dz\,e^{-z^2}=\sqrt{\pi}. \tag{17.7}$$

The result,

$$C(k)=\frac{Aa}{\sqrt{2\pi}}\exp\left[-\tfrac{1}{2}a^2(k-k_0)^2\right], \tag{17.8}$$

can easily be understood in terms of Heisenberg's uncertainty rule: In the initial state, the coordinate uncertainty of the particle is, according to Eq. (17.4), of the order of $\Delta x=a$; as (17.8) shows, to this wave function there contributes a spectrum of wave numbers $k$ or of momenta $p=\hbar k$ around $k=k_0$ of a width $\Delta k=1/a$ or $\Delta p=\hbar/a$. Therefore, independently of the choice of $a$, there holds the relation

$$\Delta x\cdot\Delta p=\hbar, \tag{17.9}$$

which is in fact Heisenberg's principle of uncertainty.

Having determined $C(k)$ from the initial state at the time $t=0$, we are now prepared to evaluate the full integral (17.3) at *any* time, viz. the integral

$$\psi(x,t)=\frac{Aa}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} dk\exp\left[-\frac{1}{2}a^2(k-k_0)^2+ikx-i\frac{\hbar t}{2m}k^2\right].$$

The exponent is a quadratic form in $k$ so that again reduction to the complete error integral (17.7) can be performed. The result is

don't write this down.

$$\psi(x,t)=\frac{A}{\left(1+i\dfrac{\hbar t}{ma^2}\right)^{\frac{1}{2}}}\exp\left[-\frac{x^2-2ia^2k_0x+i\dfrac{\hbar t}{2m}k_0^2a^2}{2a^2\left(1+i\dfrac{\hbar t}{ma^2}\right)}\right]. \tag{17.10}$$

$e^-$ spread FREE (not bound)

A good understanding of this rather cumbersome expression can be obtained by again discussing density $\rho$ and flux $s$, but now at any time. The former becomes

write this down

$$\rho(x,t)=|\psi(x,t)|^2=\frac{|A|^2}{\left[1+\left(\frac{\hbar t}{ma^2}\right)^2\right]^{\frac{1}{2}}}\exp\left[-\frac{\left(x-\frac{\hbar k_0}{m}t\right)^2}{a^2\left[1+\left(\frac{\hbar t}{ma^2}\right)^2\right]}\right]. \tag{17.11}$$

As a function of $x$, the density $\rho(x,t)$ still is a bell-shaped curve, whose maximum, however, has now shifted from $x=0$ to $x=\frac{\hbar k_0}{m}t$. The maximum of the 'wave group' represented by (17.10) therefore propagates with a velocity $v_0=\frac{\hbar k_0}{m}$ ('group velocity' = particle velocity). The denominator of the exponent in (17.11) shows that, at the same time, the wave packet has broadened from its initial width $a$ at $t=0$ to

or expand $\psi(x,t)$ around $k_0$ – see Merz to get $\left.\frac{d\omega}{dk}\right|_{k=k_0}=\frac{\hbar k_0}{m}$

$$a'=a\left[1+\left(\frac{\hbar t}{ma^2}\right)^2\right]^{\frac{1}{2}}\simeq\frac{\hbar}{ma}t$$

at $t=t$. This effect can easily be explained from the spectral function (17.8): The wave number spectrum having the width $\Delta k=1/a$, the velocities of the partial waves cover a region of width $\Delta v=\frac{\hbar}{m}\Delta k=\frac{\hbar}{ma}$ so that the packet broadens by $\Delta x=t\,\Delta v=\frac{\hbar}{ma}t$ as derived above.

The flux is obtained from (17.10) with the help of the relation

$$\frac{\partial\psi}{\partial x}=ik_0\frac{1+i\frac{x}{a^2k_0}}{1+i\frac{\hbar t}{ma^2}}\psi;$$

straightforward calculation yields by comparison with (17.11):

$$s(x,t)=\rho(x,t)v_0\frac{1+\frac{\hbar t x}{ma^4k_0}}{1+\left(\frac{\hbar t}{ma^2}\right)^2}. \tag{17.12}$$

It follows that we by no means have $s=\rho v_0$ for all times, as we had for $t=0$. This again is a consequence of the finite width of the velocity spectrum: At the packet maximum, $x_0=v_0t$, Eq. (17.12) leads to the relation $s=\rho v_0$; For $x \lessgtr x_0$, $s \lessgtr \rho v_0$ since for $x<x_0$ there arrived at time $t$ those parts of packet whose vel. is smaller than $v_0$

$$a_t^2=a^2+\frac{\hbar^2t^2}{m^2a^2}=(\Delta x)_0^2+(\Delta v)_0^2t^2$$ spread time $\tau$: $(\Delta v_0)^2\tau^2\sim a^2$

$$\tau\sim\frac{a}{\Delta v_0}=\frac{a^2m}{\hbar}$$ | $e^-$ $a\sim 1$ Å $\tau\sim 10^{-16}$ sec | $m=1$ gm $a\sim 1000$ Å $\tau\sim 3\times 10^9$ years

It should be noted that from the normalization

$$\int d^3x\,|\psi(\mathbf{r})|^2 = 1 \tag{14.7}$$

there follows

$$\int d^3k\,|f(\mathbf{k})|^2 = 1\,. \tag{14.8}$$

This can be shown by setting (14.1) into (14.7) for $\psi$:

$$\int d^3x\,|\psi(\mathbf{r})|^2 = (2\pi)^{-3}\int d^3x \int d^3k \int d^3k'\, e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} f(\mathbf{k}) f^*(\mathbf{k}')\,.$$

If here the integration over coordinate space is first performed[2] we almost immediately arrive at the expression (14.8).

## Problem 15. Momentum space: Periodic and aperiodic wave functions

To deduce the probability interpretation of momentum space wave functions in the continuous spectrum by starting from periodic wave functions $\psi(\mathbf{r})$ in ordinary space and investigating the limiting process for infinitely large periodicity cube.

**Solution.** Let $L$ be the period in each of the three space directions $x, y, z$. Then the Fourier series

$$\psi(\mathbf{r},t) = L^{-\frac{3}{2}} \sum_{\mathbf{k}} c_{\mathbf{k}}(t)\, e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}; \qquad \omega = \frac{\hbar}{2m} k^2 \tag{15.1}$$

includes terms only with components

$$k_i = \frac{2\pi}{L} n_i; \qquad n_i = 0, \pm 1, \pm 2, \ldots \tag{15.2}$$

of each vector $\mathbf{k}$. This means that in $\mathbf{k}$ space, for large $L$, a volume element $d^3k$ includes

$$d^3k \left(\frac{L}{2\pi}\right)^3 \tag{15.3}$$

states of different $\mathbf{k}$'s.

The normalization of series (15.1) can still be chosen by suitable choice of the coefficients $c_{\mathbf{k}}$. The square integral over the periodicity cube is

$$\int_{(L^3)} d^3x\,|\psi|^2 = L^{-3} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} c_{\mathbf{k}}^* c_{\mathbf{k}'}\, e^{i(\omega-\omega')t} \int d^3x\, e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}$$

[2] Cf. however, the remark at the end of the following problem.

introduca Kroneckera delta

where the last integral vanishes if $\boldsymbol{k}' \neq \boldsymbol{k}$ and becomes $= L^3$ if $\boldsymbol{k}' = \boldsymbol{k}$:

$$\int_{(L^3)} d^3x\,|\psi|^2 = \sum_{\boldsymbol{k}} |c_{\boldsymbol{k}}|^2 . \tag{15.4}$$

Let $P_L$ now be the probability of finding the particle in the periodicity cube $L^3$, then $|c_{\boldsymbol{k}}|^2\,P_L$ will be the probability of finding there the particle with momentum $\hbar\boldsymbol{k}$, and $|c_{\boldsymbol{k}}|^2$ the probability that, if the particle is found within $L^3$, its momentum will turn out to be $\hbar\boldsymbol{k}$.

We now go on to infinitely large $L$. Then we may replace the Fourier sum (15.1) by a Fourier integral over $\boldsymbol{k}$ space which according to (15.2) and (15.3) may be done by using the rule

$$\sum_{\boldsymbol{k}} \rightarrow \left(\frac{L}{2\pi}\right)^3 d^3k . \tag{15.5}$$

Eq. (15.1) then yields

$$\psi(\boldsymbol{r},t) = \frac{L^{\frac{3}{2}}}{(2\pi)^3}\int d^3k\, c(\boldsymbol{k},t)\,\mathrm{e}^{i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)} . \tag{15.6}$$

This Fourier integral describes a wave function of finite values independent of $L$ if, and only if, the quantity

$$\left(\frac{L}{2\pi}\right)^{\frac{3}{2}} c(\boldsymbol{k}) = f(\boldsymbol{k}) \qquad \text{N.B} \quad \frac{1}{(2\pi)^{1/2}} \leftarrow \tag{15.7}$$

has a finite limit for $L \rightarrow \infty$. The wave function

$$\psi(\boldsymbol{r},t) = \frac{1}{(2\pi)^{\frac{3}{2}}}\int d^3k\, f(\boldsymbol{k},t)\,\mathrm{e}^{i(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)} \tag{15.8}$$

then may be normalized according to

$$\int d^3x\,|\psi|^2 = \frac{1}{(2\pi)^3}\int d^3k \int d^3k'\, f^*(\boldsymbol{k}) f(\boldsymbol{k}')\,\mathrm{e}^{i(\omega-\omega')t}\int_{-\infty}^{+\infty} d^3x\,\mathrm{e}^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}} \tag{15.9}$$

where the last integral runs over infinite space and can be evaluated:

$$\int d^3x\,\mathrm{e}^{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}} = (2\pi)^3\,\delta(\boldsymbol{k}'-\boldsymbol{k}) , \tag{15.10}$$

so that we find for (15.9):

$$\int d^3x\,|\psi|^2 = \int d^3k\,|f(\boldsymbol{k},t)|^2 \tag{15.11}$$

which, by the way, is simply the same as translating the sum (15.4) with (15.7), according to the rule (15.5). Hence, the probability that a particle found anywhere has its momentum $\boldsymbol{k}$ within the element $d^3k$ becomes

$$dP_{\boldsymbol{k}} = d^3k\,|f(\boldsymbol{k},t)|^2 . \tag{15.12}$$

$\underline{k}\cdot\underline{r} = k_x x + k_y y + k_z z \qquad e^{i\underline{k}\cdot\underline{r}} = e^{ik_x x}\, e^{ik_y y}\, e^{ik_z z}$