CHAPTER VI

The Weyl formulation of the microscopic laws

1 *Introduction*

The various laws of electrodynamics have been derived in the preceding on the basis of a classical model of matter. The question arises in how far these results retain their validity if a more realistic model based on quantum mechanics is adopted. This programme will be carried out in this chapter and the following, at first in the non-relativistic approximation.

Quantum mechanics is usually formulated in terms of operators and state vectors in Hilbert space. In the course of the treatment it will be convenient to introduce instead an equivalent formalism which employs functions in phase space. Then the physical quantities are represented by Weyl transforms, while the Wigner function takes over the role of the density operator.

2 *The field equations and the equation of motion of a set of charged point particles*

The starting point of the theory consists in propounding the Hamilton operator for a set of charged particles. For a system consisting of N particles with masses m_i, charges e_i, coordinate operators $\boldsymbol{R}_{i,\text{op}}$ and momentum operators $\boldsymbol{P}_{i,\text{op}}$, in an external electromagnetic field with potentials $(\varphi_e, \boldsymbol{A}_e)$ one writes the Hamilton operator up to terms of order c^{-1} as:

$$H_{\text{op}} = \sum_i \frac{\boldsymbol{P}_{i,\text{op}}^2}{2m_i} + \sum_{i,j(i\neq j)} \frac{e_i e_j}{8\pi|\boldsymbol{R}_{i,\text{op}} - \boldsymbol{R}_{j,\text{op}}|} + \sum_i e_i \left[\varphi_e(\boldsymbol{R}_{i,\text{op}}, t) - \tfrac{1}{2}c^{-1} \left\{ \frac{\boldsymbol{P}_{i,\text{op}}}{m_i} \cdot, \boldsymbol{A}_e(\boldsymbol{R}_{i,\text{op}}, t) \right\} \right] \quad (1)$$

(cf. the classical expression (I.16)). In the last term the anticommutator of the momentum operator and the vector potential appears. As usual the dot indicates the scalar product of two vectors. This (hermitian) Hamilton operator governs the time development of the state vector $|\psi\rangle$ for the system via Schrödinger's equation.

The field equations, which in quantum mechanics replace the classical Lorentz equations (I.1) are the following differential equations for the hermitian operators $\boldsymbol{e}_{op}(\boldsymbol{R}, t)$ and $\boldsymbol{b}_{op}(\boldsymbol{R}, t)$ which represent the electric and magnetic fields:

$$\begin{aligned} \nabla\cdot\boldsymbol{e}_{op} &= \sum_i e_i\,\delta(\boldsymbol{R}_{i,op}-\boldsymbol{R}), \\ -\partial_0\,\boldsymbol{e}_{op}+\nabla\wedge\boldsymbol{b}_{op} &= \tfrac{1}{2}c^{-1}\sum_i e_i\{\dot{\boldsymbol{R}}_{i,op},\,\delta(\boldsymbol{R}_{i,op}-\boldsymbol{R})\}, \\ \nabla\cdot\boldsymbol{b}_{op} &= 0, \\ \partial_0\,\boldsymbol{b}_{op}+\nabla\wedge\boldsymbol{e}_{op} &= 0, \end{aligned} \tag{2}$$

where $c\partial_0$ and the fluxion dot should be interpreted as $(i/\hbar)$ times the commutator with the Hamiltonian plus the explicit time derivative:

$$\dot{A}_{op} = c\partial_0\,A_{op} = \frac{i}{\hbar}\,[H_{op},\,A_{op}]+\frac{\partial^e A_{op}}{\partial t}. \tag{3}$$

(The time derivative of the expectation value of the operator A_{op} is equal to the expectation value of $\dot{A}_{op}$, as follows from Schrödinger's equation.) In particular the fluxion $\dot{\boldsymbol{R}}_{i,op}$ is, up to order c^0, equal to $\boldsymbol{P}_{i,op}/m_i$, as follows from (1). The sources of the field equations (2) are hermitian operators, as is guaranteed by the fact that the anticommutator has been written in the second equation. From the field equations (2) one may find in principle the expressions for the electric and magnetic fields in terms of the coordinate and momentum operators of the particles.

The equation of motion for the charged particles follows by taking the second time derivative of the coordinate operator of particle i in the sense defined by (3). With the Hamilton operator (1) one finds

$$\begin{aligned} m_i\,\dot{\boldsymbol{R}}_{i,op} &= \boldsymbol{P}_{i,op}-c^{-1}e_i\,\boldsymbol{A}_e(\boldsymbol{R}_{i,op},\,t), \\ m_i\,\ddot{\boldsymbol{R}}_{i,op} &= -\nabla_{i,op}\sum_{j(\neq i)}\frac{e_i\,e_j}{4\pi|\boldsymbol{R}_{i,op}-\boldsymbol{R}_{j,op}|} \\ &\quad +e_i\left[\boldsymbol{E}_e(\boldsymbol{R}_{i,op},\,t)+\tfrac{1}{2}c^{-1}\left\{\frac{\boldsymbol{P}_{i,op}}{m_i}\wedge,\,\boldsymbol{B}_e(\boldsymbol{R}_{i,op},\,t)\right\}\right], \end{aligned} \tag{4}$$

where we used the connexions of the fields and the potentials:

$$\boldsymbol{E}_e = -\nabla\varphi_e-\partial_0\,\boldsymbol{A}_e, \qquad \boldsymbol{B}_e = \nabla\wedge\boldsymbol{A}_e. \tag{5}$$

Furthermore the symbol $\nabla_{i,op}$ denotes partial differentiation with respect to $\boldsymbol{R}_{i,op}$ and the last anticommutator with the vector product stands for $(1/m_i)(\boldsymbol{P}_{i,op}\wedge\boldsymbol{B}_e-\boldsymbol{B}_e\wedge\boldsymbol{P}_{i,op})$.

The field equations (2) and the equations of motion (4) form the basis for the derivation of the macroscopic field equations and energy–momentum laws in this chapter and the following. The equations (2) and (4) will not be used in the form given so far in view of the fact that the handling of operators, in particular of anticommutators, leads to rather unwieldy expressions. Instead we shall use Weyl transforms.

3 *The Weyl transformation and the Wigner function*

a. *The Weyl transformation*

Quantum mechanics in its usual form is concerned with the properties of vectors and operators in Hilbert space: each state of a system corresponds to a vector, each observable quantity to an operator.

However different formulations[1] are possible in which functions in a phase space are associated to both the states and the observable quantities. An example of such a formulation consists in employing for these functions the Wigner function and the Weyl transform respectively. This alternative formulation will be demonstrated for a one-particle system. The generalization to an N-particle system is trivial.

The eigenvectors $|\boldsymbol{p}\rangle$ and $|\boldsymbol{q}\rangle$ of the momentum and coordinate operators[2] $\boldsymbol{P}$ and $\boldsymbol{Q}$ satisfy the eigenvalue equations

$$\boldsymbol{P}|\boldsymbol{p}\rangle = \boldsymbol{p}|\boldsymbol{p}\rangle, \qquad \boldsymbol{Q}|\boldsymbol{q}\rangle = \boldsymbol{q}|\boldsymbol{q}\rangle, \tag{6}$$

where $\boldsymbol{p}$ and $\boldsymbol{q}$ are the eigenvalues. The complete set of eigenvectors is supposed to fulfil the closure relations

$$\begin{aligned} \int \mathrm{d}\boldsymbol{p}\,|\boldsymbol{p}\rangle\langle\boldsymbol{p}| &= I, \\ \int \mathrm{d}\boldsymbol{q}\,|\boldsymbol{q}\rangle\langle\boldsymbol{q}| &= I, \end{aligned} \tag{7}$$

[1] H. Weyl, Z. Physik **46**(1927)1; Gruppentheorie und Quantenmechanik (Hirzel, Leipzig 1931) p. 244; E. P. Wigner, Phys. Rev. **40**(1932)749; cf. also H. J. Groenewold, Physica **12**(1946)405; J. E. Moyal, Proc. Cambridge Phil. Soc. **45**(1949)99; K. Schram and B. R. A. Nijboer, Physica **25**(1959)733; B. Leaf, J. Math. Phys. **9**(1968)65, 769.

[2] In this section we use systematically capitals for operators, and lower case symbols for ordinary numbers.

(with I the unit operator in Hilbert space) and the orthogonality relations

$$\langle \boldsymbol{p}|\boldsymbol{p}'\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}'), \qquad \langle \boldsymbol{q}|\boldsymbol{q}'\rangle = \delta(\boldsymbol{q}-\boldsymbol{q}'). \tag{8}$$

The commutation rules of the operators $\boldsymbol{P}$ and $\boldsymbol{Q}$ read

$$[\boldsymbol{P}, \boldsymbol{P}] = 0, \qquad [\boldsymbol{Q}, \boldsymbol{Q}] = 0, \qquad [\boldsymbol{P}, \boldsymbol{Q}] = \frac{\hbar}{i}\,\mathsf{U}I, \tag{9}$$

where U is the unit Cartesian tensor with components $(i, j = 1, 2, 3)$. In the coordinate representation the momentum eigenvector has the wave function

$$\langle \boldsymbol{q}|\boldsymbol{p}\rangle = \frac{1}{h^{\frac{3}{2}}}\,\mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{q}}. \tag{10}$$

By using the closure relations (7) one may write the following identity[1] for an arbitrary operator A:

$$A = \int \mathrm{d}\boldsymbol{p}'\mathrm{d}\boldsymbol{p}''\mathrm{d}\boldsymbol{q}'\mathrm{d}\boldsymbol{q}''|\boldsymbol{q}''\rangle\langle \boldsymbol{q}''|\boldsymbol{p}''\rangle\langle \boldsymbol{p}''|A|\boldsymbol{p}'\rangle\langle \boldsymbol{p}'|\boldsymbol{q}'\rangle\langle \boldsymbol{q}'|. \tag{11}$$

Introducing the new integration variables

$$\begin{aligned} \boldsymbol{p}' &= \boldsymbol{p}-\tfrac{1}{2}\boldsymbol{u}, & \boldsymbol{q}' &= \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}, \\ \boldsymbol{p}'' &= \boldsymbol{p}+\tfrac{1}{2}\boldsymbol{u}, & \boldsymbol{q}'' &= \boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}, \end{aligned} \tag{12}$$

with Jacobian equal to unity, one obtains for (11), using (10)

$$A = h^{-3}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\; a(\boldsymbol{p}, \boldsymbol{q})\Delta(\boldsymbol{p}, \boldsymbol{q}) \tag{13}$$

with the function

$$a(\boldsymbol{p}, \boldsymbol{q}) \equiv \int \mathrm{d}\boldsymbol{u}\,\mathrm{e}^{(i/\hbar)\boldsymbol{q}\cdot\boldsymbol{u}}\langle \boldsymbol{p}+\tfrac{1}{2}\boldsymbol{u}|A|\boldsymbol{p}-\tfrac{1}{2}\boldsymbol{u}\rangle, \tag{14}$$

depending on A and the hermitian operator

$$\Delta(\boldsymbol{p}, \boldsymbol{q}) \equiv \int \mathrm{d}\boldsymbol{v}\,\mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}}|\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}\rangle\langle \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}|, \tag{15}$$

which is independent of the operator A.

The function $a(\boldsymbol{p}, \boldsymbol{q})$ is called the *Weyl transform* of the operator A with respect to the momentum and coordinate operators $\boldsymbol{P}$ and $\boldsymbol{Q}$. (The correspondence between an operator and its Weyl transform will be denoted by the symbol $\rightleftarrows$.) In this way one has associated a c-number to each operator. If the operator A is hermitian, the function $a(\boldsymbol{p}, \boldsymbol{q})$ is real, as follows from (14).

[1] B. Leaf, J. Math. Phys. **9**(1968)65, on which paper most of the material in this section is based.

In (14) and (15) the variables $\boldsymbol{p}$ and $\boldsymbol{q}$ have not been treated on the same footing. We may obtain symmetrical forms for (15) by noting first that

$$|\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}\rangle = \mathrm{e}^{-(i/\hbar)\boldsymbol{v}\cdot\boldsymbol{P}}|\boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}\rangle. \tag{16}$$

(The validity of this identity may be verified by multiplication with $\langle \boldsymbol{p}|$ and the use of (6) and (10).) If (16) is substituted into (15), one encounters the projection operator $|\boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}\rangle\langle \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}|$ which may be transformed with the help of the identity

$$|\boldsymbol{q}\rangle\langle \boldsymbol{q}| = h^{-3}\int \mathrm{d}\boldsymbol{u}\,\mathrm{e}^{(i/\hbar)(\boldsymbol{q}-\boldsymbol{Q})\cdot\boldsymbol{u}}. \tag{17}$$

(This identity may be verified by letting it operate on $|\boldsymbol{q}'\rangle$ and by using (6).) In that way (15) becomes

$$\Delta(\boldsymbol{p}, \boldsymbol{q}) = h^{-3}\int \mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\,\mathrm{e}^{(i/\hbar)(\boldsymbol{p}-\boldsymbol{P})\cdot\boldsymbol{v}}\mathrm{e}^{(i/\hbar)(\boldsymbol{q}-\frac{1}{2}\boldsymbol{v}-\boldsymbol{Q})\cdot\boldsymbol{u}}. \tag{18}$$

With the help of the operator identity, valid for operators A and B that commute with their commutator:

$$\mathrm{e}^{A}\mathrm{e}^{B} = \mathrm{e}^{A+B+\frac{1}{2}[A,B]} \tag{19}$$

(v. problem 1) and the commutation rule (9), one gets for (18) a symmetric form:

$$\Delta(\boldsymbol{p}, \boldsymbol{q}) = h^{-3}\int \mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\,\mathrm{e}^{(i/\hbar)\{(\boldsymbol{q}-\boldsymbol{Q})\cdot\boldsymbol{u}+(\boldsymbol{p}-\boldsymbol{P})\cdot\boldsymbol{v}\}}. \tag{20}$$

From this expression one may find, interchanging the roles of $\boldsymbol{p}$ and $\boldsymbol{q}$, and retracing the argument given above, a form for $\Delta(\boldsymbol{p}, \boldsymbol{q})$ which is the counterpart of (15):

$$\Delta(\boldsymbol{p}, \boldsymbol{q}) = \int \mathrm{d}\boldsymbol{u}\,\mathrm{e}^{(i/\hbar)\boldsymbol{q}\cdot\boldsymbol{u}}|\boldsymbol{p}-\tfrac{1}{2}\boldsymbol{u}\rangle\langle \boldsymbol{p}+\tfrac{1}{2}\boldsymbol{u}|. \tag{21}$$

The Weyl transform may also be written in different forms. Since the trace of an operator may be written in terms of the complete set $|\boldsymbol{p}\rangle$ as

$$\mathrm{Tr}\,A = \int \mathrm{d}\boldsymbol{p}\langle \boldsymbol{p}|A|\boldsymbol{p}\rangle, \tag{22}$$

one has the identity

$$\langle \boldsymbol{p}'|A|\boldsymbol{p}''\rangle = \operatorname{Tr}\,(A|\boldsymbol{p}''\rangle\langle\boldsymbol{p}'|). \tag{23}$$

From the expression (14) for $a(\boldsymbol{p}, \boldsymbol{q})$ together with the expression (21) for $\Delta(\boldsymbol{p}, \boldsymbol{q})$ one then obtains the concise formula

$$a(\boldsymbol{p}, \boldsymbol{q}) = \operatorname{Tr}\,\{A\Delta(\boldsymbol{p}, \boldsymbol{q})\}. \tag{24}$$

With (15) for $\Delta(\boldsymbol{p}, \boldsymbol{q})$ and the alternative form of the trace

$$\operatorname{Tr} A = \int \mathrm{d}\boldsymbol{q}\langle\boldsymbol{q}|A|\boldsymbol{q}\rangle, \tag{25}$$

one finds the counterpart of (14):

$$a(\boldsymbol{p}, \boldsymbol{q}) = \int \mathrm{d}\boldsymbol{v}\, \mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}}\langle \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}|A|\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}\rangle. \tag{26}$$

The formulae (14) and (26) show that the set of operators A in Hilbert space may be mapped upon a set of c-numbers: their Weyl transforms $a(\boldsymbol{p}, \boldsymbol{q})$. The reverse is also true: each function $a(\boldsymbol{p}, \boldsymbol{q})$ may generate an operator A by means of formula (13) with (15) or (20) or (21). In particular if one uses (20) for the Δ-operator, formula (13) becomes

$$A = h^{-6}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\, a(\boldsymbol{p}, \boldsymbol{q})\mathrm{e}^{(i/\hbar)\{(\boldsymbol{q}-\boldsymbol{Q})\cdot\boldsymbol{u}+(\boldsymbol{p}-\boldsymbol{P})\cdot\boldsymbol{v}\}}. \tag{27}$$

One recognizes the Fourier transform $\tilde{a}(\boldsymbol{u}, \boldsymbol{v})$ of $a(\boldsymbol{p}, \boldsymbol{q})$:

$$\tilde{a}(\boldsymbol{u}, \boldsymbol{v}) = h^{-6}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\, a(\boldsymbol{p}, \boldsymbol{q})\mathrm{e}^{(i/\hbar)(\boldsymbol{q}\cdot\boldsymbol{u}+\boldsymbol{p}\cdot\boldsymbol{v})}, \tag{28}$$

of which the inverse is

$$a(\boldsymbol{p}, \boldsymbol{q}) = \int \mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\,\tilde{a}(\boldsymbol{u}, \boldsymbol{v})\mathrm{e}^{-(i/\hbar)(\boldsymbol{q}\cdot\boldsymbol{u}+\boldsymbol{p}\cdot\boldsymbol{v})}. \tag{29}$$

The expression (27) may hence be written as

$$A = \int \mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\,\tilde{a}(\boldsymbol{u}, \boldsymbol{v})\mathrm{e}^{-(i/\hbar)(\boldsymbol{Q}\cdot\boldsymbol{u}+\boldsymbol{P}\cdot\boldsymbol{v})}. \tag{30}$$

The expressions (29) and (30) show the correspondence between an operator and its Weyl transform in an elegant way.

Weyl transforms of operators are especially simple, if the operator is a function of $\boldsymbol{P}$ or $\boldsymbol{Q}$ only. In fact the Weyl transform is then the same function of $\boldsymbol{p}$ and $\boldsymbol{q}$ respectively. An example of a Weyl correspondence which will

be used frequently in the following is

$$\tfrac{1}{2}\{\boldsymbol{P}, f(\boldsymbol{Q})\} \rightleftarrows \boldsymbol{p}f(\boldsymbol{q}), \tag{31}$$

where the curly brackets indicate the anticommutator: $\{A, B\} \equiv AB+BA$ and where f is an arbitrary function. It may be proved from (14) by insertion of a complete set $|\boldsymbol{q}'\rangle$ with the help of (7), and by application of (10).

One may ask whether taking the Weyl transform is an operation that is invariant under a change of canonical coordinates and momenta, i.e. whether one finds again the result (29) for the Weyl transform of an operator (30), if one performs first a transformation of coordinate and momentum operators in A, then takes the Weyl transform with respect to these new coordinates and momenta, and finally transforms back the Weyl transform to the old coordinates and momenta. For a linear transformation this invariance is guaranteed by the linear character of the exponentials in (29) and (30) (v. problem 2).

The operator $\Delta(\boldsymbol{p}, \boldsymbol{q})$ plays a special role in the Weyl correspondence, as is apparent from (13). By choosing in particular for A the operator $\Delta(\boldsymbol{p}', \boldsymbol{q}')$ one finds that the Weyl transform of $\Delta(\boldsymbol{p}', \boldsymbol{q}')$ is essentially a delta function:

$$\Delta(\boldsymbol{p}', \boldsymbol{q}') \rightleftarrows h^3\delta(\boldsymbol{p}-\boldsymbol{p}')\delta(\boldsymbol{q}-\boldsymbol{q}'). \tag{32}$$

The trace of the operator $\Delta(\boldsymbol{p}, \boldsymbol{q})$ and of products of Δ-operators will be used frequently in the following. In particular one finds from (25) with (8) and (15) that

$$\operatorname{Tr} \Delta(\boldsymbol{p}, \boldsymbol{q}) = 1. \tag{33}$$

Furthermore from (24) with $A = \Delta(\boldsymbol{p}', \boldsymbol{q}')$ and (32) one has

$$\operatorname{Tr}\,\{\Delta(\boldsymbol{p}, \boldsymbol{q})\Delta(\boldsymbol{p}', \boldsymbol{q}')\} = h^3\delta(\boldsymbol{p}-\boldsymbol{p}')\delta(\boldsymbol{q}-\boldsymbol{q}'). \tag{34}$$

The trace of the product of three Δ-operators will also be useful. From (25) one finds with insertion of the completeness relation (7) for $|\boldsymbol{q}\rangle$, the expression (15) for $\Delta(\boldsymbol{p}, \boldsymbol{q})$ and with the use of (8):

$$\begin{aligned}\operatorname{Tr}\,\{\Delta(\boldsymbol{p}, \boldsymbol{q})\Delta(\boldsymbol{p}', \boldsymbol{q}')\Delta(\boldsymbol{p}'', \boldsymbol{q}'')\} &= \int \mathrm{d}\boldsymbol{q}_1\,\mathrm{d}\boldsymbol{q}_2\,\mathrm{d}\boldsymbol{q}_3\,\delta(\boldsymbol{q}-\tfrac{\boldsymbol{q}_1+\boldsymbol{q}_2}{2})\delta(\boldsymbol{q}'-\tfrac{\boldsymbol{q}_2+\boldsymbol{q}_3}{2})\delta(\boldsymbol{q}''-\tfrac{\boldsymbol{q}_3+\boldsymbol{q}_1}{2})\\ &\exp\left[\frac{i}{\hbar}\{\boldsymbol{p}\cdot(\boldsymbol{q}_1-\boldsymbol{q}_2)+\boldsymbol{p}'\cdot(\boldsymbol{q}_2-\boldsymbol{q}_3)+\boldsymbol{p}''\cdot(\boldsymbol{q}_3-\boldsymbol{q}_1)\}\right]. \end{aligned} \tag{35}$$

After introduction of new variables $\frac{1}{2}(\boldsymbol{q}_1+\boldsymbol{q}_2)$, $\frac{1}{2}(\boldsymbol{q}_2+\boldsymbol{q}_3)$ and $\frac{1}{2}(\boldsymbol{q}_3+\boldsymbol{q}_1)$ the integration over the delta functions may be performed with the result

$$\operatorname{Tr}\{\Delta(\boldsymbol{p},\boldsymbol{q})\Delta(\boldsymbol{p}',\boldsymbol{q}')\Delta(\boldsymbol{p}'',\boldsymbol{q}'')\}$$
$$= 2^6 \exp\left[\frac{2i}{\hbar}\{\boldsymbol{p}\cdot(\boldsymbol{q}''-\boldsymbol{q}')+\boldsymbol{p}'\cdot(\boldsymbol{q}-\boldsymbol{q}'')+\boldsymbol{p}''\cdot(\boldsymbol{q}'-\boldsymbol{q})\}\right]. \quad (36)$$

The trace of an arbitrary operator may be expressed in terms of its Weyl transform by making use of (13) and (33):

$$\operatorname{Tr} A = h^{-3}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\, a(\boldsymbol{p},\boldsymbol{q}). \quad (37)$$

The trace of a product of two operators follows from (13) and (34):

$$\operatorname{Tr} AB = h^{-3}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\, a(\boldsymbol{p},\boldsymbol{q})b(\boldsymbol{p},\boldsymbol{q}) = \operatorname{Tr} BA. \quad (38)$$

In quantum mechanics commutators and anticommutators play an important role. To find their Weyl transform we need to study the Weyl transform of a product of operators. The latter is not in general simply the product of the Weyl transforms of the operators. To find the Weyl transform of the product of operators AB one may start from (24) and use (13) and (36):

$$AB \rightleftarrows \left(\frac{2}{h}\right)^6 \int \mathrm{d}\boldsymbol{p}'\mathrm{d}\boldsymbol{q}'\mathrm{d}\boldsymbol{p}''\mathrm{d}\boldsymbol{q}''\, a(\boldsymbol{p}',\boldsymbol{q}')b(\boldsymbol{p}'',\boldsymbol{q}'')$$
$$\exp\left[\frac{2i}{\hbar}\{(\boldsymbol{q}'-\boldsymbol{q})\cdot(\boldsymbol{p}''-\boldsymbol{p})-(\boldsymbol{p}'-\boldsymbol{p})\cdot(\boldsymbol{q}''-\boldsymbol{q})\}\right]. \quad (39)$$

Introducing new variables $\hat{\boldsymbol{p}} = \boldsymbol{p}''-\boldsymbol{p}$ and $\hat{\boldsymbol{q}} = \boldsymbol{q}''-\boldsymbol{q}$ and expanding $b(\boldsymbol{p}+\hat{\boldsymbol{p}}, \boldsymbol{q}+\hat{\boldsymbol{q}})$ into a Taylor series around $b(\boldsymbol{p},\boldsymbol{q})$, one gets

$$AB \rightleftarrows \left(\frac{2}{h}\right)^6 \int \mathrm{d}\boldsymbol{p}'\mathrm{d}\boldsymbol{q}'\mathrm{d}\hat{\boldsymbol{p}}\,\mathrm{d}\hat{\boldsymbol{q}}\, a(\boldsymbol{p}',\boldsymbol{q}')$$
$$\exp\left[\frac{2i}{\hbar}\{(\boldsymbol{q}'-\boldsymbol{q})\cdot\hat{\boldsymbol{p}}-(\boldsymbol{p}'-\boldsymbol{p})\cdot\hat{\boldsymbol{q}}\}\right]\left\{\exp\left(\hat{\boldsymbol{p}}\cdot\frac{\partial}{\partial \boldsymbol{p}}+\hat{\boldsymbol{q}}\cdot\frac{\partial}{\partial \boldsymbol{q}}\right)\right\} b(\boldsymbol{p},\boldsymbol{q}). \quad (40)$$

In the last exponential we may replace $\hat{\boldsymbol{p}}$ by the differential operator $-(\hbar/2i)\partial^{\leftarrow}/\partial\boldsymbol{q}$ and likewise $\hat{\boldsymbol{q}}$ by $(\hbar/2i)\partial^{\leftarrow}/\partial\boldsymbol{p}$, both acting to the left. Then the integration over $\hat{\boldsymbol{p}}$ and $\hat{\boldsymbol{q}}$ yields delta functions, so that the integrations over $\boldsymbol{p}'$ and $\boldsymbol{q}'$ may also be performed. In this way one gets[1]

$$AB \rightleftarrows a(\boldsymbol{p},\boldsymbol{q}) \exp\left\{\frac{\hbar}{2i}\left(\frac{\partial^{\leftarrow}}{\partial \boldsymbol{p}}\cdot\frac{\partial^{\rightarrow}}{\partial \boldsymbol{q}}-\frac{\partial^{\leftarrow}}{\partial \boldsymbol{q}}\cdot\frac{\partial^{\rightarrow}}{\partial \boldsymbol{p}}\right)\right\} b(\boldsymbol{p},\boldsymbol{q}), \quad (41)$$

where for aesthetic reasons arrows pointing to the right have been added. An alternative notation of (41) is obtained by attaching indices (a) and (b) to the differential operators, indicating their objects:

$$AB \rightleftarrows \exp\left\{\frac{\hbar}{2i}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{p}}\cdot\frac{\partial^{(b)}}{\partial \boldsymbol{q}}-\frac{\partial^{(a)}}{\partial \boldsymbol{q}}\cdot\frac{\partial^{(b)}}{\partial \boldsymbol{p}}\right)\right\} a(\boldsymbol{p},\boldsymbol{q})b(\boldsymbol{p},\boldsymbol{q}). \quad (42)$$

The right-hand side of (41) or (42) shows that the Weyl transform of a product of operators AB is not in general equal to the product $a(\boldsymbol{p},\boldsymbol{q})b(\boldsymbol{p},\boldsymbol{q})$ of their Weyl transforms.

Let us write as corollaries the Weyl transforms of the anticommutator and the commutator of A and B:

$$\{A,B\} \rightleftarrows 2\cos\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}}\cdot\frac{\partial^{(b)}}{\partial \boldsymbol{p}}-\frac{\partial^{(a)}}{\partial \boldsymbol{p}}\cdot\frac{\partial^{(b)}}{\partial \boldsymbol{q}}\right)\right\} a(\boldsymbol{p},\boldsymbol{q})b(\boldsymbol{p},\boldsymbol{q}), \quad (43)$$

$$[A,B] \rightleftarrows 2i\sin\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}}\cdot\frac{\partial^{(b)}}{\partial \boldsymbol{p}}-\frac{\partial^{(a)}}{\partial \boldsymbol{p}}\cdot\frac{\partial^{(b)}}{\partial \boldsymbol{q}}\right)\right\} a(\boldsymbol{p},\boldsymbol{q})b(\boldsymbol{p},\boldsymbol{q}). \quad (44)$$

These formulae show that the Weyl transforms of anticommutators and commutators are series in $\hbar^2$. The lowest order term of (43) is

$$2a(\boldsymbol{p},\boldsymbol{q})b(\boldsymbol{p},\boldsymbol{q}), \quad (45)$$

while that of (44) is

$$i\hbar\left(\frac{\partial a}{\partial \boldsymbol{q}}\cdot\frac{\partial b}{\partial \boldsymbol{p}}-\frac{\partial a}{\partial \boldsymbol{p}}\cdot\frac{\partial b}{\partial \boldsymbol{q}}\right). \quad (46)$$

Hence the series for the Weyl transform of $\frac{1}{2}\{A,B\}$ starts off with the product of the Weyl transforms of A and B, whereas the series for the Weyl transform of $-(i/\hbar)[A,B]$ starts off with the Poisson bracket of the Weyl transforms of A and B.

An example, which will be frequently used in the following, is furnished by the time derivative $\dot{A}$, defined in (3) as $(i/\hbar)[H,A]+\partial^{e}A/\partial t$. It follows from (44) that:

$$\dot{A} \rightleftarrows \frac{2}{\hbar}\sin\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}}\cdot\frac{\partial^{(h)}}{\partial \boldsymbol{p}}-\frac{\partial^{(a)}}{\partial \boldsymbol{p}}\cdot\frac{\partial^{(h)}}{\partial \boldsymbol{q}}\right)\right\} a(\boldsymbol{p},\boldsymbol{q};t)h(\boldsymbol{p},\boldsymbol{q})+\frac{\partial a(\boldsymbol{p},\boldsymbol{q};t)}{\partial t}. \quad (47)$$

[1] H. J. Groenewold, Physica **12**(1946)405.

Thus the Weyl transform of $\dot{A}$ is a series in $\hbar^2$, which starts off with the Poisson bracket of $a(\boldsymbol{p}, \boldsymbol{q}; t)$ and $h(\boldsymbol{p}, \boldsymbol{q})$, and the explicit time derivative of $a(\boldsymbol{p}, \boldsymbol{q}; t)$.

b. *The Wigner function*

Up to here we studied the one-to-one mapping of operators A and functions in phase space $a(\boldsymbol{p}, \boldsymbol{q})$, given by the Weyl transformation. If one wants to find expectation values of an operator, one is interested in expressions which allow to find the expectation values directly from the Weyl transform of the operator.

A system may be described by its state vector $|\psi(t)\rangle$ in Hilbert space or alternatively by the density operator

$$P(t) = |\psi(t)\rangle\langle\psi(t)|. \tag{48}$$

The expectation value $\bar{A}$ of an operator A is equal to $\langle\psi|A|\psi\rangle$ or

$$\bar{A}(t) = \mathrm{Tr}\,\{P(t)A\}. \tag{49}$$

Such a trace may be written in terms of Weyl transforms as is shown by (38). Let us denote the Weyl transform of the density operator P by $h^3\rho(\boldsymbol{p}, \boldsymbol{q}; t)$:

$$P(t) \rightleftarrows h^3\rho(\boldsymbol{p}, \boldsymbol{q}; t). \tag{50}$$

Then the expectation value (49) becomes

$$\bar{A} = \bar{a}, \tag{51}$$

where the latter quantity is an integral over the product of the Weyl transform a and the Wigner function:

$$\bar{a} \equiv \int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\; a(\boldsymbol{p}, \boldsymbol{q})\rho(\boldsymbol{p}, \boldsymbol{q}; t). \tag{52}$$

From the expression (26) it follows that the Weyl transform $h^3\rho(\boldsymbol{p}, \boldsymbol{q}; t)$ may be written as

$$h^3\rho(\boldsymbol{p}, \boldsymbol{q}; t) = \int \mathrm{d}\boldsymbol{v}\, \mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}}\langle\boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}|\psi\rangle\langle\psi|\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}\rangle \tag{53}$$

or, using the wave function notation $\psi(\boldsymbol{q}; t) \equiv \langle\boldsymbol{q}|\psi(t)\rangle$:

$$\rho(\boldsymbol{p}, \boldsymbol{q}; t) = h^{-3}\int \mathrm{d}\boldsymbol{v}\, \mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}}\psi(\boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}; t)\psi^*(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}; t). \tag{54}$$

At the right-hand side appears the function which Wigner introduced originally[1]. This formula together with (50) shows that the Wigner function is the Weyl transform of the density matrix (divided by h^3).

The Wigner function $\rho(\boldsymbol{p}, \boldsymbol{q}; t)$ is real as follows from the hermiticity of the density operator. Furthermore, since the trace of the density operator is unity:

$$\mathrm{Tr}\,P = 1, \tag{55}$$

(as follows from the normalization of the state vector $|\psi\rangle$) the Wigner function possesses the normalization property

$$\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\; \rho(\boldsymbol{p}, \boldsymbol{q}; t) = 1 \tag{56}$$

as a direct consequence of (37).

The relation (51) with (52) shows that one may calculate expectation values of an operator by evaluating an integral involving its Weyl transform and the Wigner function. In view of (51) with (52) and (56) one might be inclined to interpret the Wigner function as a probability density in phase space. However, such an interpretation is not possible since the Wigner function is not necessarily positive definite.

The time evolution of the state vector which describes the system is given by the Schrödinger equation

$$H|\psi(t)\rangle = -\frac{\hbar}{i}\frac{\partial}{\partial t}|\psi(t)\rangle, \tag{57}$$

or in terms of the density operator (48):

$$\frac{\partial P}{\partial t} = -\frac{i}{\hbar}[H, P] \tag{58}$$

(the left-hand side is the explicit time derivative denoted as $\partial^e/\partial t$ in (3)). With the help of (44) this equation may be converted into an equation in terms of the Weyl transforms $h^3\rho(\boldsymbol{p}, \boldsymbol{q}; t)$ and $h(\boldsymbol{p}, \boldsymbol{q})$, namely

$$\frac{\partial\rho(\boldsymbol{p}, \boldsymbol{q}; t)}{\partial t} = \frac{2}{\hbar}\sin\left\{\frac{\hbar}{2}\left(\frac{\partial^{(h)}}{\partial\boldsymbol{q}}\cdot\frac{\partial^{(\rho)}}{\partial\boldsymbol{p}} - \frac{\partial^{(h)}}{\partial\boldsymbol{p}}\cdot\frac{\partial^{(\rho)}}{\partial\boldsymbol{q}}\right)\right\} h(\boldsymbol{p}, \boldsymbol{q})\rho(\boldsymbol{p}, \boldsymbol{q}; t). \tag{59}$$

This equation, which gives the evolution in time of the Wigner function, may be employed to find the time derivative of an expectation value. In fact

[1] E. P. Wigner, Phys. Rev. **40**(1932)749; cf. B. Leaf, op. cit.

one finds from (52) with (59) and a partial integration

$$\frac{\mathrm{d}\bar{a}(t)}{\mathrm{d}t} = \frac{2}{\hbar}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\left[\sin\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}}\cdot\frac{\partial^{(h)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}}\cdot\frac{\partial^{(h)}}{\partial \boldsymbol{q}}\right)\right\} a(\boldsymbol{p},\boldsymbol{q})h(\boldsymbol{p},\boldsymbol{q})\right]\rho(\boldsymbol{p},\boldsymbol{q};t). \tag{60}$$

The left-hand side is equal to the time derivative of the expectation value $\bar{A}$ as follows from (51). The right-hand side is equal to the expectation value of the operator $\dot{A}$ (3) as follows from (47) and (51) with (52).

4 *The Weyl transforms of the field equations*

The field equations and the equation of motion, which have been written in operator form in section 2, will now be transformed to equations for phase space functions by using the Weyl transformation[1].

The Weyl transform of the Hamiltonian (1) follows by keeping in mind that functions of the coordinate or of the momentum operators transform into the same functions of the coordinates and momenta variables in phase space, and by using (31):

$$H_{\mathrm{op}} \rightleftarrows H(1,\dots,N;t) \equiv \sum_i \frac{\boldsymbol{P}_i^2}{2m_i} + \sum_{i,j(i\neq j)} \frac{e_i e_j}{8\pi|\boldsymbol{R}_i-\boldsymbol{R}_j|} + \sum_i e_i\left\{\varphi_e(\boldsymbol{R}_i,t) - c^{-1}\frac{\boldsymbol{P}_i}{m_i}\cdot\boldsymbol{A}_e(\boldsymbol{R}_i,t)\right\}, \tag{61}$$

where the arguments $1,\dots,N$ stand for $\boldsymbol{P}_1, \boldsymbol{R}_1 \dots \boldsymbol{P}_N, \boldsymbol{R}_N$, the variables of the N particles.

The Weyl transforms of the field equations (2) become, according to (31) and (47)

$$\begin{aligned}
\nabla\cdot\boldsymbol{e} &= \sum_i e_i\,\delta(\boldsymbol{R}_i-\boldsymbol{R}),\\
-\partial_0\,\boldsymbol{e} - c^{-1}\sin(\boldsymbol{e};H) + \nabla\wedge\boldsymbol{b} &= c^{-1}\sum_i e_i\frac{\boldsymbol{P}_i}{m_i}\,\delta(\boldsymbol{R}_i-\boldsymbol{R}),\\
\nabla\cdot\boldsymbol{b} &= 0,\\
\partial_0\,\boldsymbol{b} + c^{-1}\sin(\boldsymbol{b};H) + \nabla\wedge\boldsymbol{e} &= 0,
\end{aligned} \tag{62}$$

[1] We resume the notation op of section 2 for operators, and use symbols without this index for Weyl transforms.

where as an abbreviation we wrote

$$\sin(a;b) \equiv \sum_{i=1}^{N}\frac{2}{\hbar}\sin\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{R}_i}\cdot\frac{\partial^{(b)}}{\partial \boldsymbol{P}_i} - \frac{\partial^{(a)}}{\partial \boldsymbol{P}_i}\cdot\frac{\partial^{(b)}}{\partial \boldsymbol{R}_i}\right)\right\} a(1,\dots,N)b(1,\dots,N) \tag{63}$$

and where $\boldsymbol{e}$ and $\boldsymbol{b}$ are functions of $1,\dots,N$, $\boldsymbol{R}$ and t, while H is given by (61).

To solve these equations, we note first that the last two equations have as solutions

$$\begin{aligned}
\boldsymbol{e} &= -\nabla\varphi - \partial_0\,\boldsymbol{a} - c^{-1}\sin(\boldsymbol{a};H),\\
\boldsymbol{b} &= \nabla\wedge\boldsymbol{a}
\end{aligned} \tag{64}$$

with functions φ and $\boldsymbol{a}$ depending on $1,\dots,N$, $\boldsymbol{R}$ and t. Insertion into the first two field equations leads, up to order c^{-1}, to:

$$\begin{aligned}
\Delta\varphi + \partial_0\,\nabla\cdot\boldsymbol{a} + c^{-1}\nabla\cdot\sin(\boldsymbol{a};H) &= -\sum_i e_i\,\delta(\boldsymbol{R}_i-\boldsymbol{R}),\\
\Delta\boldsymbol{a} - \nabla\{\nabla\cdot\boldsymbol{a} + \partial_0\,\varphi + c^{-1}\sin(\varphi;H)\} &= -c^{-1}\sum_i e_i\frac{\boldsymbol{P}_i}{m_i}\,\delta(\boldsymbol{R}_i-\boldsymbol{R}).
\end{aligned} \tag{65}$$

The formulae (64) show that a gauge transformation of the potentials

$$\begin{aligned}
\varphi' &= \varphi - \partial_0\,\psi - c^{-1}\sin(\psi;H),\\
\boldsymbol{a}' &= \boldsymbol{a} + \nabla\psi,
\end{aligned} \tag{66}$$

with $\psi(1,\dots,N;\boldsymbol{R},t)$ an arbitrary function, leads to the same fields, since the Weyl transform H is independent of $\boldsymbol{R}$. Therefore it is allowed to require as a condition on the potentials

$$\partial_0\,\varphi + c^{-1}\sin(\varphi;H) + \nabla\cdot\boldsymbol{a} = 0, \tag{67}$$

because starting from potentials which do not satisfy this relation one may find ψ such that the new potentials (66) do satisfy it.

With the use of (67) the equations (65) become separated in φ and $\boldsymbol{a}$:

$$\begin{aligned}
\Delta\varphi &= -\sum_i e_i\,\delta(\boldsymbol{R}_i-\boldsymbol{R}),\\
\Delta\boldsymbol{a} &= -c^{-1}\sum_i e_i\frac{\boldsymbol{P}_i}{m_i}\,\delta(\boldsymbol{R}_i-\boldsymbol{R}),
\end{aligned} \tag{68}$$

where terms of order c^{-2} have been neglected. Solving these equations and inserting the results into (64), we get for the Weyl transforms of the fields:

$$\begin{aligned}
\boldsymbol{e} &= \sum_i \boldsymbol{e}_i, \qquad \boldsymbol{e}_i(\boldsymbol{R}_i;\boldsymbol{R}) = -\nabla\frac{e_i}{4\pi|\boldsymbol{R}_i-\boldsymbol{R}|},\\
\boldsymbol{b} &= \sum_i \boldsymbol{b}_i, \qquad \boldsymbol{b}_i(\boldsymbol{P}_i,\boldsymbol{R}_i;\boldsymbol{R}) = c^{-1}\nabla\wedge\frac{e_i\boldsymbol{P}_i}{4\pi m_i|\boldsymbol{R}_i-\boldsymbol{R}|}.
\end{aligned} \tag{69}$$

(Solutions of the sourceless equations may of course be added to these particular solutions.)

From the form of these solutions and that of the Weyl transform $H(1, \ldots, N; t)$ of the Hamiltonian it follows that the sine (63) appearing in the second equation of (62) reduces to

$$\sum_i \frac{\partial \boldsymbol{e}}{\partial \boldsymbol{R}_i} \cdot \frac{\partial H}{\partial \boldsymbol{P}_i}, \tag{70}$$

since the Weyl transform of the electric field is independent of the momenta and the Hamiltonian is quadratic in the momenta. The expression (70) is equal to the Poisson bracket of $\boldsymbol{e}$ and H, because Poisson brackets are defined as

$$\{a, b\}_{\mathrm{P}} \equiv \sum_{i=1}^{N} \left(\frac{\partial a}{\partial \boldsymbol{R}_i} \cdot \frac{\partial b}{\partial \boldsymbol{P}_i} - \frac{\partial a}{\partial \boldsymbol{P}_i} \cdot \frac{\partial b}{\partial \boldsymbol{R}_i} \right). \tag{71}$$

Let us introduce the abbreviation $\partial_{t\mathrm{P}} \equiv c\partial_{0\mathrm{P}}$ defined as

$$\partial_{t\mathrm{P}}\, a = c\partial_{0\mathrm{P}}\, a \equiv \{a, H\}_{\mathrm{P}} + \partial_t a, \tag{72}$$

where at the right-hand side the sum of the Poisson bracket of the Weyl transforms a and H, and the explicit time derivative $\partial_t a \equiv \partial^{\mathrm{e}} a/\partial t$ of a appears. Then we may write the Weyl transforms of the field equations in the form

$$\begin{aligned} \nabla \cdot \boldsymbol{e} &= \sum_i e_i \delta(\boldsymbol{R}_i - \boldsymbol{R}), \\ -\partial_{0\mathrm{P}}\, \boldsymbol{e} + \nabla \wedge \boldsymbol{b} &= c^{-1} \sum_i e_i (\partial_{t\mathrm{P}} \boldsymbol{R}_i) \delta(\boldsymbol{R}_i - \boldsymbol{R}), \\ \nabla \cdot \boldsymbol{b} &= 0, \\ \partial_0 \boldsymbol{b} + \nabla \wedge \boldsymbol{e} &= 0, \end{aligned} \tag{73}$$

where in the fourth equation only the explicit time derivative appears.

(From the solutions (69) of these equations (73) one may find, if one wishes, the operators for the fields. With (31) one obtains:

$$\begin{aligned} \boldsymbol{e}_{\mathrm{op}} &= \sum_i \boldsymbol{e}_{i,\mathrm{op}}, & \boldsymbol{e}_{i,\mathrm{op}} &= -\nabla \frac{e_i}{4\pi |\boldsymbol{R}_{i,\mathrm{op}} - \boldsymbol{R}|}, \\ \boldsymbol{b}_{\mathrm{op}} &= \sum_i \boldsymbol{b}_{i,\mathrm{op}}, & \boldsymbol{b}_{i,\mathrm{op}} &= \tfrac{1}{2} c^{-1} \left\{ \nabla \frac{e_i}{4\pi m_i |\boldsymbol{R}_{i,\mathrm{op}} - \boldsymbol{R}|} \wedge, \boldsymbol{P}_{i,\mathrm{op}} \right\}, \end{aligned} \tag{74}$$

where an anticommutator appears in the last expression.)

Equations for the expectation values may be found by multiplying (73) by a Wigner function and integrating over phase space (cf. (52)). Since (73) is equivalent to (62) one then finds with (60)

$$\begin{aligned} \nabla \cdot \bar{\boldsymbol{e}} &= \int \sum_i e_i \delta(\boldsymbol{R}_i - \boldsymbol{R}) \rho(1, \ldots, N; t) \mathrm{d}1 \ldots \mathrm{d}N, \\ -\partial_0 \bar{\boldsymbol{e}} + \nabla \wedge \bar{\boldsymbol{b}} &= c^{-1} \int \sum_i e_i \frac{\boldsymbol{P}_i}{m_i} \delta(\boldsymbol{R}_i - \boldsymbol{R}) \rho(1, \ldots, N; t) \mathrm{d}1 \ldots \mathrm{d}N, \\ \nabla \cdot \bar{\boldsymbol{b}} &= 0, \\ \partial_0 \bar{\boldsymbol{b}} + \nabla \wedge \bar{\boldsymbol{e}} &= 0, \end{aligned} \tag{75}$$

with the notations (52):

$$\begin{aligned} \bar{\boldsymbol{e}}(\boldsymbol{R}, t) &= \int \boldsymbol{e}(1, \ldots, N; \boldsymbol{R}) \rho(1, \ldots, N; t) \mathrm{d}1 \ldots \mathrm{d}N, \\ \bar{\boldsymbol{b}}(\boldsymbol{R}, t) &= \int \boldsymbol{b}(1, \ldots, N; \boldsymbol{R}) \rho(1, \ldots, N; t) \mathrm{d}1 \ldots \mathrm{d}N, \end{aligned} \tag{76}$$

where $1, \ldots, N$ stands for all phase variables of the N-point system. (If external fields are present, the fields $\boldsymbol{e}$ and $\boldsymbol{b}$ depend also on t.)

It stands to reason that these results could also have been obtained directly from the operator equations (2) by taking the expectation values, as follows from (51–52) together with (31). The advantage of using the Weyl transform and the Wigner function will become apparent in the following when the atomic and macroscopic theories will be dealt with.

5 *The Weyl transform of the equation of motion*

The equation of motion in operator form has been given in (4). Its Weyl transform is obtained with the help of (31) and (47):

$$\begin{aligned} & m_i \sin\{\sin(\boldsymbol{R}_i; H); H\} + m_i \frac{\partial}{\partial t} \{\sin(\boldsymbol{R}_i; H)\} \\ &= -\nabla_i \sum_{j(\neq i)} \frac{e_i e_j}{4\pi |\boldsymbol{R}_i - \boldsymbol{R}_j|} + e_i \left\{ \boldsymbol{E}_{\mathrm{e}}(\boldsymbol{R}_i, t) + c^{-1} \frac{\boldsymbol{P}_i}{m_i} \wedge \boldsymbol{B}_{\mathrm{e}}(\boldsymbol{R}_i, t) \right\}, \end{aligned} \tag{77}$$

where the abbreviation (63) has been used. At the right-hand side one recognizes the total fields (cf. (69)) up to order c^{-1} and c^0 respectively:

$$\begin{aligned} \boldsymbol{e}_t(\boldsymbol{R}_i, t) &= \sum_{j(\neq i)} \boldsymbol{e}_j(\boldsymbol{R}_j; \boldsymbol{R}_i) + \boldsymbol{E}_{\mathrm{e}}(\boldsymbol{R}_i, t), \\ \boldsymbol{b}_t(\boldsymbol{R}_i, t) &= \boldsymbol{B}_{\mathrm{e}}(\boldsymbol{R}_i, t). \end{aligned} \tag{78}$$

The equation (77) may thus also be written as

$$m_i \sin \{\sin (\boldsymbol{R}_i; H); H\} + m_i \frac{\partial}{\partial t} \{\sin (\boldsymbol{R}_i; H)\}$$
$$= e_i \left\{ \boldsymbol{e}_t(\boldsymbol{R}_i, t) + c^{-1} \frac{\boldsymbol{P}_i}{m_i} \wedge \boldsymbol{b}_t(\boldsymbol{R}_i, t) \right\}. \quad (79)$$

From the form of the Weyl transform H (61) of the Hamiltonian and the definition (63) of the sine symbol it follows that the latter reduces here to Poisson brackets (71). This is most easily seen by writing the sine symbol (63) as

$$\sin (a; b) = \sum_{i=1}^{N} \frac{2}{\hbar} \left\{ \sin \left(\frac{\hbar}{2} \frac{\partial^{(a)}}{\partial \boldsymbol{R}_i} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{P}_i} \right) \cos \left(\frac{\hbar}{2} \frac{\partial^{(a)}}{\partial \boldsymbol{P}_i} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{R}_i} \right) \right.$$
$$\left. - \cos \left(\frac{\hbar}{2} \frac{\partial^{(a)}}{\partial \boldsymbol{R}_i} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{P}_i} \right) \sin \left(\frac{\hbar}{2} \frac{\partial^{(a)}}{\partial \boldsymbol{P}_i} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{R}_i} \right) \right\} a(1, \ldots, N) b(1, \ldots, N). \quad (80)$$

Therefore we find the Weyl transform (79) of the equation of motion as

$$m_i \partial_{t\mathrm{P}}^2 \boldsymbol{R}_i = e_i \{ \boldsymbol{e}_t(\boldsymbol{R}_i, t) + c^{-1} (\partial_{t\mathrm{P}} \boldsymbol{R}_i) \wedge \boldsymbol{b}_t(\boldsymbol{R}_i, t) \}. \quad (81)$$

where the abbreviation (72) has been introduced. (An alternative way to derive this equation would have been to calculate directly the repeated Poisson bracket of $\boldsymbol{R}_i$ and H.)

An equation for the expectation value follows from (81) by multiplying with a Wigner function and integrating over phase space. Because of the equivalence of (81) and (79) one obtains in this way with (60)

$$m_i \frac{\mathrm{d}^2 \overline{\boldsymbol{R}}_i}{\mathrm{d}t^2} = e_i \int \left\{ \boldsymbol{e}_t(1, \ldots, N; \boldsymbol{R}_i, t) + c^{-1} \frac{\boldsymbol{P}_i}{m_i} \wedge \boldsymbol{b}_t(1, \ldots, N; \boldsymbol{R}_i, t) \right\}$$
$$\rho(1, \ldots, N; t) \mathrm{d}1 \ldots \mathrm{d}N \quad (82)$$

with the notation (52):

$$\overline{\boldsymbol{R}}_i = \int \boldsymbol{R}_i \rho(1, \ldots, N; t) \mathrm{d}1 \ldots \mathrm{d}N. \quad (83)$$

Again it may be remarked that the result (82) can be obtained in a more straightforward way by taking the expectation value of equation (4), as follows from (51–52), (31) and (78).

The Weyl transforms (73) of the field equations and (81) of the equation of motion have the same forms as the corresponding classical equations (I.1) and (I.12) respectively. This fact will be exploited in the following sections.

6 *The equations for the fields of composite particles*

In the preceding sections we derived the field equations and the equation of motion for a set of charged point particles in an external field. Their Weyl transforms turned out to have the same form as the classical equations. As a consequence of this feature we may now find the equations that govern the behaviour of stable groups of charged particles in a way completely analogous to the classical treatment. In this fashion the 'atomic level' of the quantum-mechanical theory will be reached.

The Weyl transforms of the field equations at the 'sub-atomic' level have been given in (73). They have the same form as the corresponding classical equations (I.1). Indeed, in the latter one may read, if one wishes so, the time derivations denoted by $c\partial_0$ or by a dot as the sum of a Poisson bracket with the Hamilton function (I.16) and an explicit time derivative. Since the Hamilton function (I.16) has the same form as the Weyl transform (61) of the quantum-mechanical Hamiltonian, the classical time derivation $c\partial_0$ (or the dot) acts on classical functions in exactly the same way as the operator $\partial_{t\mathrm{P}} \equiv c\partial_{0\mathrm{P}}$ (72) acts on Weyl transforms.

The right-hand sides of the Weyl transforms of the field equations may now be handled in the same way as the classical equations. In particular we expand the sources that are functions of $\boldsymbol{R}_i$ or, with a double indexing, of $\boldsymbol{R}_{ki}$ (k numbering the atoms, i their constituent particles) around a privileged coordinate $\boldsymbol{R}_k$ of atom k (e.g. one may take for $\boldsymbol{R}_k$ the Weyl transform of the position operator of the nucleus or the centre of mass). Then with the same mathematical steps as in the classical treatment, we obtain for the Weyl transforms of the field equations (cf. (I.35)):

$$\begin{aligned} \nabla \cdot \boldsymbol{e} &= \rho^{\mathrm{e}} - \nabla \cdot \boldsymbol{p}, \\ -\partial_{0\mathrm{P}} \boldsymbol{e} + \nabla \wedge \boldsymbol{b} &= c^{-1} \boldsymbol{j} + \partial_{0\mathrm{P}} \boldsymbol{p} + \nabla \wedge \boldsymbol{m}, \\ \nabla \cdot \boldsymbol{b} &= 0, \\ \partial_0 \boldsymbol{b} + \nabla \wedge \boldsymbol{e} &= 0, \end{aligned} \quad (84)$$

where ρ^{e} and $\boldsymbol{j}$ are given by (cf. (I.33))

$$\begin{aligned} \rho^{\mathrm{e}} &= \sum_k e_k \delta(\boldsymbol{R}_k - \boldsymbol{R}), \\ \boldsymbol{j} &= \sum_k e_k \boldsymbol{v}_k \delta(\boldsymbol{R}_k - \boldsymbol{R}) \end{aligned} \quad (85)$$

(with the abbreviation $\boldsymbol{v}_k \equiv \partial_{t\mathrm{P}} \boldsymbol{R}_k$, v. (72)) and where $\boldsymbol{p}$ and $\boldsymbol{m}$ are the series (cf. (I.34))[1]:

$$
\begin{aligned}
\boldsymbol{p} &= \sum_{n=1}^{\infty} (-1)^{n-1}\nabla^{n-1} : \sum_k \overline{\boldsymbol{\mu}}_k^{(n)} \delta(\boldsymbol{R}_k - \boldsymbol{R}), \\
\boldsymbol{m} &= \sum_{n=1}^{\infty} (-1)^{n-1}\nabla^{n-1} : \sum_k (\overline{\boldsymbol{\nu}}_k^{(n)} + c^{-1}\overline{\boldsymbol{\mu}}_k^{(n)} \wedge \boldsymbol{v}_k)\delta(\boldsymbol{R}_k - \boldsymbol{R}).
\end{aligned} \tag{86}
$$

In these formulae we used the abbreviations (cf. I.31–32):

$$
\begin{aligned}
\overline{\boldsymbol{\mu}}_k^{(n)} &= \frac{1}{n!} \sum_i e_{ki} \boldsymbol{r}_{ki}^n, \qquad (n = 1, 2, \ldots), \\
\overline{\boldsymbol{\nu}}_k^{(n)} &= \frac{n}{(n+1)!} \sum_i e_{ki} \boldsymbol{r}_{ki}^n \wedge (\partial_{0\mathrm{P}} \boldsymbol{r}_{ki}), \qquad (n = 1, 2, \ldots),
\end{aligned} \tag{87}
$$

with $\boldsymbol{r}_{ki} \equiv \boldsymbol{R}_{ki} - \boldsymbol{R}_k$.

Thanks to the use of Weyl transforms we did not need to give the derivations since formally they are exactly the same as in classical theory. There is one difference with classical theory connected with the convergence of the series expansion. In the classical theory we considered only those points $\boldsymbol{R}$ that are outside the atoms (i.e. for which $|\boldsymbol{R}_{ki} - \boldsymbol{R}_k| < |\boldsymbol{R}_k - \boldsymbol{R}|$), since only then the series expansion of the sources converges. In the quantum-mechanical treatment convergence is guaranteed under (formally) the same condition that $|\boldsymbol{R}_{ki} - \boldsymbol{R}_k| < |\boldsymbol{R}_k - \boldsymbol{R}|$. Here $\boldsymbol{R}_{ki}$ is a running variable, so that the condition means that the equations are only valid in part of phase space. If expectation values are taken, i.e. if integrals (52) over the Weyl transforms multiplied by a Wigner function are calculated, the condition gets the meaning that only points $\boldsymbol{R}$ may be considered which have the property that the Wigner function is negligible for phase space points $\boldsymbol{R}_{ki}$ that do not satisfy the inequality given above. The condition on $\boldsymbol{R}$ is thus the quantum-mechanical version of the classical condition that the observation point should be outside the atoms.

From the Weyl transform (84) of the field equations one may derive equations for expectation values. In fact by multiplying with a Wigner function and integrating over phase space one obtains, with the notation (52)

$$
\begin{aligned}
\nabla\cdot\overline{\boldsymbol{e}} &= \overline{\rho^{\mathrm{e}}} - \nabla\cdot\overline{\boldsymbol{p}}, \\
-\overline{\partial_{0\mathrm{P}}\boldsymbol{e}} + \nabla\wedge\overline{\boldsymbol{b}} &= c^{-1}\overline{\boldsymbol{j}} + \overline{\partial_{0\mathrm{P}}\boldsymbol{p}} + \nabla\wedge\overline{\boldsymbol{m}}, \\
\nabla\cdot\overline{\boldsymbol{b}} &= 0, \\
\overline{\partial_0\boldsymbol{b}} + \nabla\wedge\overline{\boldsymbol{e}} &= 0.
\end{aligned} \tag{88}
$$

[1] The bars over the symbols $\boldsymbol{\mu}$ and $\boldsymbol{\nu}$ indicate non-relativistic multipole moments, in the same fashion as in classical theory. They should not be confused with the symbol for expectation values.

Here the space derivations ∇ could be written before the symbols with the bar, since the Wigner function does not depend upon $\boldsymbol{R}$. Furthermore the time derivative in the fourth equation can also be written in the form of $\partial_0 \overline{\boldsymbol{b}}$, because $\overline{\boldsymbol{b}} = \boldsymbol{b} = \boldsymbol{B}_{\mathrm{e}}$, the external field in the present non-relativistic theory. It remains to discuss the quantities $\overline{\partial_{0\mathrm{P}}\boldsymbol{e}}$ and $\overline{\partial_{0\mathrm{P}}\boldsymbol{p}}$. Since both $\boldsymbol{e}$ and $\boldsymbol{p}$ are independent of the momenta (as follows from the first line of (86) for $\boldsymbol{p}$, and for $\boldsymbol{e}$ from the fact that it is the multipole expansion of the first line of (69)) and since moreover the Hamiltonian (61) is of second degree in the momenta, it follows from (60) that

$$
\begin{aligned}
\overline{\partial_{0\mathrm{P}}\boldsymbol{e}} &= \partial_0 \overline{\boldsymbol{e}}, \\
\overline{\partial_{0\mathrm{P}}\boldsymbol{p}} &= \partial_0 \overline{\boldsymbol{p}}.
\end{aligned} \tag{89}
$$

Therefore the atomic field equations (88) for the expectation values get the form

$$
\begin{aligned}
\nabla\cdot\overline{\boldsymbol{e}} &= \overline{\rho^{\mathrm{e}}} - \nabla\cdot\overline{\boldsymbol{p}}, \\
-\partial_0\overline{\boldsymbol{e}} + \nabla\wedge\overline{\boldsymbol{b}} &= c^{-1}\overline{\boldsymbol{j}} + \partial_0\overline{\boldsymbol{p}} + \nabla\wedge\overline{\boldsymbol{m}}, \\
\nabla\cdot\overline{\boldsymbol{b}} &= 0, \\
\partial_0\overline{\boldsymbol{b}} + \nabla\wedge\overline{\boldsymbol{e}} &= 0.
\end{aligned} \tag{90}
$$

These atomic equations contain at the right-hand side expectation values of operators of which the Weyl transforms have been given in (85) and (86). From (85) and (31) it follows that the operators corresponding to ρ^{e} and $\boldsymbol{j}$ are

$$
\begin{aligned}
\rho^{\mathrm{e}}_{\mathrm{op}} &= \sum_k e_k \delta(\boldsymbol{R}_{k,\mathrm{op}} - \boldsymbol{R}), \\
\boldsymbol{j}_{\mathrm{op}} &= \tfrac{1}{2} \sum_k e_k \{\boldsymbol{v}_{k,\mathrm{op}}, \delta(\boldsymbol{R}_{k,\mathrm{op}} - \boldsymbol{R})\},
\end{aligned} \tag{91}
$$

where the velocity operator $\boldsymbol{v}_{k,\mathrm{op}}$, which has the Weyl transform $\boldsymbol{v}_k \equiv \partial_{t\mathrm{P}}\boldsymbol{R}_k$, is equal to

$$
\boldsymbol{v}_{k,\mathrm{op}} = \frac{i}{\hbar}[H_{\mathrm{op}}, \boldsymbol{R}_{k,\mathrm{op}}] = \frac{1}{m_k} \sum_i \{\boldsymbol{P}_{ki,\mathrm{op}} - c^{-1} e_{ki} \boldsymbol{A}_{\mathrm{e}}(\boldsymbol{R}_{ki,\mathrm{op}}, t)\}, \tag{92}
$$

if one chooses the centre of mass as the central point, as follows from (44), (61) and (72). In view of the way in which the expectation values of these operators occur in the equations (90), they may be called the operators for the charge and current densities. Furthermore it follows from (86) and (31) that the operators corresponding to $\boldsymbol{p}$ and $\boldsymbol{m}$ are

$$
\begin{aligned}
\boldsymbol{p}_{\mathrm{op}} &= \sum_{n=1}^{\infty} (-1)^{n-1} \nabla^{n-1} : \sum_k \overline{\boldsymbol{\mu}}_{k,\mathrm{op}}^{(n)} \delta(\boldsymbol{R}_{k,\mathrm{op}} - \boldsymbol{R}), \\
\boldsymbol{m}_{\mathrm{op}} &= \tfrac{1}{2} \sum_{n=1}^{\infty} (-1)^{n-1} \nabla^{n-1} : \sum_k \{\overline{\boldsymbol{\nu}}_{k,\mathrm{op}}^{(n)} + \tfrac{1}{2} c^{-1} \{\overline{\boldsymbol{\mu}}_{k,\mathrm{op}}^{(n)} \wedge, \boldsymbol{v}_{k,\mathrm{op}}\}, \delta(\boldsymbol{R}_{k,\mathrm{op}} - \boldsymbol{R})\},
\end{aligned} \tag{93}
$$

which will be called the operators for the polarization densities. The atomic multipole moment operators that occur here are

$$
\begin{aligned}
\overline{\boldsymbol{\mu}}_{k,\mathrm{op}}^{(n)} &= \frac{1}{n!} \sum_i e_{ki} \boldsymbol{r}_{ki,\mathrm{op}}^n, \\
\overline{\boldsymbol{\nu}}_{k,\mathrm{op}}^{(n)} &= \tfrac{1}{2} c^{-1} \frac{n}{(n+1)!} \sum_i e_{ki} \{\boldsymbol{r}_{ki,\mathrm{op}}^n \wedge, \dot{\boldsymbol{r}}_{ki,\mathrm{op}}\},
\end{aligned} \tag{94}
$$

with the notation (3):

$$
\dot{\boldsymbol{r}}_{ki,\mathrm{op}} \equiv \frac{i}{\hbar} [H_{\mathrm{op}}, \boldsymbol{r}_{ki,\mathrm{op}}]. \tag{95}
$$

7 *The momentum and energy equations for composite particles*

a. *The equation of motion*

The starting point to derive the equation of motion for composite particles is the 'sub-atomic' equation (81). Again replacing the index i by a double index ki, where k numbers the atoms, and i their constituent particles, one finds after a summation over i

$$
m_k \partial_{tP}^2 \boldsymbol{R}_k = \sum_i e_{ki} \{\boldsymbol{e}_t(\boldsymbol{R}_{ki}, t) + (\partial_{0P} \boldsymbol{R}_{ki}) \wedge \boldsymbol{b}_t(\boldsymbol{R}_{ki}, t)\}, \tag{96}
$$

where we introduced the total mass $m_k = \sum_i m_{ki}$ of the atom and the Weyl transform $\boldsymbol{R}_k$ of the centre of mass operator

$$
\boldsymbol{R}_k = \sum_i m_{ki} \boldsymbol{R}_{ki} / m_k. \tag{97}
$$

Following the same procedure as in the classical theory we obtain from (96) for the atomic equation of motion (cf. (I.50) with (I.54) and (I.52)):

$$
m_k \partial_{tP} \boldsymbol{v}_k = \boldsymbol{f}_k^{\mathrm{L}} + \boldsymbol{f}_k^{\mathrm{S}} \tag{98}
$$

with the long range force

$$
\begin{aligned}
\boldsymbol{f}_k^{\mathrm{L}} = &- \sum_{l(\neq k)} \sum_{n,m=0}^{\infty} \overline{\boldsymbol{\mu}}_k^{(n)} : \nabla_k^n \overline{\boldsymbol{\mu}}_l^{(m)} : \nabla_l^m \nabla_k \frac{1}{4\pi |\boldsymbol{R}_k - \boldsymbol{R}_l|} \\
&+ e_k \{\boldsymbol{E}_{\mathrm{e}}(\boldsymbol{R}_k, t) + c^{-1} \boldsymbol{v}_k \wedge \boldsymbol{B}_{\mathrm{e}}(\boldsymbol{R}_k, t)\} + \{\nabla_k \boldsymbol{E}_{\mathrm{e}}(\boldsymbol{R}_k, t)\} \cdot \overline{\boldsymbol{\mu}}_k^{(1)} \\
&+ \{\nabla_k \boldsymbol{B}_{\mathrm{e}}(\boldsymbol{R}_k, t)\} \cdot (\overline{\boldsymbol{\nu}}_k^{(1)} + c^{-1} \overline{\boldsymbol{\mu}}_k^{(1)} \wedge \boldsymbol{v}_k) + \partial_{0P} \{\overline{\boldsymbol{\mu}}_k^{(1)} \wedge \boldsymbol{B}_{\mathrm{e}}(\boldsymbol{R}_k, t)\},
\end{aligned} \tag{99}
$$

and the short range force:

$$
\begin{aligned}
\boldsymbol{f}_k^{\mathrm{S}} = &- \sum_{l(\neq k)i,j} \nabla_{ki} \frac{e_{ki} e_{lj}}{4\pi |\boldsymbol{R}_{ki} - \boldsymbol{R}_{lj}|} \\
&+ \sum_{l(\neq k)} \sum_{n,m=0}^{\infty} \overline{\boldsymbol{\mu}}_k^{(n)} : \nabla_k^n \overline{\boldsymbol{\mu}}_l^{(m)} : \nabla_l^m \nabla_k \frac{1}{4\pi |\boldsymbol{R}_k - \boldsymbol{R}_l|}.
\end{aligned} \tag{100}
$$

Here ∂_{0P} and ∂_{tP} have been defined in (72), while $\boldsymbol{v}_k$ stands for $\partial_{tP} \boldsymbol{R}_k$. Furthermore the multipole moments $\overline{\boldsymbol{\mu}}_k$ and $\overline{\boldsymbol{\nu}}_k$, defined in (87), occur.

Thus it turns out that the Weyl transform (98) of the quantum-mechanical equation of motion has the same form as the classical equation with time derivatives replaced by the derivatives of the type (72). The latter contain the sum of an explicit derivative and the Poisson bracket with the Weyl transform of the Hamiltonian.

From (98) one finds an equation for the expectation values by multiplying with a Wigner function and integrating over phase space. Then, with the notation (52), one obtains

$$
m_k \overline{\partial_{tP} \boldsymbol{v}_k} = \overline{\boldsymbol{f}_k^{\mathrm{L}}} + \overline{\boldsymbol{f}_k^{\mathrm{S}}}. \tag{101}
$$

From the form of the Weyl transform of the Hamiltonian (61), the definition $\boldsymbol{v}_k \equiv \partial_{tP} \boldsymbol{R}_k$ (with ∂_{tP} defined in (72)), it follows with the expression (80) for the sine symbol that

$$
\partial_{tP} \boldsymbol{v}_k = \sin(\boldsymbol{v}_k; H) + \frac{\partial \boldsymbol{v}_k}{\partial t}. \tag{102}
$$

Then with (60) we get for the equation (101)

$$
m_k \frac{\mathrm{d} \overline{\boldsymbol{v}}_k}{\mathrm{d} t} = \overline{\boldsymbol{f}_k^{\mathrm{L}}} + \overline{\boldsymbol{f}_k^{\mathrm{S}}}. \tag{103}
$$

At the left-hand side the time derivative of the expectation value of the velocity operator $\boldsymbol{v}_{k,\mathrm{op}}$ (92) appears, with $\boldsymbol{R}_{k,\mathrm{op}}$ the operator that has the Weyl transform $\boldsymbol{R}_k$, i.e. the right-hand side of (97) with $\boldsymbol{R}_{ki,\mathrm{op}}$ for $\boldsymbol{R}_{ki}$. Furthermore, at the right-hand side the expectation values of the operators that have the Weyl transforms (99) and (100) occur.

b. *The energy equation*

By scalar multiplication of the Weyl transformed equation of motion (81) (where i is to be replaced by ki) by the quantity $\partial_{tP}\boldsymbol{R}_{ki}$ one finds after summation over i:

$$\sum_i \tfrac{1}{2}m_{ki}\,\partial_{tP}\{(\partial_{tP}\boldsymbol{R}_{ki})^2\} = \sum_i e_{ki}\,\boldsymbol{e}_t(\boldsymbol{R}_{ki},t)\cdot(\partial_{tP}\boldsymbol{R}_{ki}). \tag{104}$$

With the same steps as have been taken to obtain the classical atomic energy equation we get then (cf. (I.63) with (I.65–66)):

$$\partial_{tP}\left\{\tfrac{1}{2}m_k\,\boldsymbol{v}_k^2+\tfrac{1}{2}\sum_i m_{ki}(\partial_{tP}\boldsymbol{r}_{ki})^2+\sum_{i,j(i\neq j)}\frac{e_{ki}e_{kj}}{8\pi|\boldsymbol{r}_{ki}-\boldsymbol{r}_{kj}|}\right\} = \psi_k^{\mathrm{L}}+\psi_k^{\mathrm{S}} \tag{105}$$

with two terms representing work exerted on the composite particle per unit of time: a long range term

$$\begin{aligned}\psi_k^{\mathrm{L}} = &-\sum_{l(\neq k)}\sum_{m=0}^{\infty}\Big\{\sum_{n=0}^{\infty}\bar{\boldsymbol{\mu}}_k^{(n)}\,\vdots\,\boldsymbol{\nabla}_k^n\boldsymbol{v}_k\cdot\boldsymbol{\nabla}_k+\sum_{n=1}^{\infty}(\partial_{tP}\bar{\boldsymbol{\mu}}_k^{(n)})\,\vdots\,\boldsymbol{\nabla}_k^n\Big\}\\ &\bar{\boldsymbol{\mu}}_l^{(m)}\,\vdots\,\boldsymbol{\nabla}_l^m\frac{1}{4\pi|\boldsymbol{R}_k-\boldsymbol{R}_l|}+e_k\,\boldsymbol{v}_k\cdot\boldsymbol{E}_e(\boldsymbol{R}_k,t)+\boldsymbol{v}_k\cdot\{\boldsymbol{\nabla}_k\boldsymbol{E}_e(\boldsymbol{R}_k,t)\}\cdot\bar{\boldsymbol{\mu}}_k^{(1)}\\ &+(\partial_{tP}\bar{\boldsymbol{\mu}}_k^{(1)})\cdot\boldsymbol{E}_e(\boldsymbol{R}_k,t)-(\bar{\boldsymbol{v}}_k^{(1)}+c^{-1}\bar{\boldsymbol{\mu}}_k^{(1)}\wedge\boldsymbol{v}_k)\cdot\frac{\partial\boldsymbol{B}_e(\boldsymbol{R}_k,t)}{\partial t},\end{aligned} \tag{106}$$

and a short range term

$$\begin{aligned}\psi_k^{\mathrm{S}} = &-\sum_{l(\neq k)i,j}(\partial_{tP}\boldsymbol{R}_{ki})\cdot\boldsymbol{\nabla}_{ki}\frac{e_{ki}e_{lj}}{4\pi|\boldsymbol{R}_{ki}-\boldsymbol{R}_{lj}|}\\ &+\sum_{l(\neq k)}\sum_{m=0}^{\infty}\Big\{\sum_{n=0}^{\infty}\bar{\boldsymbol{\mu}}_k^{(n)}\,\vdots\,\boldsymbol{\nabla}_k^n\boldsymbol{v}_k\cdot\boldsymbol{\nabla}_k+\sum_{n=1}^{\infty}(\partial_{tP}\bar{\boldsymbol{\mu}}_k^{(n)})\,\vdots\,\boldsymbol{\nabla}_k^n\Big\}\\ &\bar{\boldsymbol{\mu}}_l^{(m)}\,\vdots\,\boldsymbol{\nabla}_l^m\frac{1}{4\pi|\boldsymbol{R}_k-\boldsymbol{R}_l|},\end{aligned} \tag{107}$$

with $\boldsymbol{v}_k = \partial_{tP}\boldsymbol{R}_k$ and $\partial_{0P} = c^{-1}\partial_{tP}$ defined by (72). Again formally this result is the same as that of the classical theory.

The corresponding equation for expectation values may be obtained from (105) by multiplying with a Wigner function and integrating over phase space. Then with the help of (60), (61), (72) and (80) one finds:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\{\tfrac{1}{2}m_k\,\overline{\boldsymbol{v}_k^2}+\tfrac{1}{2}\sum_i m_{ki}\overline{(\partial_{tP}\boldsymbol{r}_{ki})^2}+\sum_{i,j(i\neq j)}\overline{\frac{e_{ki}e_{kj}}{8\pi|\boldsymbol{R}_{ki}-\boldsymbol{R}_{kj}|}}\right\} = \overline{\psi_k^{\mathrm{L}}}+\overline{\psi_k^{\mathrm{S}}}, \tag{108}$$

where the notation (52) has been employed. Since $\boldsymbol{v}_k$ is the Weyl transform

of $\boldsymbol{v}_{k,\mathrm{op}}$ given by (92) and $\partial_{tP}\boldsymbol{r}_{ki}$ is the Weyl transform of $\dot{\boldsymbol{r}}_{ki,\mathrm{op}}$ given by (95), one obtains with the help of (43) that the left-hand side contains the expectation values of the kinetic energy operator $\frac{1}{2}m_k\,\boldsymbol{v}_{k,\mathrm{op}}^2$, the internal kinetic energy operator $\frac{1}{2}\sum_i m_{ki}\dot{\boldsymbol{r}}_{ki,\mathrm{op}}^2$ and the internal Coulomb energy operator. At the right-hand side the expectation values of two operators appear of which the Weyl transforms are (106) and (107).

8 *The inner angular momentum equation for composite particles*

By vectorial multiplication of the Weyl transformed equation of motion (81) (with i replaced by ki) with $\boldsymbol{r}_{ki} \equiv \boldsymbol{R}_{ki}-\boldsymbol{R}_k$, one finds with the help of (97) and a summation over i:

$$\partial_{tP}\,\bar{\boldsymbol{s}}_k = \sum_i e_{ki}\,\boldsymbol{r}_{ki}\wedge\{\boldsymbol{e}_t(\boldsymbol{R}_{ki},t)+(\partial_{0P}\boldsymbol{R}_{ki})\wedge\boldsymbol{b}_t(\boldsymbol{R}_{ki},t)\}, \tag{109}$$

where we introduced the quantity[1]

$$\bar{\boldsymbol{s}}_k \equiv \sum_i m_{ki}\,\boldsymbol{r}_{ki}\wedge(\partial_{tP}\boldsymbol{r}_{ki}). \tag{110}$$

Just as in the classical case one finds from this equation (cf. (I.76) with (I.77–78))

$$\partial_{tP}\,\bar{\boldsymbol{s}}_k = \boldsymbol{d}_k^{\mathrm{L}}+\boldsymbol{d}_k^{\mathrm{S}} \tag{111}$$

with the long range moment

$$\begin{aligned}\boldsymbol{d}_k^{\mathrm{L}} = &\sum_{l(\neq k)}\sum_{n,m=0}^{\infty} n\boldsymbol{\nabla}_k\wedge\bar{\boldsymbol{\mu}}_k^{(n)}\,\vdots\,\boldsymbol{\nabla}_k^{n-1}\bar{\boldsymbol{\mu}}_l^{(m)}\,\vdots\,\boldsymbol{\nabla}_l^m\frac{1}{4\pi|\boldsymbol{R}_k-\boldsymbol{R}_l|}\\ &+\bar{\boldsymbol{\mu}}_k^{(1)}\wedge\{\boldsymbol{E}_e(\boldsymbol{R}_k,t)+c^{-1}\boldsymbol{v}_k\wedge\boldsymbol{B}_e(\boldsymbol{R}_k,t)\}+\bar{\boldsymbol{v}}_k^{(1)}\wedge\boldsymbol{B}_e(\boldsymbol{R}_k,t)\end{aligned} \tag{112}$$

and the short range moment

$$\begin{aligned}\boldsymbol{d}_k^{\mathrm{S}} = &-\sum_{l(\neq k)i,j}\boldsymbol{r}_{ki}\wedge\boldsymbol{\nabla}_{ki}\frac{e_{ki}e_{lj}}{4\pi|\boldsymbol{R}_{ki}-\boldsymbol{R}_{lj}|}\\ &-\sum_{l(\neq k)}\sum_{n,m=0}^{\infty} n\boldsymbol{\nabla}_k\wedge\bar{\boldsymbol{\mu}}_k^{(n)}\,\vdots\,\boldsymbol{\nabla}_k^{n-1}\bar{\boldsymbol{\mu}}_l^{(m)}\,\vdots\,\boldsymbol{\nabla}_l^m\frac{1}{4\pi|\boldsymbol{R}_k-\boldsymbol{R}_l|},\end{aligned} \tag{113}$$

with $\boldsymbol{v}_k = \partial_{tP}\boldsymbol{R}_k$ and $\partial_{0P} = c^{-1}\partial_{tP}$ defined in (72).

[1] The bar denotes a non-relativistic quantity, not an expectation value.

Multiplying (111) by a Wigner function and integrating over phase space one obtains

$$\overline{\partial_{tP}\bar{s}_k} = \overline{d_k^L} + \overline{d_k^S}, \tag{114}$$

where the notation (52) has been employed. With the help of (60), (61), (72), (80) and (110) we get for this equation

$$\frac{d\overline{\bar{s}_k}}{dt} = \overline{d_k^L} + \overline{d_k^S}. \tag{115}$$

At the left-hand side the time derivative of the expectation value of the operator $\bar{s}_{k,\text{op}}$ for the internal angular momentum, with Weyl transform (110), occurs, while the right-hand side contains the expectation values of two operators for long and short range moments of which the Weyl transforms have been given in (112) and (113).

The field equations and the equation of motion for composite particles, as well as the ensuing energy and angular momentum equations, were obtained from the equations for point particles in formally the same fashion as in the classical treatment. This could be achieved because already at the sub-atomic level we translated the quantum-mechanical operator equations into their Weyl transforms. Therefore at this stage it becomes apparent that a transcription which leads away from the usual operator language gives rise to considerable formal simplification since *mutatis mutandis* the classical derivation may be taken over as such.

APPENDIX

Properties of the Weyl transformation and the Wigner function

1. *A reformulation of quantum mechanics*

In the usual formulation of quantum mechanics one associates a vector in Hilbert space to each state of the system and to each physical quantity an operator acting in this Hilbert space. It is possible however to give an alternative description of quantum mechanics by using only ordinary functions in phase space for both the states and the physical quantities. An example of such an approach consists in introducing Weyl transforms instead of operators, and simultaneously the Wigner function instead of the state vector.

This programme will be carried out in the following appendix for a one-particle system. The reason for this limitation is merely to reduce slightly the length of the formulae. Indeed if N-particle systems are considered indices that label the particles and summation signs have to be added.

2. *The Weyl transformation*

a. *Preliminaries*

A few notions of ordinary quantum mechanics will be summarized here for use in the following. The momentum and coordinate operators[1] $\boldsymbol{P}$ and $\boldsymbol{Q}$ for a single point particle satisfy the commutation relations

$$[\boldsymbol{P}, \boldsymbol{P}] = 0, \qquad [\boldsymbol{Q}, \boldsymbol{Q}] = 0, \qquad [\boldsymbol{P}, \boldsymbol{Q}] = \frac{\hbar}{i}\,\mathbf{U}I, \tag{A1}$$

with $\mathbf{U}$ the unit three-tensor and I the unit operator in Hilbert space. Their eigenvectors $|\boldsymbol{p}\rangle$ and $|\boldsymbol{q}\rangle$, defined by the eigenvalue equations

$$\boldsymbol{P}|\boldsymbol{p}\rangle = \boldsymbol{p}|\boldsymbol{p}\rangle, \qquad \boldsymbol{Q}|\boldsymbol{q}\rangle = \boldsymbol{q}|\boldsymbol{q}\rangle, \tag{A2}$$

[1] Throughout this appendix we use capitals to denote operators and lower case symbols for ordinary numbers.

satisfy completeness relations

$$\int \mathrm{d}\boldsymbol{p}|\boldsymbol{p}\rangle\langle\boldsymbol{p}| = I, \qquad \int \mathrm{d}\boldsymbol{q}|\boldsymbol{q}\rangle\langle\boldsymbol{q}| = I \tag{A3}$$

and inner product relations

$$\langle\boldsymbol{p}|\boldsymbol{p}'\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}'), \qquad \langle\boldsymbol{q}|\boldsymbol{q}'\rangle = \delta(\boldsymbol{q}-\boldsymbol{q}'), \qquad \langle\boldsymbol{q}|\boldsymbol{p}\rangle = \frac{1}{h^{\frac{3}{2}}}\,\mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{q}}. \tag{A4}$$

The trace of an operator may be expressed in terms of the complete sets $|\boldsymbol{p}\rangle$ or $|\boldsymbol{q}\rangle$ as

$$\mathrm{Tr}\,A = \int \mathrm{d}\boldsymbol{p}\langle\boldsymbol{p}|A|\boldsymbol{p}\rangle = \int \mathrm{d}\boldsymbol{q}\langle\boldsymbol{q}|A|\boldsymbol{q}\rangle. \tag{A5}$$

b. *Definition*[1]

The Weyl transform of a quantum-mechanical operator A for a single point particle is a scalar function $a(\boldsymbol{p}, \boldsymbol{q})$ defined as

$$a(\boldsymbol{p}, \boldsymbol{q}) = \int \mathrm{d}\boldsymbol{u}\,\mathrm{e}^{(i/\hbar)\boldsymbol{q}\cdot\boldsymbol{u}}\langle\boldsymbol{p}+\tfrac{1}{2}\boldsymbol{u}|A|\boldsymbol{p}-\tfrac{1}{2}\boldsymbol{u}\rangle, \tag{A6}$$

where $|\boldsymbol{p}\rangle$ is the eigenvector of the momentum operator with eigenvalue $\boldsymbol{p}$. Alternatively one may write

$$a(\boldsymbol{p}, \boldsymbol{q}) = \int \mathrm{d}\boldsymbol{v}\,\mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}}\langle\boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}|A|\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}\rangle, \tag{A7}$$

where $|\boldsymbol{q}\rangle$ is the eigenvector of the coordinate operator with eigenvalue $\boldsymbol{q}$. From (A6) or (A7) it follows that the Weyl transform $a(\boldsymbol{p}, \boldsymbol{q})$ is real if the operator A is hermitian.

The operator A reads, in terms of the Weyl transform:

$$A = h^{-3}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\,a(\boldsymbol{p}, \boldsymbol{q})\Delta(\boldsymbol{p}, \boldsymbol{q}), \tag{A8}$$

where the hermitian operator $\Delta(\boldsymbol{p}, \boldsymbol{q})$ is defined as

$$\Delta(\boldsymbol{p}, \boldsymbol{q}) = h^{-3}\int \mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\,\mathrm{e}^{(i/\hbar)\{(\boldsymbol{q}-\boldsymbol{Q})\cdot\boldsymbol{u}+(\boldsymbol{p}-\boldsymbol{P})\cdot\boldsymbol{v}\}} \tag{A9}$$

[1] The derivations of (A6–A14) and of (A54) have been given in § 3 and will not be repeated here.

or alternatively as

$$\Delta(\boldsymbol{p}, \boldsymbol{q}) = \int \mathrm{d}\boldsymbol{u}\,\mathrm{e}^{(i/\hbar)\boldsymbol{q}\cdot\boldsymbol{u}}|\boldsymbol{p}-\tfrac{1}{2}\boldsymbol{u}\rangle\langle\boldsymbol{p}+\tfrac{1}{2}\boldsymbol{u}|, \tag{A10}$$

$$\Delta(\boldsymbol{p}, \boldsymbol{q}) = \int \mathrm{d}\boldsymbol{v}\,\mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}}|\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}\rangle\langle\boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}|. \tag{A11}$$

The Weyl transform may also be written as a trace involving this operator $\Delta(\boldsymbol{p}, \boldsymbol{q})$

$$a(\boldsymbol{p}, \boldsymbol{q}) = \mathrm{Tr}\,\{A\Delta(\boldsymbol{p}, \boldsymbol{q})\}. \tag{A12}$$

A different formulation of the Weyl correspondence consists in giving both the operator and the Weyl transform as a Fourier integral

$$A = \int \mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\,\tilde{a}(\boldsymbol{u}, \boldsymbol{v})\mathrm{e}^{-(i/\hbar)(\boldsymbol{Q}\cdot\boldsymbol{u}+\boldsymbol{P}\cdot\boldsymbol{v})}, \tag{A13}$$

$$a(\boldsymbol{p}, \boldsymbol{q}) = \int \mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\,\tilde{a}(\boldsymbol{u}, \boldsymbol{v})\mathrm{e}^{-(i/\hbar)(\boldsymbol{q}\cdot\boldsymbol{u}+\boldsymbol{p}\cdot\boldsymbol{v})}, \tag{A14}$$

with the same function $\tilde{a}(\boldsymbol{u}, \boldsymbol{v})$ in both integrands.

A still different way to get the Weyl transform $a(\boldsymbol{p}, \boldsymbol{q})$ from the operator A is obtained by starting from (A12) with (A9). Application of the identity

$$\mathrm{e}^{A+B} = \mathrm{e}^{A}\mathrm{e}^{B}\mathrm{e}^{-\frac{1}{2}[A,B]} \tag{A15}$$

for operators A and B that commute with their commutator (v. problem 1) yields with the help of (A5) and (A2)

$$a(\boldsymbol{p}, \boldsymbol{q}) = \frac{1}{h^3}\int \mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\,\mathrm{d}\boldsymbol{p}'\,\mathrm{d}\boldsymbol{q}'\,\exp\left(-\frac{i}{2\hbar}\,\boldsymbol{u}\cdot\boldsymbol{v}\right)\exp\left[\frac{i}{\hbar}\,\{(\boldsymbol{p}-\boldsymbol{p}')\cdot\boldsymbol{v}+(\boldsymbol{q}-\boldsymbol{q}')\cdot\boldsymbol{u}\}\right] \langle\boldsymbol{q}'|A|\boldsymbol{p}'\rangle\langle\boldsymbol{p}'|\boldsymbol{q}'\rangle. \tag{A16}$$

The product $\boldsymbol{u}\cdot\boldsymbol{v}$ in the first exponent may be replaced by $-\hbar^2(\partial/\partial\boldsymbol{p}')\cdot(\partial/\partial\boldsymbol{q}')$ acting on the second exponential, or, by partial integration, by the same operator acting on the rest of the integrand. The integration over $\boldsymbol{u}$ and $\boldsymbol{v}$ then yields delta functions, so that the integration over $\boldsymbol{p}'$ and $\boldsymbol{q}'$ may also be performed, with the result

$$a(\boldsymbol{p}, \boldsymbol{q}) = h^3\exp\left(-\frac{\hbar}{2i}\,\frac{\partial}{\partial\boldsymbol{p}}\cdot\frac{\partial}{\partial\boldsymbol{q}}\right)\langle\boldsymbol{q}|A|\boldsymbol{p}\rangle\langle\boldsymbol{p}|\boldsymbol{q}\rangle, \tag{A17}$$

or alternatively, if the roles of $\boldsymbol{p}$ and $\boldsymbol{q}$ are interchanged in the proof,

$$a(\boldsymbol{p}, \boldsymbol{q}) = h^3\exp\left(\frac{\hbar}{2i}\,\frac{\partial}{\partial\boldsymbol{p}}\cdot\frac{\partial}{\partial\boldsymbol{q}}\right)\langle\boldsymbol{p}|A|\boldsymbol{q}\rangle\langle\boldsymbol{q}|\boldsymbol{p}\rangle. \tag{A18}$$

Finding the operator A from the Weyl transform $a(\boldsymbol{p}, \boldsymbol{q})$ is in principle possible from the formulae (A8) with (A9), (A10) or (A11), or otherwise from (A13) with (A14). A method which is often more convenient will be indicated now. From (A8) with (A9) and the identity (A15) it follows that

$$A = \frac{1}{h^6}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\,\mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\, a(\boldsymbol{p}, \boldsymbol{q})\mathrm{e}^{(i/\hbar)(\boldsymbol{q}-\boldsymbol{Q})\cdot\boldsymbol{u}}\mathrm{e}^{(i/\hbar)(\boldsymbol{p}-\boldsymbol{P})\cdot\boldsymbol{v}}\mathrm{e}^{(i/2\hbar)\boldsymbol{u}\cdot\boldsymbol{v}}. \quad \text{(A19)}$$

Again the product $\boldsymbol{u}\cdot\boldsymbol{v}$ may be replaced by $-\hbar^2(\partial/\partial\boldsymbol{p})\cdot(\partial/\partial\boldsymbol{q})$ acting on the first two exponentials, or, after a partial integration, by the same operator acting on $a(\boldsymbol{p}, \boldsymbol{q})$, so that one has, after integration over $\boldsymbol{u}$ and $\boldsymbol{v}$,

$$A = \int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\,\delta(\boldsymbol{q}-\boldsymbol{Q})\delta(\boldsymbol{p}-\boldsymbol{P})a_0(\boldsymbol{p}, \boldsymbol{q}) \quad \text{(A20)}$$

with

$$a_0(\boldsymbol{p}, \boldsymbol{q}) \equiv \exp\left(\frac{\hbar}{2i}\frac{\partial}{\partial\boldsymbol{p}}\cdot\frac{\partial}{\partial\boldsymbol{q}}\right)a(\boldsymbol{p}, \boldsymbol{q}). \quad \text{(A21)}$$

These formulae show that one may find the operator A from its Weyl transform $a(\boldsymbol{p}, \boldsymbol{q})$ by calculating first $a_0(\boldsymbol{p}, \boldsymbol{q})$ from (A21) and then replacing the variables $\boldsymbol{q}$ and $\boldsymbol{p}$ by the operators $\boldsymbol{Q}$ and $\boldsymbol{P}$, always writing the coordinate operators at the left of the momentum operators. This shows that the procedure is only convenient if one has to do with binomials of $\boldsymbol{P}$ and $\boldsymbol{Q}$.

The Weyl transform $a(\boldsymbol{p}, \boldsymbol{q})$ of a quantum-mechanical operator A may be employed to find the function in classical mechanics that corresponds to the operator A. This function is in general not simply the Weyl transform itself (since the latter depends in general on Planck's constant $\hbar$), but is obtained if one takes the limit for $\hbar \to 0$:

$$A \overset{\mathrm{cl}}{\to} a_{\mathrm{cl}}(\boldsymbol{p}, \boldsymbol{q}) = \lim_{\hbar\to 0} a(\boldsymbol{p}, \boldsymbol{q}). \quad \text{(A22)}$$

c. *Examples*

One often encounters physical operators of which the Weyl transforms are of the form

$$a(p, q) = f(q)p^n \quad \text{(A23)}$$

with f an arbitrary function and n a natural number (for convenience we limit ourselves to the one-dimensional case in this subsection). Application of (A21) gives

$$a_0(p, q) = \sum_{k=0}^{n}\binom{n}{k}\left(\frac{\hbar}{2i}\right)^k \frac{\mathrm{d}^k f(q)}{\mathrm{d}q^k}\, p^{n-k}. \quad \text{(A24)}$$

Hence according to (A20) the corresponding operator is

$$A = \sum_{k=0}^{n}\binom{n}{k}\left(\frac{\hbar}{2i}\right)^k \frac{\mathrm{d}^k f(Q)}{\mathrm{d}Q^k}\, P^{n-k}. \quad \text{(A25)}$$

The result may be cast into the form:

$$A = \frac{1}{2^n}\sum_{k=0}^{n}\binom{n}{k} P^k f(Q) P^{n-k}, \quad \text{(A26)}$$

as may be seen in the following way. From the commutation relations (A1) one finds

$$P^k f(Q) = \sum_{j=0}^{k}\left(\frac{\hbar}{i}\right)^j \binom{k}{j} \frac{\mathrm{d}^j f(Q)}{\mathrm{d}Q^j}\, P^{k-j}. \quad \text{(A27)}$$

Inserting this expression into (A26) and using the identities

$$\binom{n}{k}\binom{k}{j} = \binom{n}{j}\binom{n-j}{k-j}, \qquad \frac{1}{2^m}\sum_{n=0}^{m}\binom{m}{n} = 1, \quad \text{(A28)}$$

one recovers indeed (A25), so that we have established the Weyl correspondence

$$f(q)p^n \rightleftarrows \frac{1}{2^n}\sum_{k=0}^{n}\binom{n}{k} P^k f(Q) P^{n-k}. \quad \text{(A29)}$$

It may also be formulated in terms of repeated anticommutators:

$$f(q)p^n \rightleftarrows \frac{1}{2^n}\{\{\ldots\{f(Q), P\}, P\}, \ldots, P\}. \quad \text{(A30)}$$

Special cases are for instance

$$p \rightleftarrows P, \quad \text{(A31)}$$

$$q \rightleftarrows Q, \quad \text{(A32)}$$

$$pq \rightleftarrows \tfrac{1}{2}(PQ+QP), \quad \text{(A33)}$$

$$p^2 q \rightleftarrows \tfrac{1}{4}(QP^2+2PQP+P^2Q), \quad \text{(A34)}$$

$$p^2 q^2 \rightleftarrows \tfrac{1}{4}(Q^2P^2+2PQ^2P+P^2Q^2). \quad \text{(A35)}$$

d. *The Δ-operator*

The Δ-operator (A9), (A10) or (A11) has as Weyl transform a product of delta functions as follows from (A8):

$$\Delta(\boldsymbol{p}', \boldsymbol{q}') \rightleftarrows h^3 \delta(\boldsymbol{p}-\boldsymbol{p}')\delta(\boldsymbol{q}-\boldsymbol{q}'). \tag{A36}$$

Its matrix elements between eigenvectors of the coordinate and momentum operators follow with (A10), (A11) and (A4)

$$\langle \boldsymbol{q}'|\Delta(\boldsymbol{p}, \boldsymbol{q})|\boldsymbol{q}''\rangle = \delta\left(\boldsymbol{q} - \frac{\boldsymbol{q}'+\boldsymbol{q}''}{2}\right) \mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot(\boldsymbol{q}'-\boldsymbol{q}'')}, \tag{A37}$$

$$\langle \boldsymbol{p}'|\Delta(\boldsymbol{p}, \boldsymbol{q})|\boldsymbol{p}''\rangle = \delta\left(\boldsymbol{p} - \frac{\boldsymbol{p}'+\boldsymbol{p}''}{2}\right) \mathrm{e}^{-(i/\hbar)\boldsymbol{q}\cdot(\boldsymbol{p}'-\boldsymbol{p}'')}. \tag{A38}$$

In particular the diagonal elements are

$$\langle \boldsymbol{q}'|\Delta(\boldsymbol{p}, \boldsymbol{q})|\boldsymbol{q}'\rangle = \delta(\boldsymbol{q}-\boldsymbol{q}'), \tag{A39}$$

$$\langle \boldsymbol{p}'|\Delta(\boldsymbol{p}, \boldsymbol{q})|\boldsymbol{p}'\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}'). \tag{A40}$$

Mixed matrix elements are found by using (A17) for $A = \Delta(\boldsymbol{p}', \boldsymbol{q}')$. Then with (A36) and (A4) one finds

$$\langle \boldsymbol{q}'|\Delta(\boldsymbol{p}, \boldsymbol{q})|\boldsymbol{p}'\rangle = \exp\left(\frac{i}{\hbar}\, \boldsymbol{p}'\cdot\boldsymbol{q}'\right) \exp\left(\frac{\hbar}{2i}\, \frac{\partial}{\partial \boldsymbol{p}} \cdot \frac{\partial}{\partial \boldsymbol{q}}\right) \delta(\boldsymbol{p}-\boldsymbol{p}')\delta(\boldsymbol{q}-\boldsymbol{q}'). \tag{A41}$$

Integration of the Δ-operator (A11) or (A10) over $\boldsymbol{p}$ or $\boldsymbol{q}$ respectively yields

$$\int \mathrm{d}\boldsymbol{p}\, \Delta(\boldsymbol{p}, \boldsymbol{q}) = h^3 |\boldsymbol{q}\rangle\langle \boldsymbol{q}|, \tag{A42}$$

$$\int \mathrm{d}\boldsymbol{q}\, \Delta(\boldsymbol{p}, \boldsymbol{q}) = h^3 |\boldsymbol{p}\rangle\langle \boldsymbol{p}|, \tag{A43}$$

i.e. projection operators on a particular member of the complete set of eigenvectors of the coordinate and momentum operators. A second integration yields according to the closure relations (A3)

$$h^{-3}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\, \Delta(\boldsymbol{p}, \boldsymbol{q}) = I. \tag{A44}$$

The trace of a product of Δ-operators has different general forms for an even and an odd number of factors[1]:

$$\mathrm{Tr}\,\{\Delta(\boldsymbol{p}_1, \boldsymbol{q}_1) \dots \Delta(\boldsymbol{p}_n, \boldsymbol{q}_n)\}$$
$$= 2^{3(n-1)} \exp\left\{\frac{2i}{\hbar} \sum_{j,k=1(j<k)}^{n} (-1)^{j+k}(\boldsymbol{p}_j\cdot\boldsymbol{q}_k - \boldsymbol{p}_k\cdot\boldsymbol{q}_j)\right\}, \qquad (n \text{ odd}), \tag{A45}$$

[1] R. L. Stratonovich, Soviet Phys. JETP 4(1957)891.

$$\mathrm{Tr}\,\{\Delta(\boldsymbol{p}_1, \boldsymbol{q}_1) \dots \Delta(\boldsymbol{p}_n, \boldsymbol{q}_n)\}$$
$$= h^3\delta(\boldsymbol{p}_1 - \boldsymbol{p}_2 + \dots - \boldsymbol{p}_n)\delta(\boldsymbol{q}_1 - \boldsymbol{q}_2 + \dots - \boldsymbol{q}_n)$$
$$\mathrm{Tr}\,\{\Delta(\boldsymbol{p}_1, \boldsymbol{q}_1) \dots \Delta(\boldsymbol{p}_{n-1}, \boldsymbol{q}_{n-1})\}, \qquad (n \text{ even}), \tag{A46}$$

Proof: With (A5), insertion of complete sets $|\boldsymbol{q}_i'\rangle$ $(i = 2, \dots, n)$ by means of (A3) and the use of (A37) we may write the left-hand side of (A45) or (A46) as

$$\int \mathrm{d}\boldsymbol{q}_1' \dots \mathrm{d}\boldsymbol{q}_n'\, \delta\left(\boldsymbol{q}_1 - \frac{\boldsymbol{q}_1'+\boldsymbol{q}_2'}{2}\right) \dots \delta\left(\boldsymbol{q}_n - \frac{\boldsymbol{q}_n'+\boldsymbol{q}_1'}{2}\right)$$
$$\exp\left[\frac{i}{\hbar}\{\boldsymbol{p}_1\cdot(\boldsymbol{q}_1'-\boldsymbol{q}_2') + \dots \boldsymbol{p}_n\cdot(\boldsymbol{q}_n'-\boldsymbol{q}_1')\}\right]. \tag{A47}$$

It is convenient to introduce as new integration variables $\boldsymbol{q}_i'' = \frac{1}{2}(\boldsymbol{q}_i'+\boldsymbol{q}_{i+1}')$ with $i = 1, \dots, n$ $(\boldsymbol{q}_{n+1}' \equiv \boldsymbol{q}_1')$. The Jacobian of this transformation is equal to $2^{-3(n-1)}$ for n = odd and 0 for n = even. Therefore the proof continues for n = odd only. In that case we obtain, writing also the exponential in terms of the new variables and performing the integrations, the right-hand side of (A45).

To find the result for n even we use formula (A45) for $n+1$, and formula (A44) to write

$$\mathrm{Tr}\,\{\Delta(\boldsymbol{p}_1, \boldsymbol{q}_1) \dots \Delta(\boldsymbol{p}_n, \boldsymbol{q}_n)\}$$
$$= \left(\frac{2^n}{h}\right)^3 \int \mathrm{d}\boldsymbol{p}_{n+1}\,\mathrm{d}\boldsymbol{q}_{n+1} \exp\left[\frac{2i}{\hbar}\{ \sum_{j,k=1(j<k)}^{n} (-1)^{j+k}(\boldsymbol{p}_j\cdot\boldsymbol{q}_k - \boldsymbol{p}_k\cdot\boldsymbol{q}_j)\right.$$
$$\left. + \sum_{j=1}^{n} (-1)^{j+1}(\boldsymbol{p}_j\cdot\boldsymbol{q}_{n+1} - \boldsymbol{p}_{n+1}\cdot\boldsymbol{q}_j)\}\right]. \tag{A48}$$

The integration over $\boldsymbol{p}_{n+1}$ and $\boldsymbol{q}_{n+1}$ may be performed to yield a product of two delta functions. In the remaining exponential the part with $k = n$ in the double sum vanishes because of the occurrence of the delta functions. Then one is left with the right-hand side of (A46) with the expression (A45) for $n-1$ inserted. Q.E.D.

The special cases n = 1, 2 and 3 of (A45–46) have already been mentioned in the main text (33, 34, 36):

$$\mathrm{Tr}\, \Delta(\boldsymbol{p}_1, \boldsymbol{q}_1) = 1, \tag{A49}$$

$$\mathrm{Tr}\,\{\Delta(\boldsymbol{p}_1, \boldsymbol{q}_1)\Delta(\boldsymbol{p}_2, \boldsymbol{q}_2)\} = h^3\delta(\boldsymbol{p}_1-\boldsymbol{p}_2)\delta(\boldsymbol{q}_1-\boldsymbol{q}_2), \tag{A50}$$

$$\mathrm{Tr}\,\{\Delta(\boldsymbol{p}_1, \boldsymbol{q}_1)\Delta(\boldsymbol{p}_2, \boldsymbol{q}_2)\Delta(\boldsymbol{p}_3, \boldsymbol{q}_3)\}$$
$$= 2^6 \exp\left[\frac{2i}{\hbar}\{\boldsymbol{p}_1\cdot(\boldsymbol{q}_3-\boldsymbol{q}_2)+\boldsymbol{p}_2\cdot(\boldsymbol{q}_1-\boldsymbol{q}_3)+\boldsymbol{p}_3\cdot(\boldsymbol{q}_2-\boldsymbol{q}_1)\}\right]. \qquad \text{(A51)}$$

The traces of products of operators follow by application of (A8), (A45) and (A46). In particular one finds thus from (A8), (A49) and (A50):

$$\mathrm{Tr}\, A = h^{-3}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\, a(\boldsymbol{p}, \boldsymbol{q}), \qquad \text{(A52)}$$

$$\mathrm{Tr}\, AB = h^{-3}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\, a(\boldsymbol{p}, \boldsymbol{q})b(\boldsymbol{p}, \boldsymbol{q}) = \mathrm{Tr}\, BA. \qquad \text{(A53)}$$

e. *Products of operators*

The Weyl transform of a product of the operators A and B follows from (A12), (A8) and (A51). One then obtains

$$AB \rightleftarrows \exp\left\{\frac{i\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}}\cdot\frac{\partial^{(b)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}}\cdot\frac{\partial^{(b)}}{\partial \boldsymbol{q}}\right)\right\} a(\boldsymbol{p}, \boldsymbol{q})b(\boldsymbol{p}, \boldsymbol{q}), \qquad \text{(A54)}$$

where the indices (a) and (b) at the differential operators indicate which functions have to be differentiated. From this correspondence it follows that the Weyl transforms of the anticommutator and the commutator are given by

$$\tfrac{1}{2}\{A, B\} \rightleftarrows \cos\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}}\cdot\frac{\partial^{(b)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}}\cdot\frac{\partial^{(b)}}{\partial \boldsymbol{q}}\right)\right\} a(\boldsymbol{p}, \boldsymbol{q})b(\boldsymbol{p}, \boldsymbol{q}), \qquad \text{(A55)}$$

$$-\frac{i}{\hbar}[A, B] \rightleftarrows \frac{2}{\hbar}\sin\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}}\cdot\frac{\partial^{(b)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}}\cdot\frac{\partial^{(b)}}{\partial \boldsymbol{q}}\right)\right\} a(\boldsymbol{p}, \boldsymbol{q})b(\boldsymbol{p}, \boldsymbol{q}). \qquad \text{(A56)}$$

While the transform (A54) of a product AB of operators is a series in $\hbar$, both (half) the anticommutator and $(-i/\hbar)$ times the commutator are series in $\hbar^2$.

The classical functions that correspond to the product AB and the operators $\frac{1}{2}\{A, B\}$ and $-(i/\hbar)[A, B]$ are, according to (A22), the limits for $\hbar \to 0$ of the right-hand sides of (A54), (A55) and (A56)

$$AB \overset{\mathrm{cl}}{\to} a_{\mathrm{cl}}(\boldsymbol{p}, \boldsymbol{q})b_{\mathrm{cl}}(\boldsymbol{p}, \boldsymbol{q}), \qquad \text{(A57)}$$

$$\tfrac{1}{2}\{A, B\} \overset{\mathrm{cl}}{\to} a_{\mathrm{cl}}(\boldsymbol{p}, \boldsymbol{q})b_{\mathrm{cl}}(\boldsymbol{p}, \boldsymbol{q}), \qquad \text{(A58)}$$

$$-\frac{i}{\hbar}[A, B] \overset{\mathrm{cl}}{\to} \frac{\partial a_{\mathrm{cl}}(\boldsymbol{p}, \boldsymbol{q})}{\partial \boldsymbol{q}}\cdot\frac{\partial b_{\mathrm{cl}}(\boldsymbol{p}, \boldsymbol{q})}{\partial \boldsymbol{p}} - \frac{\partial a_{\mathrm{cl}}(\boldsymbol{p}, \boldsymbol{q})}{\partial \boldsymbol{p}}\cdot\frac{\partial b_{\mathrm{cl}}(\boldsymbol{p}, \boldsymbol{q})}{\partial \boldsymbol{q}}. \qquad \text{(A59)}$$

The last expression obtained is the Poisson bracket of the classical functions $a_{\mathrm{cl}}(\boldsymbol{p}, \boldsymbol{q})$ and $b_{\mathrm{cl}}(\boldsymbol{p}, \boldsymbol{q})$.

3. *The Wigner function*

a. *Definition*

The state of a quantum-mechanical system may be described by means of a density operator

$$P(t) = |\psi(t)\rangle\langle\psi(t)|, \qquad \text{(A60)}$$

where $|\psi(t)\rangle$ is the state vector in Hilbert space. The expectation value of an operator A may be written in terms of this density operator as:

$$\bar{A}(t) = \mathrm{Tr}\,\{P(t)A\}. \qquad \text{(A61)}$$

With the use of (A53) this expectation value becomes

$$\bar{A} = \bar{a} \qquad \text{(A62)}$$

with the abbreviation

$$\bar{a}(t) \equiv \int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\, a(\boldsymbol{p}, \boldsymbol{q})\rho(\boldsymbol{p}, \boldsymbol{q}; t). \qquad \text{(A63)}$$

Here $h^3\rho(\boldsymbol{p}, \boldsymbol{q}; t)$ is the Weyl transform of the density operator

$$P(t) \rightleftarrows h^3\rho(\boldsymbol{p}, \boldsymbol{q}; t). \qquad \text{(A64)}$$

Since the density operator is hermitian its Weyl transform $\rho(\boldsymbol{p}, \boldsymbol{q}; t)$ is real.

The function $\rho(\boldsymbol{p}, \boldsymbol{q}; t)$ is called the Wigner function. Its original form[1] follows from (A7) with (A60) inserted:

$$\rho(\boldsymbol{p}, \boldsymbol{q}; t) = h^{-3}\int \mathrm{d}\boldsymbol{v}\, e^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}}\psi(\boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}; t)\psi^*(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}; t) \qquad \text{(A65)}$$

with the notation $\psi(\boldsymbol{q}; t) \equiv \langle \boldsymbol{q}|\psi(t)\rangle$, the wave function in the coordinate representation. From (A6), with (A60) inserted, one gets the Wigner function in terms of the wave functions $\varphi(\boldsymbol{p}; t) \equiv \langle \boldsymbol{p}|\psi(t)\rangle$ in the momentum representation

$$\rho(\boldsymbol{p}, \boldsymbol{q}; t) = h^{-3}\int \mathrm{d}\boldsymbol{u}\, e^{(i/\hbar)\boldsymbol{q}\cdot\boldsymbol{u}}\varphi(\boldsymbol{p}+\tfrac{1}{2}\boldsymbol{u}; t)\varphi^*(\boldsymbol{p}-\tfrac{1}{2}\boldsymbol{u}; t). \qquad \text{(A66)}$$

[1] E. P. Wigner, Phys. Rev. **40**(1932)749.

A third form is obtained by inserting (A60) into (A18) and using (A4). One then obtains (omitting the time dependence from now on):

$$\rho(\boldsymbol{p}, \boldsymbol{q}) = h^{-\frac{3}{2}} \exp\left(\frac{\hbar}{2i}\frac{\partial}{\partial \boldsymbol{p}} \cdot \frac{\partial}{\partial \boldsymbol{q}}\right) \{\varphi(\boldsymbol{p})\psi^*(\boldsymbol{q})\mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{q}}\}. \tag{A67}$$

Since ρ is real one may also write the complex conjugate of the right-hand side:

$$\rho(\boldsymbol{p}, \boldsymbol{q}) = h^{-\frac{3}{2}} \exp\left(-\frac{\hbar}{2i}\frac{\partial}{\partial \boldsymbol{p}} \cdot \frac{\partial}{\partial \boldsymbol{q}}\right) \{\varphi^*(\boldsymbol{p})\psi(\boldsymbol{q})\mathrm{e}^{-(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{q}}\}. \tag{A68}$$

The fact that the trace of the density operator is unity is reflected by the property that the Wigner function is normalized

$$\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\, \rho(\boldsymbol{p}, \boldsymbol{q}) = 1, \tag{A69}$$

as follows from (A52).

Expectation values of an operator A are thus obtained as integrals (A62) with (A63) over its Weyl transform $a(\boldsymbol{p}, \boldsymbol{q})$ and the Wigner function $\rho(\boldsymbol{p}, \boldsymbol{q})$, which is normalized according to (A69).

b. *Properties*

The function $\rho(\boldsymbol{p}, \boldsymbol{q})$ is real and normalized, but not necessarily positive definite. The integrals over the coordinates or momenta however are positive definite as follows from (A65) and (A66)

$$\int \rho(\boldsymbol{p}, \boldsymbol{q})\mathrm{d}\boldsymbol{p} = |\psi(\boldsymbol{q})|^2 \geqslant 0, \tag{A70}$$

$$\int \rho(\boldsymbol{p}, \boldsymbol{q})\mathrm{d}\boldsymbol{q} = |\varphi(\boldsymbol{p})|^2 \geqslant 0. \tag{A71}$$

Thus, in contrast to the function $\rho(\boldsymbol{p}, \boldsymbol{q})$ itself, these integrals may be interpreted as probability densities. (They are indeed normalized to unity.)

One may show that the Wigner function is limited: it satisfies the inequality

$$|\rho(\boldsymbol{p}, \boldsymbol{q})| \leqslant (2/h)^3. \tag{A72}$$

To prove this one starts from Schwarz's inequality, applied to the expression (A65) for the Wigner function

$$|\rho(\boldsymbol{p}, \boldsymbol{q})|^2 \leqslant h^{-6}\left\{\int \mathrm{d}\boldsymbol{v}|\mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}}\psi(\boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v})|^2\right\}\left\{\int \mathrm{d}\boldsymbol{v}|\psi^*(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v})|^2\right\}. \tag{A73}$$

From the normalization of the wave function it follows that the right-hand side of (A73) is indeed the square of the right-hand side of (A72).

Since ρ is normalized, it follows from the inequality (A72) that ρ is different from zero in a region of which the volume in phase space is at least equal to $(h/2)^3$, in other words its support has a volume larger than this volume. Hence the Wigner function can never be sharply localized both in $\boldsymbol{p}$ and $\boldsymbol{q}$: a delta function character is thus excluded. (This situation is a reflection of the uncertainty principle.)

The density operator has the form of a projection operator, so that

$$P^2 = P. \tag{A74}$$

As a consequence the trace of P^2 is equal to unity (since the trace of P is unity). In terms of the Wigner function this property is

$$\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\{\rho(\boldsymbol{p}, \boldsymbol{q})\}^2 = h^{-3}, \tag{A75}$$

as follows from (A53).

The property (A74) has as a counterpart for the Wigner function

$$\rho(\boldsymbol{p}, \boldsymbol{q}) = h^3 \exp\left\{\frac{i\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{q}}\right)\right\} \rho^{(a)}(\boldsymbol{p}, \boldsymbol{q})\rho^{(b)}(\boldsymbol{p}, \boldsymbol{q}), \tag{A76}$$

as follows from (A54). The two factors ρ at the right-hand side are in fact the same, but indices (a) and (b) have been employed to indicate the way in which the differential operators are acting.

To every wave function $\psi(\boldsymbol{q})$ corresponds one single Wigner function as is apparent from the expression (A65). The inverse is also true[1]: to every real function $f(\boldsymbol{p}, \boldsymbol{q})$ in phase space, which satisfies equations of the form (A69) and (A76) corresponds one single normalized complex function $g(\boldsymbol{q})$ of the coordinates (apart from a phase factor), in such a way that (cf. (A65)):

$$f(\boldsymbol{p}, \boldsymbol{q}) = h^{-3}\int \mathrm{d}\boldsymbol{v}\, \mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}} g(\boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v})g^*(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}). \tag{A77}$$

In other words every real function in phase space, satisfying (A69) and (A76), may play the role of a Wigner function. To prove (A77) we first define the function

$$\mathscr{K}(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}, \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}) = \int \mathrm{d}\boldsymbol{p}\, \mathrm{e}^{-(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}} f(\boldsymbol{p}, \boldsymbol{q}). \tag{A78}$$

[1] G. A. Baker jr., Phys. Rev. **109**(1958)2198.

Its inverse is

$$f(\boldsymbol{p}, \boldsymbol{q}) = h^{-3}\int \mathrm{d}\boldsymbol{v}\, \mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}}\mathcal{K}(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}, \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}). \tag{A79}$$

We shall have to show that the kernel $\mathcal{K}(\boldsymbol{q}+\frac{1}{2}\boldsymbol{v}, \boldsymbol{q}-\frac{1}{2}\boldsymbol{v})$ factorizes, so that (A79) reduces to (A77). To that purpose we write the properties (A69) and (A76) for $f(\boldsymbol{p}, \boldsymbol{q})$ in terms of the kernel $\mathcal{K}$. Inserting (A78) and (A79) into (A69) and (A76) one finds:

$$\int \mathcal{K}(\boldsymbol{q}, \boldsymbol{q})\mathrm{d}\boldsymbol{q} = 1, \tag{A80}$$

$$\begin{aligned}\mathcal{K}&(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}, \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}) \\ &= h^{-3}\int \mathrm{d}\boldsymbol{v}'\mathrm{d}\boldsymbol{v}''\mathrm{d}\boldsymbol{p}\, \exp\left\{-\frac{i}{\hbar}\,\boldsymbol{p}\cdot\boldsymbol{v}+\tfrac{1}{2}i\hbar\left(\frac{\partial^{(a)}}{\partial\boldsymbol{q}}\cdot\frac{\partial^{(b)}}{\partial\boldsymbol{p}}-\frac{\partial^{(a)}}{\partial\boldsymbol{p}}\cdot\frac{\partial^{(b)}}{\partial\boldsymbol{q}}\right)\right\} \\ &\quad \exp\left\{\frac{i}{\hbar}\,(\boldsymbol{p}^{(a)}\cdot\boldsymbol{v}'+\boldsymbol{p}^{(b)}\cdot\boldsymbol{v}'')\right\}\mathcal{K}^{(a)}(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}', \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}')\mathcal{K}^{(b)}(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}'', \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}'').\end{aligned} \tag{A81}$$

If the differentiations in (A81) with respect to the momentum variables are performed, the integration over these variables may be carried out. This gives

$$\begin{aligned}\mathcal{K}(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}, \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}) &= \int \mathrm{d}\boldsymbol{v}'\mathrm{d}\boldsymbol{v}''\delta(\boldsymbol{v}'+\boldsymbol{v}''-\boldsymbol{v})\exp\left\{\frac{1}{2}\left(\boldsymbol{v}'\cdot\frac{\partial^{(b)}}{\partial\boldsymbol{q}}-\boldsymbol{v}''\cdot\frac{\partial^{(a)}}{\partial\boldsymbol{q}}\right)\right\} \\ &\qquad \mathcal{K}^{(a)}(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}', \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}')\mathcal{K}^{(b)}(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}'', \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}'').\end{aligned} \tag{A82}$$

The exponential acting on the kernel may be seen as the operator which yields a Taylor expansion. Hence we may write now

$$\begin{aligned}\mathcal{K}(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}, \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}) &= \int \mathrm{d}\boldsymbol{v}'\mathrm{d}\boldsymbol{v}''\delta(\boldsymbol{v}'+\boldsymbol{v}''-\boldsymbol{v})\mathcal{K}\{\boldsymbol{q}+\tfrac{1}{2}(\boldsymbol{v}'-\boldsymbol{v}''), \boldsymbol{q}-\tfrac{1}{2}(\boldsymbol{v}'+\boldsymbol{v}'')\} \\ &\qquad \mathcal{K}\{\boldsymbol{q}+\tfrac{1}{2}(\boldsymbol{v}'+\boldsymbol{v}''), \boldsymbol{q}+\tfrac{1}{2}(\boldsymbol{v}'-\boldsymbol{v}'')\}.\end{aligned} \tag{A83}$$

With new integration variables $\boldsymbol{v}''' = \frac{1}{2}(\boldsymbol{v}'-\boldsymbol{v}'')$, $\boldsymbol{v}'''' = \boldsymbol{v}'+\boldsymbol{v}''$ one finds, writing $\boldsymbol{v}'$ instead of $\boldsymbol{q}+\boldsymbol{v}'''$,

$$\mathcal{K}(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}, \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}) = \int \mathrm{d}\boldsymbol{v}'\,\mathcal{K}(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}, \boldsymbol{v}')\mathcal{K}(\boldsymbol{v}', \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}). \tag{A84}$$

A third property of the kernel $\mathcal{K}$ is its hermitian character:

$$\mathcal{K}^*(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}, \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}) = \mathcal{K}(\boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}, \boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}), \tag{A85}$$

as follows from (A78). From (A84) it is seen that the eigenvalues λ of the kernel $\mathcal{K}$ satisfy the equation $\lambda = \lambda^2$, so that λ is 0 or 1. Furthermore it follows from (A80) that the sum of the eigenvalues is unity. Therefore only one eigenvalue is 1, and the rest 0. This means that the kernel may be expressed in terms of the normalized eigenfunction g' that corresponds to the single eigenvalue 1:

$$\mathcal{K}(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}, \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}) = g'(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v})g'^*(\boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}), \tag{A86}$$

or, writing g instead of g'^* (g is likewise normalized to unity),

$$\mathcal{K}(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}, \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}) = g(\boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v})g^*(\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}), \tag{A87}$$

which completes the proof of (A77).

c. *Development in time*

The time evolution of the Wigner function is a direct consequence of the equation

$$\frac{\partial P}{\partial t} = -\frac{i}{\hbar}[H, P], \tag{A88}$$

which governs the time evolution of the density operator. In fact one finds from (A56) for the Weyl transform $h^3\rho(\boldsymbol{p}, \boldsymbol{q}; t)$ of the density operator:

$$\frac{\partial\rho(\boldsymbol{p}, \boldsymbol{q}; t)}{\partial t} = \frac{2}{\hbar}\sin\left\{\frac{\hbar}{2}\left(\frac{\partial^{(h)}}{\partial\boldsymbol{q}}\cdot\frac{\partial^{(\rho)}}{\partial\boldsymbol{p}}-\frac{\partial^{(h)}}{\partial\boldsymbol{p}}\cdot\frac{\partial^{(\rho)}}{\partial\boldsymbol{q}}\right)\right\}h(\boldsymbol{p}, \boldsymbol{q})\rho(\boldsymbol{p}, \boldsymbol{q}; t), \tag{A89}$$

where $h(\boldsymbol{p}, \boldsymbol{q})$ is the Weyl transform of the Hamilton operator. One may introduce a Liouville operator defined as

$$\mathcal{L}(\boldsymbol{p}, \boldsymbol{q}) \equiv -\frac{2}{\hbar}\sin\left\{\frac{\hbar}{2}\left(\frac{\partial^{(h)}}{\partial\boldsymbol{q}}\cdot\frac{\partial}{\partial\boldsymbol{p}}-\frac{\partial^{(h)}}{\partial\boldsymbol{p}}\cdot\frac{\partial}{\partial\boldsymbol{q}}\right)\right\}h(\boldsymbol{p}, \boldsymbol{q}). \tag{A90}$$

Then the time evolution of the Wigner function is described by

$$\frac{\partial\rho(\boldsymbol{p}, \boldsymbol{q}; t)}{\partial t} = -\mathcal{L}(\boldsymbol{p}, \boldsymbol{q})\rho(\boldsymbol{p}, \boldsymbol{q}; t). \tag{A91}$$

It has the formal solution, for a time-independent Hamiltonian,

$$\rho(\boldsymbol{p}, \boldsymbol{q}; t) = \exp\{-\mathcal{L}(\boldsymbol{p}, \boldsymbol{q})(t-t_0)\}\rho(\boldsymbol{p}, \boldsymbol{q}; t_0). \tag{A92}$$

The equation (A91) may be used to find an expression for the time derivative of the expectation value (A62) with (A63) of an operator A:

$$\frac{\mathrm{d}\bar{a}(t)}{\mathrm{d}t} = -\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\, a(\boldsymbol{p}, \boldsymbol{q})\mathcal{L}(\boldsymbol{p}, \boldsymbol{q})\rho(\boldsymbol{p}, \boldsymbol{q}; t). \tag{A93}$$

Partial integration gives

$$\frac{\mathrm{d}\bar{a}(t)}{\mathrm{d}t} = \int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\{\mathscr{L}(\boldsymbol{p},\boldsymbol{q})a(\boldsymbol{p},\boldsymbol{q})\}\rho(\boldsymbol{p},\boldsymbol{q};t), \tag{A94}$$

or with the explicit Liouvillean (A90)

$$\frac{\mathrm{d}\bar{a}(t)}{\mathrm{d}t} = \frac{2}{\hbar}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\left[\sin\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}}\cdot\frac{\partial^{(h)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}}\cdot\frac{\partial^{(h)}}{\partial \boldsymbol{q}}\right)\right\} a(\boldsymbol{p},\boldsymbol{q})h(\boldsymbol{p},\boldsymbol{q})\right] \rho(\boldsymbol{p},\boldsymbol{q};t). \tag{A95}$$

In particular if one chooses for $a(\boldsymbol{p},\boldsymbol{q})$ the Weyl transforms $\boldsymbol{p}$ and $\boldsymbol{q}$ of the momentum and coordinate operators this relation gets the simple form

$$\frac{\mathrm{d}\bar{\boldsymbol{p}}(t)}{\mathrm{d}t} = -\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\,\frac{\partial h}{\partial \boldsymbol{q}}\,\rho(\boldsymbol{p},\boldsymbol{q};t), \tag{A96}$$

$$\frac{\mathrm{d}\bar{\boldsymbol{q}}(t)}{\mathrm{d}t} = \int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\,\frac{\partial h}{\partial \boldsymbol{p}}\,\rho(\boldsymbol{p},\boldsymbol{q};t). \tag{A97}$$

These equations are the Weyl transform versions of the Ehrenfest equations of the ordinary formulation of quantum mechanics. Their connexion with the Hamilton equations will be discussed in the next subsection.

d. *The classical limit*

Let us try to find those Wigner functions which are products of functions of the coordinates and momenta[1]

$$\rho(\boldsymbol{p},\boldsymbol{q}) = \rho_1(\boldsymbol{p})\rho_2(\boldsymbol{q}). \tag{A98}$$

From the form (A65) of the Wigner function one finds for the Fourier transform of (A98), replacing $\frac{1}{2}\boldsymbol{v}$ by $\boldsymbol{v}$ for convenience,

$$\psi(\boldsymbol{q}-\boldsymbol{v})\psi^*(\boldsymbol{q}+\boldsymbol{v}) = \left\{\int \mathrm{d}\boldsymbol{p}\,\mathrm{e}^{-(2i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}}\rho_1(\boldsymbol{p})\right\}\rho_2(\boldsymbol{q}), \tag{A99}$$

where the expression at the right-hand side is a product of a function of $\boldsymbol{v}$ and a function of $\boldsymbol{q}$. Writing

$$\psi(\boldsymbol{q}) = \mathrm{e}^{\chi(\boldsymbol{q})}, \tag{A100}$$

$$\int \mathrm{d}\boldsymbol{p}\,\mathrm{e}^{-(2i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}}\rho_1(\boldsymbol{p}) = \mathrm{e}^{\alpha(\boldsymbol{v})}, \tag{A101}$$

$$\rho_2(\boldsymbol{q}) = \mathrm{e}^{\beta(\boldsymbol{q})}, \tag{A102}$$

[1] T. Takabayasi, Progr. Theor. Phys. **11**(1954)341.

one gets for the logarithm of (A99)

$$\chi(\boldsymbol{q}-\boldsymbol{v})+\chi^*(\boldsymbol{q}+\boldsymbol{v}) = \alpha(\boldsymbol{v})+\beta(\boldsymbol{q}). \tag{A103}$$

Developing the functions in the left-hand side in powers of $\boldsymbol{v}$, we get the identity in $\boldsymbol{q}$ and $\boldsymbol{v}$

$$\mathrm{re}\,\chi(\boldsymbol{q}) - i\boldsymbol{v}\cdot\frac{\partial}{\partial \boldsymbol{q}}\{\mathrm{im}\,\chi(\boldsymbol{q})\} + \tfrac{1}{2}\boldsymbol{v}\boldsymbol{v} : \frac{\partial^2}{\partial \boldsymbol{q}\,\partial \boldsymbol{q}}\{\mathrm{re}\,\chi(\boldsymbol{q})\} - \ldots = \tfrac{1}{2}\alpha(\boldsymbol{v}) + \tfrac{1}{2}\beta(\boldsymbol{q}). \tag{A104}$$

From this identity it follows that

$$\begin{aligned} \frac{\partial^n}{\partial \boldsymbol{q}^n}\{\mathrm{re}\,\chi(\boldsymbol{q})\} &= \mathbf{c}_n, \qquad (n = 2, 4, \ldots), \\ \frac{\partial^n}{\partial \boldsymbol{q}^n}\{\mathrm{im}\,\chi(\boldsymbol{q})\} &= \mathbf{c}_n, \qquad (n = 1, 3, \ldots), \end{aligned} \tag{A105}$$

with (real) constants $\mathbf{c}_n$ independent of $\boldsymbol{q}$. These formulae yield for $n = 1$ and $n = 2$ respectively:

$$\begin{aligned} \mathrm{im}\,\chi(\boldsymbol{q}) &= \boldsymbol{c}_1\cdot\boldsymbol{q} + d_0, \\ \mathrm{re}\,\chi(\boldsymbol{q}) &= \tfrac{1}{2}\mathbf{c}_2 : \boldsymbol{q}\boldsymbol{q} + \boldsymbol{d}_1\cdot\boldsymbol{q} + d_2, \end{aligned} \tag{A106}$$

with $\boldsymbol{c}_1$ and $\mathbf{c}_2$ constants which already occurred, and d_0, $\boldsymbol{d}_1$ and d_2 other real constant quantities. The expressions (A106) satisfy (A105) also for $n = 3, 4, \ldots$. From (A106) and (A100) one finds

$$\psi(\boldsymbol{q}) = \exp\left(\mathbf{a}_2 : \boldsymbol{q}\boldsymbol{q} + \boldsymbol{a}_1\cdot\boldsymbol{q} + a_0\right) \tag{A107}$$

with $\mathbf{a}_2 = \frac{1}{2}\mathbf{c}_2$ real, and $\boldsymbol{a}_1 = \boldsymbol{d}_1 + i\boldsymbol{c}_1$, $a_0 = d_2 + id_0$ complex constants. By a rotation of the coordinate axes one may bring the quadratic expression in diagonal form. Subsequently the real part of the linear term is taken together with the quadratic term so as to form a square. In this way one finds

$$\psi(\boldsymbol{q}) = C\exp\left\{-\sum_{i=1}^{3}\frac{(\boldsymbol{q}-\boldsymbol{q}_0)_i^2}{4\Delta_i^2} + \frac{i\boldsymbol{p}_0\cdot\boldsymbol{q}}{\hbar}\right\} \tag{A108}$$

with real constants $\boldsymbol{p}_0$, $\boldsymbol{q}_0$ and Δ_i and a normalization constant C, which may be chosen to be real. If, for simplicity, we limit ourselves to the case $\Delta_1 = \Delta_2 = \Delta_3 = \Delta$, we have the wave function

$$\psi(\boldsymbol{q}) = \frac{1}{(2\pi)^{\frac{3}{4}}\Delta^{\frac{3}{2}}}\exp\left\{-\frac{(\boldsymbol{q}-\boldsymbol{q}_0)^2}{4\Delta^2} + \frac{i\boldsymbol{p}_0\cdot\boldsymbol{q}}{\hbar}\right\}, \tag{A109}$$

a 'minimum wave packet'. The Wigner function (A65) which corresponds to this wave function is

$$\rho(\boldsymbol{p}, \boldsymbol{q}) = (2/h)^3 \exp\left\{-\frac{(\boldsymbol{q}-\boldsymbol{q}_0)^2}{2\Delta^2} - \frac{2\Delta^2}{\hbar^2}(\boldsymbol{p}-\boldsymbol{p}_0)^2\right\}. \tag{A110}$$

This expression is the product of two Gaussians, one in the coordinate and one in the momentum space. The integrals of (A110) over $\boldsymbol{p}$ or $\boldsymbol{q}$ are the probability densities (A70) and (A71). They are Gaussians with widths Δ and $\hbar/2\Delta$ respectively. The product of their widths is $\frac{1}{2}\hbar$, which explains the name 'minimum wave packet' for (A109).

In the preceding section the classical limit of a physical quantity was defined as the limit, for $\hbar$ tending to zero, of the Weyl transform of the corresponding operator (v. (A22)). The situation is not exactly the same for the density operator, since physical states exist in quantum mechanics which have no classical counterpart. This means that taking the limit $\hbar \to 0$ of the Wigner function will not always lead to a classical function. Even if one utilizes minimum wave packets in their form (A110), the limit $\hbar \to 0$ has to be taken in a special way so as to obtain the classical limit. In fact one must let tend both $\hbar$ and Δ to zero, but the latter in such a way that $\hbar/\Delta$ tends to zero as well. In this way one finds from (A110) as the classical limit of the Wigner function

$$\rho(\boldsymbol{p}, \boldsymbol{q}) \overset{\text{cl}}{\to} \rho_{\text{cl}}(\boldsymbol{p}, \boldsymbol{q}) = \delta(\boldsymbol{p}-\boldsymbol{p}_0)\delta(\boldsymbol{q}-\boldsymbol{q}_0). \tag{A111}$$

With this classical function and (A22) we obtain as the classical limit of the expectation value from (A62) with (A63)

$$\bar{A} = \bar{a} \overset{\text{cl}}{\to} a_{\text{cl}}(\boldsymbol{p}_0, \boldsymbol{q}_0). \tag{A112}$$

The time derivative of an expectation value follows from (A94) with (A90). In the classical limit one finds then with (A111) and (A22)

$$\frac{\mathrm{d}\bar{a}(t)}{\mathrm{d}t} \overset{\text{cl}}{\to} \mathscr{L}_{\text{cl}}(\boldsymbol{p}_0, \boldsymbol{q}_0)a_{\text{cl}}(\boldsymbol{p}_0, \boldsymbol{q}_0). \tag{A113}$$

Here the classical Liouville operator is

$$\mathscr{L}_{\text{cl}}(\boldsymbol{p}, \boldsymbol{q}) \equiv \lim_{\hbar\to 0} \mathscr{L}(\boldsymbol{p}, \boldsymbol{q}) = \frac{\partial h_{\text{cl}}}{\partial \boldsymbol{p}}\cdot\frac{\partial}{\partial \boldsymbol{q}} - \frac{\partial h_{\text{cl}}}{\partial \boldsymbol{q}}\cdot\frac{\partial}{\partial \boldsymbol{p}}, \tag{A114}$$

where $h_{\text{cl}}(\boldsymbol{p}, \boldsymbol{q})$ is the classical limit (A22) of the Hamiltonian. Thus (A113) becomes

$$\frac{\mathrm{d}\bar{a}(t)}{\mathrm{d}t} \overset{\text{cl}}{\to} \frac{\partial h_{\text{cl}}(\boldsymbol{p}_0, \boldsymbol{q}_0)}{\partial \boldsymbol{p}_0}\cdot\frac{\partial a_{\text{cl}}(\boldsymbol{p}_0, \boldsymbol{q}_0)}{\partial \boldsymbol{q}_0} - \frac{\partial h_{\text{cl}}(\boldsymbol{p}_0, \boldsymbol{q}_0)}{\partial \boldsymbol{q}_0}\cdot\frac{\partial a_{\text{cl}}(\boldsymbol{p}_0, \boldsymbol{q}_0)}{\partial \boldsymbol{p}_0}, \tag{A115}$$

which is the Poisson bracket. With the help of (A112) we may write the classical limit of the left-hand side as:

$$\frac{\mathrm{d}\bar{a}(t)}{\mathrm{d}t} \overset{\text{cl}}{\to} \frac{\mathrm{d}a_{\text{cl}}(\boldsymbol{p}_0, \boldsymbol{q}_0)}{\mathrm{d}t}. \tag{A116}$$

Comparing (A115) and (A116) we obtain the classical equation:

$$\frac{\mathrm{d}a_{\text{cl}}(\boldsymbol{p}_0, \boldsymbol{q}_0)}{\mathrm{d}t} = \frac{\partial h_{\text{cl}}(\boldsymbol{p}_0, \boldsymbol{q}_0)}{\partial \boldsymbol{p}_0}\cdot\frac{\partial a_{\text{cl}}(\boldsymbol{p}_0, \boldsymbol{q}_0)}{\partial \boldsymbol{q}_0} - \frac{\partial h_{\text{cl}}(\boldsymbol{p}_0, \boldsymbol{q}_0)}{\partial \boldsymbol{q}_0}\cdot\frac{\partial a_{\text{cl}}(\boldsymbol{p}_0, \boldsymbol{q}_0)}{\partial \boldsymbol{p}_0}. \tag{A117}$$

In particular for the momenta and coordinates we get

$$\frac{\mathrm{d}\boldsymbol{p}_0}{\mathrm{d}t} = -\frac{\partial h_{\text{cl}}(\boldsymbol{p}_0, \boldsymbol{q}_0)}{\partial \boldsymbol{q}_0}, \tag{A118}$$

$$\frac{\mathrm{d}\boldsymbol{q}_0}{\mathrm{d}t} = \frac{\partial h_{\text{cl}}(\boldsymbol{p}_0, \boldsymbol{q}_0)}{\partial \boldsymbol{p}_0}, \tag{A119}$$

which are the classical Hamilton equations.

e. *The propagator*

The density operator at time t follows from the density operator at time t_0 with the help of the expression

$$P(t) = U(t, t_0)P(t_0)U^{\dagger}(t, t_0). \tag{A120}$$

The evolution operator $U(t, t_0)$ follows from the Schrödinger equation (for a time-independent Hamiltonian)

$$-\frac{\hbar}{i}\frac{\partial U(t, t_0)}{\partial t} = HU(t, t_0) \tag{A121}$$

with the initial condition $U(t_0, t_0) = 1$:

$$U(t, t_0) = \mathrm{e}^{-(i/\hbar)H(t-t_0)}. \tag{A122}$$

The Wigner function, which is the Weyl transform of the density operator (times h^{-3}) follows from (A12), with (A120) inserted,

$$\rho(\boldsymbol{p}, \boldsymbol{q}; t) = h^{-3}\,\mathrm{Tr}\,\{\Delta(\boldsymbol{p}, \boldsymbol{q})U(t, t_0)P(t_0)U^{\dagger}(t, t_0)\}. \tag{A123}$$

According to (A8) the third factor between the brackets may be written as an integral with a Wigner function at the time t_0, so that one has for (A123):

$$\rho(\boldsymbol{p}, \boldsymbol{q}; t) = \int \mathrm{d}\boldsymbol{p}_0 \, \mathrm{d}\boldsymbol{q}_0 \, \mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0) \rho(\boldsymbol{p}_0, \boldsymbol{q}_0; t_0) \quad \text{(A124)}$$

with the propagator of the Wigner function, defined as

$$\mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0) = h^{-3} \operatorname{Tr} \{\Delta(\boldsymbol{p}, \boldsymbol{q}) U(t, t_0) \Delta(\boldsymbol{p}_0, \boldsymbol{q}_0) U^\dagger(t, t_0)\}. \quad \text{(A125)}$$

The propagator, which is a real function (as follows from its definition and the hermiticity of the Δ-operator) is not necessarily positive. Hence an interpretation as a conditional probability is not justified. From the definition (A125) and (A12) it follows that it may be looked upon as the Weyl transform of the operator $h^{-3}U(t, t_0)\Delta(\boldsymbol{p}_0, \boldsymbol{q}_0)U^\dagger(t, t_0)$. Then as a consequence of (A8) one has

$$U(t, t_0)\Delta(\boldsymbol{p}_0, \boldsymbol{q}_0)U^\dagger(t, t_0) = \int \mathrm{d}\boldsymbol{p} \, \mathrm{d}\boldsymbol{q} \, \mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0) \Delta(\boldsymbol{p}, \boldsymbol{q}). \quad \text{(A126)}$$

In a similar way one finds:

$$U^\dagger(t, t_0)\Delta(\boldsymbol{p}, \boldsymbol{q})U(t, t_0) = \int \mathrm{d}\boldsymbol{p}_0 \, \mathrm{d}\boldsymbol{q}_0 \, \mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0) \Delta(\boldsymbol{p}_0, \boldsymbol{q}_0). \quad \text{(A127)}$$

The propagator is normalized, as follows from (A44) with (A49):

$$\int \mathrm{d}\boldsymbol{p}_0 \, \mathrm{d}\boldsymbol{q}_0 \, \mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0) = 1,$$
$$\int \mathrm{d}\boldsymbol{p} \, \mathrm{d}\boldsymbol{q} \, \mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0) = 1. \quad \text{(A128)}$$

The symmetry of the propagator:

$$\mathscr{P}(\boldsymbol{p}_0, \boldsymbol{q}_0, t_0 | \boldsymbol{p}, \boldsymbol{q}, t) = \mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0) \quad \text{(A129)}$$

follows from its definition with (A122).

For the initial value of the propagator one finds from (A122) and (A50):

$$\mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t_0 | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0) = \delta(\boldsymbol{p}-\boldsymbol{p}_0)\delta(\boldsymbol{q}-\boldsymbol{q}_0). \quad \text{(A130)}$$

Since the propagator $\mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0)$ is the Weyl transform of the operator $h^{-3}U(t, t_0)\Delta(\boldsymbol{p}_0, \boldsymbol{q}_0)U^\dagger(t, t_0)$ one may write, with (A53), (A122) and (A50), the orthogonality property:

$$\int \mathrm{d}\boldsymbol{p} \, \mathrm{d}\boldsymbol{q} \, \mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0) \mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0', \boldsymbol{q}_0', t_0) = \delta(\boldsymbol{p}_0-\boldsymbol{p}_0')\delta(\boldsymbol{q}_0-\boldsymbol{q}_0'), \quad \text{(A131)}$$

and similarly

$$\int \mathrm{d}\boldsymbol{p}_0 \, \mathrm{d}\boldsymbol{q}_0 \, \mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0) \mathscr{P}(\boldsymbol{p}', \boldsymbol{q}', t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0) = \delta(\boldsymbol{p}-\boldsymbol{p}')\delta(\boldsymbol{q}-\boldsymbol{q}'). \quad \text{(A132)}$$

From the definition (A125) and the explicit form (A122) for the evolution operator it follows that one may write for arbitrary t_1:

$$\mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0) = h^{-3} \operatorname{Tr} \{U^\dagger(t, t_1)\Delta(\boldsymbol{p}, \boldsymbol{q})U(t, t_1)U(t_1, t_0)\Delta(\boldsymbol{p}_0, \boldsymbol{q}_0) U^\dagger(t_1, t_0)\}. \quad \text{(A133)}$$

With (A126), (A127) and (A50) this gives the convolution property

$$\mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0) = \int \mathrm{d}\boldsymbol{p}_1 \, \mathrm{d}\boldsymbol{q}_1 \, \mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_1, \boldsymbol{q}_1, t_1) \mathscr{P}(\boldsymbol{p}_1, \boldsymbol{q}_1, t_1 | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0). \quad \text{(A134)}$$

Since $\mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0)$ is the propagator of the Wigner function, it satisfies the same equation for the time evolution as the Wigner function itself, i.e. (A91):

$$\frac{\partial \mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0)}{\partial t} = -\mathscr{L}(\boldsymbol{p}, \boldsymbol{q}) \mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0). \quad \text{(A135)}$$

Its formal solution follows with (A130):

$$\mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0) = \exp\{-\mathscr{L}(\boldsymbol{p}, \boldsymbol{q})(t-t_0)\}\delta(\boldsymbol{p}-\boldsymbol{p}_0)\delta(\boldsymbol{q}-\boldsymbol{q}_0). \quad \text{(A136)}$$

The symmetry (A129) permits to write this alternatively as

$$\mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0) = \exp\{\mathscr{L}(\boldsymbol{p}_0, \boldsymbol{q}_0)(t-t_0)\}\delta(\boldsymbol{p}-\boldsymbol{p}_0)\delta(\boldsymbol{q}-\boldsymbol{q}_0), \quad \text{(A137)}$$

which is the solution of

$$\frac{\partial \mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0)}{\partial t} = \mathscr{L}(\boldsymbol{p}_0, \boldsymbol{q}_0) \mathscr{P}(\boldsymbol{p}, \boldsymbol{q}, t | \boldsymbol{p}_0, \boldsymbol{q}_0, t_0). \quad \text{(A138)}$$

4. *Generalization to particles with spin*

a. *Introduction*

In the preceding we confined ourselves to the consideration of quantum mechanics for single point particles. In that case the three coordinate (or momentum) operators form a complete set of commuting operators. The eigenstates that could be characterized by the eigenvalues of the coordinate (or momentum) operators formed a basis of the complete Hilbert space of all possible states of the particle.

For particles with internal degrees of freedom this holds no longer true. Then several eigenstates correspond to each eigenvalue of the coordinate (or momentum) operator. They may be labelled by a new index κ. The eigenvalue equations for the momentum and coordinate operators $\boldsymbol{P}$ and $\boldsymbol{Q}$ read in this case

$$\boldsymbol{P}|\boldsymbol{p}, \kappa\rangle = \boldsymbol{p}|\boldsymbol{p}, \kappa\rangle, \qquad \boldsymbol{Q}|\boldsymbol{q}, \kappa\rangle = \boldsymbol{q}|\boldsymbol{q}, \kappa\rangle, \tag{A139}$$

with eigenvalues $\boldsymbol{p}$ and $\boldsymbol{q}$ and $\kappa = 1, 2, \ldots, n$. (For particles with spin for instance, which are described by the Schrödinger–Pauli theory one has $n = 2$, while in Dirac's relativistic theory of spin particles $n = 4$.) The vectors $|\boldsymbol{p}, \kappa\rangle$ or $|\boldsymbol{q}, \kappa\rangle$ with κ one of the numbers $1, 2, \ldots, n$ form n bases in n Hilbert spaces of the same structure. The total Hilbert space is the direct sum of these n spaces.

The closure relations for the bases $|\boldsymbol{p}, \kappa\rangle$ and $|\boldsymbol{q}, \kappa\rangle$ read now

$$\begin{aligned} \sum_\kappa \int \mathrm{d}\boldsymbol{p}|\boldsymbol{p}, \kappa\rangle\langle \boldsymbol{p}, \kappa| &= I, \\ \sum_\kappa \int \mathrm{d}\boldsymbol{q}|\boldsymbol{q}, \kappa\rangle\langle \boldsymbol{q}, \kappa| &= I, \end{aligned} \tag{A140}$$

while their inner products are

$$\begin{aligned} \langle \boldsymbol{p}, \kappa|\boldsymbol{p}', \kappa'\rangle &= \delta(\boldsymbol{p}-\boldsymbol{p}')\delta_{\kappa\kappa'}, \\ \langle \boldsymbol{q}, \kappa|\boldsymbol{q}', \kappa'\rangle &= \delta(\boldsymbol{q}-\boldsymbol{q}')\delta_{\kappa\kappa'}, \\ \langle \boldsymbol{q}, \kappa|\boldsymbol{p}, \kappa'\rangle &= \frac{1}{h^{\frac{3}{2}}} \mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{q}}\delta_{\kappa\kappa'}. \end{aligned} \tag{A141}$$

In the following we need the operator $\Omega_{\kappa\lambda}$ which is defined as

$$\Omega_{\kappa\lambda} = \int \mathrm{d}\boldsymbol{p}|\boldsymbol{p}, \kappa\rangle\langle \boldsymbol{p}, \lambda| = \int \mathrm{d}\boldsymbol{q}|\boldsymbol{q}, \kappa\rangle\langle \boldsymbol{q}, \lambda|. \tag{A142}$$

The last equality follows directly if one forms matrix elements of the operator $\Omega_{\kappa\lambda}$.

The trace of an operator may be expressed in terms of the bases $|\boldsymbol{p}, \kappa\rangle$ or $|\boldsymbol{q}, \kappa\rangle$:

$$\operatorname{Tr} A = \sum_\kappa \int \mathrm{d}\boldsymbol{p}\langle \boldsymbol{p}, \kappa|A|\boldsymbol{p}, \kappa\rangle = \sum_\kappa \int \mathrm{d}\boldsymbol{q}\langle \boldsymbol{q}, \kappa|A|\boldsymbol{q}, \kappa\rangle. \tag{A143}$$

b. *The Weyl transform*

The above generalization of the formulae for point particles permits to repeat the derivations of section 2 and 3 for the Weyl transforms and the Wigner functions. In the results the indices of the inner degrees of freedom will appear now and then.

Thus one finds for the Weyl transform of an operator A, instead of (A6), (A7) and (A12)

$$a_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q}) = \int \mathrm{d}\boldsymbol{u}\, \mathrm{e}^{(i/\hbar)\boldsymbol{q}\cdot\boldsymbol{u}}\langle \boldsymbol{p}+\tfrac{1}{2}\boldsymbol{u}, \kappa|A|\boldsymbol{p}-\tfrac{1}{2}\boldsymbol{u}, \lambda\rangle, \tag{A144}$$

$$a_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q}) = \int \mathrm{d}\boldsymbol{v}\, \mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}}\langle \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}, \kappa|A|\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}, \lambda\rangle, \tag{A145}$$

$$a_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q}) = \operatorname{Tr}\{A\Delta_{\lambda\kappa}(\boldsymbol{p}, \boldsymbol{q})\}. \tag{A146}$$

The Δ-operator which occurs here is given by

$$\Delta_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q}) = h^{-3}\int \mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\, \mathrm{e}^{(i/\hbar)\{(\boldsymbol{q}-\boldsymbol{Q})\cdot\boldsymbol{u}+(\boldsymbol{p}-\boldsymbol{P})\cdot\boldsymbol{v}\}}\Omega_{\kappa\lambda} \equiv \Delta(\boldsymbol{p}, \boldsymbol{q})\Omega_{\kappa\lambda}, \tag{A147}$$

with $\Delta(\boldsymbol{p}, \boldsymbol{q})$ as given in (A9). Alternative forms for $\Delta_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q})$ are:

$$\Delta_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q}) = \int \mathrm{d}\boldsymbol{u}\, \mathrm{e}^{(i/\hbar)\boldsymbol{q}\cdot\boldsymbol{u}}|\boldsymbol{p}-\tfrac{1}{2}\boldsymbol{u}, \kappa\rangle\langle \boldsymbol{p}+\tfrac{1}{2}\boldsymbol{u}, \lambda|, \tag{A148}$$

$$\Delta_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q}) = \int \mathrm{d}\boldsymbol{v}\, \mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}}|\boldsymbol{q}+\tfrac{1}{2}\boldsymbol{v}, \kappa\rangle\langle \boldsymbol{q}-\tfrac{1}{2}\boldsymbol{v}, \lambda|, \tag{A149}$$

instead of (A10) and (A11). The operator A is now a sum of integrals:

$$A = h^{-3}\sum_{\kappa,\lambda}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\, a_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q})\Delta_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q}) \tag{A150}$$

instead of (A8). The Weyl correspondence may also be expressed, as in (A13–14), by

$$A = \sum_{\kappa,\lambda}\int \mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\, \tilde{a}_{\kappa\lambda}(\boldsymbol{u}, \boldsymbol{v})\mathrm{e}^{-(i/\hbar)(\boldsymbol{Q}\cdot\boldsymbol{u}+\boldsymbol{P}\cdot\boldsymbol{v})}\Omega_{\kappa\lambda}, \tag{A151}$$

$$a_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q}) = \int \mathrm{d}\boldsymbol{u}\,\mathrm{d}\boldsymbol{v}\, \tilde{a}_{\kappa\lambda}(\boldsymbol{u}, \boldsymbol{v})\mathrm{e}^{-(i/\hbar)(\boldsymbol{q}\cdot\boldsymbol{u}+\boldsymbol{p}\cdot\boldsymbol{v})}. \tag{A152}$$

If an operator A does not connect the different parts of Hilbert space labelled by κ, its Weyl transform is diagonal in the discrete indices, as follows from (A144) (or (A145)):

$$a_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q}) = \delta_{\kappa\lambda}\int \mathrm{d}\boldsymbol{u}\, \mathrm{e}^{(i/\hbar)\boldsymbol{q}\cdot\boldsymbol{u}}\langle \boldsymbol{p}+\tfrac{1}{2}\boldsymbol{u}, \kappa|A|\boldsymbol{p}-\tfrac{1}{2}\boldsymbol{u}, \kappa\rangle. \tag{A153}$$

If the operator moreover acts in the same way in each subspace, the integral is independent of κ and may be denoted as $a(\boldsymbol{p}, \boldsymbol{q})$:

$$a_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q}) = \delta_{\kappa\lambda}\, a(\boldsymbol{p}, \boldsymbol{q}). \tag{A154}$$

Upon introduction into (A150) and the use of the relation $\sum_\kappa \Omega_{\kappa\kappa} = I$ that follows from (A140) and (A142), one recovers (A8).

As a different special case we consider operators A which are independent of the coordinate and momentum operators, as for instance the spin operator. Then the Weyl transform (A144) or (A145) is independent of $\boldsymbol{p}$ and $\boldsymbol{q}$:

$$a_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q}) = a_{\kappa\lambda}\,. \tag{A155}$$

Upon introduction into (A150) one finds with the help of (A44) that the operator may be written as

$$A = \sum_{\kappa,\lambda} a_{\kappa\lambda}\, \Omega_{\kappa\lambda}\,. \tag{A156}$$

As formula (A147) showed the basic operator $\Delta_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q})$ has the simple form $\Delta_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q}) = \Delta(\boldsymbol{p}, \boldsymbol{q})\Omega_{\kappa\lambda}$. Therefore one may derive properties for the $\Delta_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q})$-operator from those of the $\Delta(\boldsymbol{p}, \boldsymbol{q})$-operator derived in section 2*d*. As corollaries one finds for the traces of an operator and a product of two operators (cf. (A52–53)):

$$\mathrm{Tr}\, A = h^{-3} \sum_\kappa \int \mathrm{d}\boldsymbol{p}\, \mathrm{d}\boldsymbol{q}\, a_{\kappa\kappa}(\boldsymbol{p}, \boldsymbol{q}), \tag{A157}$$

$$\mathrm{Tr}\, AB = h^{-3} \sum_{\kappa,\lambda} \int \mathrm{d}\boldsymbol{p}\, \mathrm{d}\boldsymbol{q}\, a_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q}) b_{\lambda\kappa}(\boldsymbol{p}, \boldsymbol{q}) = \mathrm{Tr}\, BA. \tag{A158}$$

Furthermore one finds for the Weyl transform of a product of two operators (cf. (A54))

$$AB \rightleftarrows \exp\left\{\frac{i\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{q}}\right)\right\} \sum_\mu a_{\kappa\mu}(\boldsymbol{p}, \boldsymbol{q}) b_{\mu\lambda}(\boldsymbol{p}, \boldsymbol{q}). \tag{A159}$$

The commutator and the anticommutator of two operators are given by (cf. (A55) and (A56)):

$$\begin{aligned}\tfrac{1}{2}\{A, B\} \rightleftarrows \tfrac{1}{2} \cos\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{q}}\right)\right\} &\sum_\mu \{a_{\kappa\mu}(\boldsymbol{p}, \boldsymbol{q}) b_{\mu\lambda}(\boldsymbol{p}, \boldsymbol{q}) \\ &+ b_{\kappa\mu}(\boldsymbol{p}, \boldsymbol{q}) a_{\mu\lambda}(\boldsymbol{p}, \boldsymbol{q})\} \\ + \frac{i}{2} \sin\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{q}}\right)\right\} &\sum_\mu \{a_{\kappa\mu}(\boldsymbol{p}, \boldsymbol{q}) b_{\mu\lambda}(\boldsymbol{p}, \boldsymbol{q}) \\ &- b_{\kappa\mu}(\boldsymbol{p}, \boldsymbol{q}) a_{\mu\lambda}(\boldsymbol{p}, \boldsymbol{q})\},\end{aligned} \tag{A160}$$

$$\begin{aligned}-\frac{i}{\hbar}[A, B] \rightleftarrows \frac{1}{\hbar} \sin\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{q}}\right)\right\} &\sum_\mu \{a_{\kappa\mu}(\boldsymbol{p}, \boldsymbol{q}) b_{\mu\lambda}(\boldsymbol{p}, \boldsymbol{q}) \\ &+ b_{\kappa\mu}(\boldsymbol{p}, \boldsymbol{q}) a_{\mu\lambda}(\boldsymbol{p}, \boldsymbol{q})\} \\ - \frac{i}{\hbar} \cos\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{q}}\right)\right\} &\sum_\mu \{a_{\kappa\mu}(\boldsymbol{p}, \boldsymbol{q}) b_{\mu\lambda}(\boldsymbol{p}, \boldsymbol{q}) \\ &- b_{\kappa\mu}(\boldsymbol{p}, \boldsymbol{q}) a_{\mu\lambda}(\boldsymbol{p}, \boldsymbol{q})\}.\end{aligned} \tag{A161}$$

In the special case that the operators A and B do not act on the indices κ, i.e. if they have Weyl transforms of the type (A154), the expressions (A160) and (A161) reduce to

$$\tfrac{1}{2}\{A, B\} \rightleftarrows \cos\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{q}}\right)\right\} a(\boldsymbol{p}, \boldsymbol{q}) b(\boldsymbol{p}, \boldsymbol{q}) \delta_{\kappa\lambda}, \tag{A162}$$

$$-\frac{i}{\hbar}[A, B] \rightleftarrows \frac{2}{\hbar} \sin\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}} \cdot \frac{\partial^{(b)}}{\partial \boldsymbol{q}}\right)\right\} a(\boldsymbol{p}, \boldsymbol{q}) b(\boldsymbol{p}, \boldsymbol{q}) \delta_{\kappa\lambda}, \tag{A163}$$

which have the same form as the right-hand sides of (A55) and (A56), apart from the trivial Kronecker deltas.

In the special case that the operators are independent of the coordinate and momentum operators, i.e. if their Weyl transforms are of the type (A155), one finds from (A160) and (A161)

$$\tfrac{1}{2}\{A, B\} \rightleftarrows \tfrac{1}{2} \sum_\mu (a_{\kappa\mu} b_{\mu\lambda} + b_{\kappa\mu} a_{\mu\lambda}), \tag{A164}$$

$$-\frac{i}{\hbar}[A, B] \rightleftarrows -\frac{i}{\hbar} \sum_\mu (a_{\kappa\mu} b_{\mu\lambda} - b_{\kappa\mu} a_{\mu\lambda}). \tag{A165}$$

While the special case (A162–163) has a classical limit of the form (A58–59), the special case (A164–165) has no classical limit.

c. *The Wigner function*

As the Weyl transform of the density operator $P(t) = |\psi(t)\rangle\langle\psi(t)|$ the Wigner function will be equipped with indices if one considers a particle with internal degrees of freedom. Indeed from (A145) one finds (cf. (A65)):

$$\rho_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q}; t) = h^{-3} \int \mathrm{d}\boldsymbol{v}\, \mathrm{e}^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{v}} \psi_\kappa(\boldsymbol{q} - \tfrac{1}{2}\boldsymbol{v}; t) \psi_\lambda^*(\boldsymbol{q} + \tfrac{1}{2}\boldsymbol{v}; t), \tag{A166}$$

where the wave function $\langle \boldsymbol{q}, \kappa | \psi(t) \rangle$ in the coordinate representation has been written as $\psi_\kappa(\boldsymbol{q}; t)$. The expectation value of an operator A follows now from (A158):

$$\bar{A}(t) = \bar{a}(t) \equiv \sum_{\kappa,\lambda} \int \mathrm{d}\boldsymbol{p}\, \mathrm{d}\boldsymbol{q}\, \rho_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q}; t) a_{\lambda\kappa}(\boldsymbol{p}, \boldsymbol{q}) \tag{A167}$$

(cf. (A62) with (A63)). The Wigner function is normalized to unity (cf. (A69)) as follows from $\mathrm{Tr}\,P(t) = 1$ and (A157):

$$\sum_\kappa \int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\,\rho_{\kappa\kappa}(\boldsymbol{p},\boldsymbol{q};t) = 1. \tag{A168}$$

The time evolution of the Wigner function follows by taking the Weyl transform of the equation for the time evolution of the density operator (A88):

$$\frac{\partial \rho_{\kappa\lambda}(\boldsymbol{p},\boldsymbol{q};t)}{\partial t} = \frac{1}{\hbar}\sin\left\{\frac{\hbar}{2}\left(\frac{\partial^{(h)}}{\partial \boldsymbol{q}}\cdot\frac{\partial^{(\rho)}}{\partial \boldsymbol{p}} - \frac{\partial^{(h)}}{\partial \boldsymbol{p}}\cdot\frac{\partial^{(\rho)}}{\partial \boldsymbol{q}}\right)\right\}\sum_\mu (h_{\kappa\mu}\rho_{\mu\lambda}+\rho_{\kappa\mu}h_{\mu\lambda})$$
$$-\frac{i}{\hbar}\cos\left\{\frac{\hbar}{2}\left(\frac{\partial^{(h)}}{\partial \boldsymbol{q}}\cdot\frac{\partial^{(\rho)}}{\partial \boldsymbol{p}} - \frac{\partial^{(h)}}{\partial \boldsymbol{p}}\cdot\frac{\partial^{(\rho)}}{\partial \boldsymbol{q}}\right)\right\}\sum_\mu (h_{\kappa\mu}\rho_{\mu\lambda}-\rho_{\kappa\mu}h_{\mu\lambda}), \tag{A169}$$

where $h_{\kappa\lambda}$ depends on $\boldsymbol{p}$ and $\boldsymbol{q}$ and $\rho_{\kappa\lambda}$ on $\boldsymbol{p}$, $\boldsymbol{q}$ and t. This equation may be used to find an expression for the time derivative of the expectation value of an operator (cf. (A95))

$$\frac{\mathrm{d}\bar{a}(t)}{\mathrm{d}t} = \frac{1}{\hbar}\sum_{\kappa,\lambda,\mu}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\,\rho_{\lambda\kappa}\left[\sin\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}}\cdot\frac{\partial^{(h)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}}\cdot\frac{\partial^{(h)}}{\partial \boldsymbol{q}}\right)\right\}(a_{\kappa\mu}h_{\mu\lambda}+h_{\kappa\mu}a_{\mu\lambda})\right.$$
$$\left.-i\cos\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}}\cdot\frac{\partial^{(h)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}}\cdot\frac{\partial^{(h)}}{\partial \boldsymbol{q}}\right)\right\}(a_{\kappa\mu}h_{\mu\lambda}-h_{\kappa\mu}a_{\mu\lambda})\right], \tag{A170}$$

where $a_{\kappa\lambda}$ and $h_{\kappa\lambda}$ depend on $\boldsymbol{p}$ and $\boldsymbol{q}$, and $\rho_{\kappa\lambda}$ on $\boldsymbol{p}$, $\boldsymbol{q}$ and t.

If the operator A does not act on the spin indices, i.e. if its Weyl transform is of the type (A154), expression (A170) becomes

$$\frac{\mathrm{d}\bar{a}(t)}{\mathrm{d}t} = \frac{2}{\hbar}\sum_{\kappa,\lambda}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\left[\sin\left\{\frac{\hbar}{2}\left(\frac{\partial^{(a)}}{\partial \boldsymbol{q}}\cdot\frac{\partial^{(h)}}{\partial \boldsymbol{p}} - \frac{\partial^{(a)}}{\partial \boldsymbol{p}}\cdot\frac{\partial^{(h)}}{\partial \boldsymbol{q}}\right)\right\} a h_{\kappa\lambda}\right]\rho_{\lambda\kappa}, \tag{A171}$$

where a, $h_{\kappa\lambda}$ and $\rho_{\kappa\lambda}$ depend on $\boldsymbol{p}$ and $\boldsymbol{q}$, and $\rho_{\kappa\lambda}$ moreover on t. If on the other hand the operator A is independent of the coordinate and momentum operators, so that its Weyl transform is of the type (A155), one has for (A170)

$$\frac{\mathrm{d}\bar{a}(t)}{\mathrm{d}t} = \frac{i}{\hbar}\sum_{\kappa,\lambda,\mu}\int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}(h_{\kappa\mu}a_{\mu\lambda}-a_{\kappa\lambda}h_{\mu\lambda})\rho_{\lambda\kappa} \tag{A172}$$

with $h_{\kappa\lambda}$ depending on $\boldsymbol{p}$, $\boldsymbol{q}$ and $\rho_{\kappa\lambda}$ on $\boldsymbol{p}$, $\boldsymbol{q}$ and t. If the Weyl transform of the Hamiltonian is such that

$$\lim_{\hbar\to 0} h_{\kappa\lambda}(\boldsymbol{p},\boldsymbol{q}) = \delta_{\kappa\lambda}h_{\mathrm{cl}}(\boldsymbol{p},\boldsymbol{q}), \tag{A173}$$

the expression (A171) has a classical limit. The expression (A172) however has no classical limit.

PROBLEMS

1. Prove the following theorems on exponentials of operators A and B, which commute with their commutator $[A, B]$:

$$\mathrm{e}^{A+B} = \mathrm{e}^A\mathrm{e}^B\mathrm{e}^{-\frac{1}{2}[A,B]} = \mathrm{e}^B\mathrm{e}^A\mathrm{e}^{\frac{1}{2}[A,B]}, \tag{P1}$$
$$\mathrm{e}^{A+B} = \mathrm{e}^{\frac{1}{2}A}\mathrm{e}^B\mathrm{e}^{\frac{1}{2}A} = \mathrm{e}^{\frac{1}{2}B}\mathrm{e}^A\mathrm{e}^{\frac{1}{2}B}. \tag{P2}$$

Hint: Prove first the lemma (λ is a number)

$$f(\lambda) \equiv \mathrm{e}^{\lambda A}B\mathrm{e}^{-\lambda A} = B+\lambda[A, B]. \tag{P3}$$

This follows by integration of $\partial f/\partial\lambda$. In the same way it follows, using also (P3), that

$$g(\lambda) \equiv \mathrm{e}^{\lambda A}\mathrm{e}^{\lambda B} = \mathrm{e}^{\lambda(A+B)}\mathrm{e}^{\frac{1}{2}\lambda^2[A,B]}, \tag{P4}$$

of which (P1) is a special case. Note the useful corollary of (P1):

$$\mathrm{e}^A\mathrm{e}^B = \mathrm{e}^B\mathrm{e}^A\mathrm{e}^{[A,B]}. \tag{P5}$$

The relation (P2) follows if (P5) is used at the right-hand side, and then (P1) applied.

2. Show that taking the Weyl transform of an operator $A(\boldsymbol{P}, \boldsymbol{Q})$ and performing a linear transformation of the coordinate and momentum operators $\hat{\boldsymbol{Q}} = \mathbf{c}\cdot\boldsymbol{Q}$ and $\hat{\boldsymbol{P}} = \boldsymbol{P}\cdot\mathbf{c}^{-1}$ ($\mathbf{c}$ is a matrix of c-numbers) (or $\hat{\boldsymbol{q}} = \mathbf{c}\cdot\boldsymbol{q}$, $\hat{\boldsymbol{p}} = \boldsymbol{p}\cdot\mathbf{c}^{-1}$ of their Weyl transforms) are commuting operations. The proof consists in showing – on the basis of (29) and (30) – that one gets the same result if one takes the Weyl transform of the operator and then transforms $\boldsymbol{q}$ and $\boldsymbol{p}$ or if one transforms $\boldsymbol{Q}$ and $\boldsymbol{P}$ and then takes the Weyl transform.

3. Prove the relation (38) from (37) and (41).

4. A relation like (A29), but with the operator P interchanged with Q and the Weyl transform p interchanged with q, is valid also. An example of this relation is

$$p^2q \rightleftarrows \tfrac{1}{2}(P^2Q+QP^2).$$

Compare this result with (A34) and show that they are identical.

5. Prove from (A33) and (A35) that the square of the operator of which the Weyl transform is pq is different from the operator of which the Weyl transform is $(pq)^2$ by explicitly evaluating both operators in terms of the operators P and Q.

6. Prove the relation (A30) by making use of the Weyl transform (A55).

7. Prove that for the propagator

$$\mathscr{K} \equiv \langle \boldsymbol{q} | U(t, t_0) | \boldsymbol{q}_0 \rangle$$

of the Schrödinger equation $|\psi(t)\rangle = U(t, t_0)|\psi(t_0)\rangle$ with $U(t, t_0) = \exp\{-(i/\hbar)H(t-t_0)\}$ and the Hamiltonian operator $H = \boldsymbol{P}^2/2m + V(\boldsymbol{Q})$, with Weyl transform $h = \boldsymbol{p}^2/2m + V(\boldsymbol{q})$, one can derive the Feynman path integral

$$\mathscr{K} = \lim_{n\to\infty} \int \ldots \int \mathrm{d}\boldsymbol{q}_1 \ldots \mathrm{d}\boldsymbol{q}_{n-1} \prod_{j=0}^{n-1} \left\{ \frac{m}{ih(t_{j+1}-t_j)} \right\}^{\frac{3}{2}} \mathrm{e}^{(i/\hbar)(t_{j+1}-t_j)l_j}$$

with

$$l_j \equiv l\left(\frac{\boldsymbol{q}_{j+1}-\boldsymbol{q}_j}{t_{j+1}-t_j}, \frac{\boldsymbol{q}_j+\boldsymbol{q}_{j+1}}{2}\right) = \tfrac{1}{2}m\left(\frac{\boldsymbol{q}_{j+1}-\boldsymbol{q}_j}{t_{j+1}-t_j}\right)^2 - V\left(\frac{\boldsymbol{q}_j+\boldsymbol{q}_{j+1}}{2}\right),$$

which is sometimes[1] symbolically written as

$$\mathscr{K} = \sum_{\text{all paths}} \mathrm{e}^{(i/\hbar)\int l(\dot{q},q)\mathrm{d}t}.$$

Hint: The propagator may first be written as

$$\mathscr{K} = \lim_{n\to\infty} \int \ldots \int \mathrm{d}\boldsymbol{q}_1 \ldots \mathrm{d}\boldsymbol{q}_{n-1} \prod_{j=0}^{n-1} \langle \boldsymbol{q}_{j+1} | U(t_{j+1}, t_j) | \boldsymbol{q}_j \rangle$$

with $\boldsymbol{q}_n \equiv \boldsymbol{q}$ and $t \equiv t_n > t_{n-1} > \ldots > t_1 > t_0$. Now use (13) for $U(t_{j+1}, t_j) = 1-(i/\hbar)(t_{j+1}-t_j)H$ up to terms linear in $t_{j+1}-t_j$ (its Weyl transform may be written again as an exponential) and apply the relation (A37). Integration over $\boldsymbol{p}$ will then yield the result.

Note: The result may be generalized to the case of a particle in a field, described by a Hamilton operator

$$H = \left(\boldsymbol{P} - \frac{e}{c}\boldsymbol{A}\right)^2 /2m + V(\boldsymbol{Q}).$$

The theorem is not true for arbitrary Hamiltonians (v. Groenewold, loc. cit.).

[1] R. P. Feynman, Rev. Mod. Phys. **20**(1948)367; H. J. Groenewold, Mat. Fys. Medd. Dan. Vid. Selsk. **30**(1956)no. 19.

8. Show that for a free particle the wave packet, which at time t_0 is described by the Wigner function (A110) as a minimum wave packet, is at time $t \neq t_0$ described by the Wigner function

$$\rho(\boldsymbol{p}, \boldsymbol{q}; t) = (2/h)^3 \exp\left[-\frac{\{\boldsymbol{q}-\boldsymbol{q}_0-(\boldsymbol{p}/m)(t-t_0)\}^2}{2\Delta^2} - \frac{2\Delta^2(\boldsymbol{p}-\boldsymbol{p}_0)^2}{\hbar^2}\right],$$

by using the time evolution equation (A89) with $h = \boldsymbol{p}^2/2m$. Note that at times $t \neq t_0$ the wave packet shows correlations between the variables $\boldsymbol{p}$ and $\boldsymbol{q}$; in other words it is only a minimum wave packet at time $t = t_0$.

9. Prove that for Hamiltonians, which are at most quadratic in the coordinates and momenta the time evolution equation (A89) for the Wigner function reduces to the simple form

$$\frac{\partial\rho}{\partial t} = \{h, \rho\}_{\mathrm{P}}$$

with the Poisson bracket of the Weyl transform h of the Hamiltonian and the Wigner function. Physical examples are: the free particle ($h = \boldsymbol{p}^2/2m$), the particle in a constant force field ($h = \boldsymbol{p}^2/2m - \boldsymbol{a}\cdot\boldsymbol{q}$) and the harmonic oscillator ($h = \boldsymbol{p}^2/2m + \frac{1}{2}m\omega^2\boldsymbol{q}^2$). It is well known that not all aspects of quantum mechanics show up clearly for these examples. The fact that the time evolution equation for the Wigner function, although quantum-mechanical, looks formally like the classical equation for the time evolution of a classical distribution function (h is then to be replaced by the classical Hamiltonian) is another illustration of this feature.

Prove also that for these Hamiltonians the expression (A95) for the time derivative of an expectation value reduces to

$$\frac{\mathrm{d}\bar{a}(t)}{\mathrm{d}t} = \int \mathrm{d}\boldsymbol{p}\,\mathrm{d}\boldsymbol{q}\{a, h\}\rho(\boldsymbol{p}, \boldsymbol{q}; t),$$

which is again analogous to, but different from the classical case.

10. Prove the Weyl correspondence

$$ABC \rightleftarrows \exp\left\{\frac{i\hbar}{2}\left(\frac{\partial^{(a)}}{\partial\boldsymbol{q}}\cdot\frac{\partial^{(b)}}{\partial\boldsymbol{p}} - \frac{\partial^{(a)}}{\partial\boldsymbol{p}}\cdot\frac{\partial^{(b)}}{\partial\boldsymbol{q}} + \frac{\partial^{(a)}}{\partial\boldsymbol{q}}\cdot\frac{\partial^{(c)}}{\partial\boldsymbol{p}} - \frac{\partial^{(a)}}{\partial\boldsymbol{p}}\cdot\frac{\partial^{(c)}}{\partial\boldsymbol{q}} + \frac{\partial^{(b)}}{\partial\boldsymbol{q}}\cdot\frac{\partial^{(c)}}{\partial\boldsymbol{p}} - \frac{\partial^{(b)}}{\partial\boldsymbol{p}}\cdot\frac{\partial^{(c)}}{\partial\boldsymbol{q}}\right)\right\} \sum_{\mu,\nu} a_{\kappa\mu}(\boldsymbol{p}, \boldsymbol{q}) b_{\mu\nu}(\boldsymbol{p}, \boldsymbol{q}) c_{\nu\lambda}(\boldsymbol{p}, \boldsymbol{q}),$$

valid for the product of three operators A, B and C, acting on a spinor, with Weyl transforms $a_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q})$, $b_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q})$ and $c_{\kappa\lambda}(\boldsymbol{p}, \boldsymbol{q})$.

11. Verify that the expressions (74) for the field operators satisfy the equations (2).