

1.4: Continuity Equation

The wave mechanics postulates survive one more sanity check: they satisfy the natural requirement that the particle does not appear or vanish in the course of the quantum evolution.³³ Indeed, let us use Eq. (22b) to calculate the rate of change of the probability W to find a particle within a certain volume V :

$$\frac{dW}{dt} = \frac{d}{dt} \int_V \Psi \Psi^* d^3r \quad (1.4.1)$$

Assuming for simplicity that the boundaries of the volume V do not move, it is sufficient to carry out the partial differentiation of the product $\Psi \Psi^*$ inside the integral. Using the Schrödinger equation (25), together with its complex conjugate,

$$-i\hbar \frac{\partial \Psi^*}{\partial t} = (\hat{H}\Psi)^* \quad (1.4.2)$$

we readily get

$$\frac{dW}{dt} = \int_V \frac{\partial}{\partial t} (\Psi \Psi^*) d^3r \equiv \int_V \left(\Psi^* \frac{\partial \Psi}{\partial t} + \Psi \frac{\partial \Psi^*}{\partial t} \right) d^3r = \frac{1}{i\hbar} \int_V \left[\Psi^* (\hat{H}\Psi) - \Psi (\hat{H}\Psi)^* \right] d^3r \quad (1.4.3)$$

Let the particle move in a field of external forces (not necessarily constant in time), so that its classical Hamiltonian function H is the sum of the particle's kinetic energy $T = p^2/2m$ and its potential energy $U(\mathbf{r}, t)$.³⁴ According to the correspondence principle, and Eq. (27), the Hamiltonian operator may be represented as the sum³⁵,

$$\hat{H} = \hat{T} + \hat{U} = \frac{\hat{p}^2}{2m} + U(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \nabla^2 + U(\mathbf{r}, t). \quad (1.4.4)$$

At this stage, we should notice that this operator, when acting on a real function, returns a real function.³⁶ Hence, the result of its action on an arbitrary complex function $\Psi = a + ib$ (where a and b are real) is

$$\hat{H}\Psi = \hat{H}(a + ib) = \hat{H}a + i\hat{H}b, \quad (1.4.5)$$

where $\hat{H}a$ and $\hat{H}b$ are also real, while

$$(\hat{H}\Psi)^* = (\hat{H}a + i\hat{H}b)^* = \hat{H}a - i\hat{H}b = \hat{H}(a - ib) = \hat{H}\Psi^*. \quad (1.4.6)$$

This means that Eq. (40) may be rewritten as

$$\frac{dW}{dt} = \frac{1}{i\hbar} \int_V \left[\Psi^* \hat{H}\Psi - \Psi \hat{H}\Psi^* \right] d^3r = -\frac{\hbar^2}{2m} \frac{1}{i\hbar} \int_V \left[\Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^* \right] d^3r. \quad (1.4.7)$$

Now let us use general rules of vector calculus³⁷ to write the following identity:

$$\nabla \cdot (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*) = \Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^*, \quad (1.4.8)$$

A comparison of Eqs. (44) and (45) shows that we may write

$$\frac{dW}{dt} = - \int_V (\nabla \cdot \mathbf{j}) d^3r, \quad (1.4.9)$$

where the vector \mathbf{j} is defined as

$$\mathbf{j} \equiv \frac{i\hbar}{2m} (\Psi \nabla \Psi^* - \text{c.c.}) \equiv \frac{\hbar}{m} \text{Im}(\Psi^* \nabla \Psi), \quad (1.4.10)$$

where c.c. means the complex conjugate of the previous expression - in this case, $(\Psi \nabla \Psi^*)^*$, i.e. $\Psi^* \nabla \Psi$. Now using the well-known divergence theorem,³⁸ Eq. (46) may be rewritten as the continuity equation

$$\frac{dW}{dt} + I = 0, \quad \text{with } I \equiv \int_S j_n d^2r, \quad (1.4.11)$$

where j_n is the component of the vector \mathbf{j} , along the outwardly directed normal to the closed surface S that limits the volume V , i.e. the scalar product $\mathbf{j} \cdot \mathbf{n}$, where \mathbf{n} is the unit vector along this normal.

Equalities (47) and (48) show that if the wavefunction on the surface vanishes, the total probability W of finding the particle within the volume does not change, providing the intended sanity check. In the general case, Eq. (48) says that dW/dt equals the flux I of the vector \mathbf{j} through the surface, with the minus sign. It is clear that this vector may be interpreted as the probability current density and I , as the total probability current through the surface S . This interpretation may be further supported by rewriting Eq. (47) for the wavefunction represented in the polar form $\Psi = ae^{i\varphi}$, with real a and φ :

$$\mathbf{j} = a^2 \frac{\hbar}{m} \nabla \varphi \quad (1.4.12)$$

Note that for a real wavefunction, or even for a wavefunction with an arbitrary but space-constant phase φ , the probability current density vanishes. On the contrary, for the traveling wave (29), with a constant probability density $w = a^2$, Eq. (49) yields a non-zero (and physically very transparent) result:

$$\mathbf{j} = w \frac{\hbar}{m} \mathbf{k} = w \frac{\mathbf{p}}{m} = w \mathbf{v}, \quad (1.4.13)$$

where $\mathbf{v} = \mathbf{p}/m$ is particle's velocity. If multiplied by the particle's mass m , the probability density w turns into the (average) mass density ρ , and the probability current density, into the mass flux density $\rho \mathbf{v}$. Similarly, if multiplied by the total electric charge q of the particle, with w turning into the charge density σ , \mathbf{j} becomes the electric current density. As the reader (hopefully :-)) knows, both these currents satisfy classical continuity equations similar to Eq. (48).³⁹

Finally, let us recast the continuity equation, rewriting Eq. (46) as

$$\int_V \left(\frac{\partial w}{\partial t} + \nabla \cdot \mathbf{j} \right) d^3r = 0. \quad (1.4.14)$$

Now we may argue that this equality may be true for any choice of the volume V only if the expression under the integral vanishes everywhere, i.e. if

$$\frac{\partial w}{\partial t} + \nabla \cdot \mathbf{j} = 0 \quad (1.4.15)$$

This differential form of the continuity equation may be more convenient than its integral form (48)

³² The reader should not be surprised by the use of the notion of "knowledge" (or "information") in this context. Indeed, due to the statistical character of experiment outcomes, quantum mechanics (or at least its relation to experiment) is intimately related to information theory. In contrast to much of classical physics, which may be discussed without any reference to information, in quantum mechanics, as in classical statistical physics, such abstraction is possible only in some very special (and not the most interesting) cases.

³³ Note that this requirement may be violated in the relativistic quantum theory - see Chapter 9.

³⁴ As a reminder, such description is valid not only for conservative forces (in that case U has to be timeindependent), but also for any force $\mathbf{F}(\mathbf{r}, t)$ that may be expressed via the gradient of $U(\mathbf{r}, t)$ - see, e.g., CM Chapters 2 and 10. (A good example when such a description is impossible is given by the magnetic component of the Lorentz force - see, e.g., EM Sec. 9.7, and also Sec. 3.1 below.)

³⁵ Historically, this was the main step made (in 1926) by E. Schrödinger on the background of L. de Broglie's idea. The probabilistic interpretation of the wavefunction was put forward, almost simultaneously, by M. Born.

³⁶ In Chapter 4, we will discuss a more general family of Hermitian operators, which have this property.

³⁷ See, e.g., MA Eq. (11.4a), combined with the del operator's definition $\nabla^2 \equiv \nabla \cdot \nabla$.

³⁸ See, e.g., MA Eq. (12.2).

³⁹ See, e.g., respectively, CM 8.3 and EM Sec. 4.1.