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Schrödinger equation from an exact uncertainty principle

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Abstract
An exact uncertainty principle, formulated as the assumption that a classical ensemble is subject to random momentum fluctuations of a strength which is determined by and scales inversely with uncertainty in position, leads from the classical equations of motion to the Schrödinger equation.

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1. Introduction

The uncertainty principle is generally considered to be a fundamental conceptual tool for understanding differences between classical and quantum mechanics. As first argued by Heisenberg in 1927 [1], the fact that quantum states do not admit simultaneously precise values of conjugate observables, such as position and momentum, does not necessarily imply an incompleteness of the theory, but rather is consistent with not being able to simultaneously determine such observables experimentally to an arbitrary accuracy.

Corresponding uncertainty relations such as $\Delta x \Delta p \geqslant \hbar/2$ 'give us that measure of freedom from the limitations of classical concepts which is necessary for a consistent description of atomic processes' [2]. The uncertainty principle provides the basis of the Copenhagen interpretation of quantum mechanics, famously used by Bohr in defending the completeness of the theory against critics such as Einstein [3].

If regarded as merely asserting a physical limit on the degree to which classical concepts can be applied, the uncertainty principle is not sufficiently restrictive in content to supply a means for moving from classical mechanics to quantum mechanics. Thus Landau and Lifschitz write that 'this principle in itself does not suffice as a basis on which to construct a new mechanics of particles' [4]. In particular, uncertainty relations expressed as imprecise inequalities are not enough to pin down the essence of what is nonclassical about quantum mechanics. Authors have tended to point instead, for example, to the commutation relation

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$[\hat{x}, \hat{p}] = \mathrm{i}\hbar$ for quantum observables [5], or to the principle of superposition of wavefunctions [4, 6], in this regard.

However, it will be shown here that an *exact* form of the uncertainty principle may in fact be formulated, which provides the *single* key element in moving from the equations of motion of a classical ensemble to those of a quantum ensemble. In particular, if it is assumed that a classical ensemble is subject to random momentum fluctuations, *where the strength of these fluctuations is precisely determined by and scales inversely with uncertainty in position* (as characterized by the position probability density), then the resulting modified equations of motion are equivalent to the Schrödinger equation. Thus, surprisingly, there is an exact formulation of the uncertainty principle which does in fact capture the essence of what is 'quantum' about quantum mechanics.

In the following section we recall the description of a classical ensemble in terms of a pair of equations in configuration space (the Hamilton–Jacobi equation and the continuity equation), and provide the corresponding Lagrangian from which these equations follow. In section 3 we show that the above exact uncertainty principle leads to a modification of this Lagrangian (essentially incorporating the kinetic energy of the random momentum fluctuations), the form of which yields equations of motion equivalent to the Schrödinger equation. Further, an exact uncertainty *relation* for position and momentum uncertainties is derived, corresponding to the exact uncertainty principle, from which the usual Heisenberg inequality follows as a consequence.

Of course, equations of motion equivalent to the Schrödinger equation do not in themselves imply the full quantum formalism. Accordingly, in section 4 a Hamiltonian formulation is provided for the equations of motion, which leads naturally to the usual wavefunction representation as corresponding to the normal modes of the modified system. Conclusions are presented in section 5.

2. Classical mechanics

For simplicity, we limit ourselves to the case of a single particle, described in a configuration space of n dimensions. In the Hamilton–Jacobi formulation of classical mechanics, the equation of motion takes the form [7]

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\nabla S \cdot \nabla S + V = 0. \tag{1}$$

The velocity field $\boldsymbol{u}(\boldsymbol{x}, t)$ that describes the motion of the particle is related to the momentum potential $S(\boldsymbol{x}, t)$ by

$$\boldsymbol{u} = \frac{1}{m}\nabla S. \tag{2}$$

We assume that the initial conditions are not known exactly, and that the probability of finding the particle in a given volume of the configuration space is described by a probability density $P(\boldsymbol{x}, t)$. The probability density must satisfy the following two conditions: it must be normalized,

$$\int P \, \mathrm{d}^n x = 1$$

and it must satisfy a continuity equation,

$$\frac{\partial P}{\partial t} + \nabla \cdot \left(P \frac{1}{m} \nabla S \right) = 0. \tag{3}$$

Equations (1) and (3), together with (2), completely determine the motion of the classical ensemble. Equations (1) and (3) can be derived from the Lagrangian

$$L_C = \int P \left\{ \frac{\partial S}{\partial t} + \frac{1}{2m} \nabla S \cdot \nabla S + V \right\} \mathrm{d}^n x \, \mathrm{d}t \tag{4}$$

by fixed end-point variation ($\delta P = \delta S = 0$ at the boundaries) with respect to S and P.

3. The transition from classical mechanics to quantum mechanics

3.1. Momentum fluctuations

Consider now the possibility that the classical Lagrangian is not quite right, because ∇S is actually an average momentum: one also has a fluctuation $\boldsymbol{N}$ about ∇S. Thus the physical momentum is

$$\boldsymbol{p} = \nabla S + \boldsymbol{N}.$$

No particular underlying physical model will be assumed for the momentum fluctuation $\boldsymbol{N}$. Indeed, one could instead regard the fluctuations as fundamentally nonanalysable, being introduced as a simple device to remove the notion of individual particle trajectories (since $\boldsymbol{u}$ in equation (2) is no longer ascertainable).

Since the momentum fluctuation $\boldsymbol{N}$ may conceivably depend on position, the average over such fluctuations for a given quantity A at point $\boldsymbol{x}$ will be denoted by $\bar{A}$, while the average over fluctuations *and* position will be denoted by $\langle A \rangle$. One hence has the general relation $\langle A \rangle = \int P \bar{A} \, \mathrm{d}^n x$. A physically very reasonable *randomness* assumption for the momentum fluctuation $\boldsymbol{N}$ is that it vanishes on average everywhere, i.e. $\bar{\boldsymbol{N}} \equiv 0$. However, here only two weaker assumptions will be made:

$$\langle \boldsymbol{N} \rangle = 0 \qquad \langle \nabla S \cdot \boldsymbol{N} \rangle = 0. \tag{5}$$

The first of these states that the fluctuations are unbiased and the second that the fluctuations are linearly uncorrelated with the average momentum ∇S.

It follows that when the momentum fluctuations are significant, the kinetic energy term $\left\langle \frac{1}{2m} \nabla S \cdot \nabla S \right\rangle$ in the Lagrangian should be replaced by $\left\langle \frac{1}{2m} (\nabla S + \boldsymbol{N}) \cdot (\nabla S + \boldsymbol{N}) \right\rangle$, yielding the modified Lagrangian

$$\begin{aligned} L &= \int P \left\{ \frac{\partial S}{\partial t} + \frac{1}{2m} \overline{(\nabla S + \boldsymbol{N}) \cdot (\nabla S + \boldsymbol{N})} + V \right\} \mathrm{d}^n x \, \mathrm{d}t \\ &= \int P \left\{ \frac{\partial S}{\partial t} + \frac{1}{2m} \nabla S \cdot \nabla S + V \right\} \mathrm{d}^n x \, \mathrm{d}t + \frac{1}{2m} \int P \overline{\boldsymbol{N} \cdot \boldsymbol{N}} \, \mathrm{d}^n x \, \mathrm{d}t \\ &\equiv L_C + \frac{1}{2m} \int (\Delta N)^2 \, \mathrm{d}t \end{aligned} \tag{6}$$

where ΔN is the average rms momentum fluctuation, given by $\langle \boldsymbol{N} \cdot \boldsymbol{N} \rangle^{1/2}$. Thus the consequence of taking into consideration the momentum fluctuations is to add a positive term to the Lagrangian, arising from the additional kinetic energy due to the fluctuations.

3.2. Exact uncertainty principle

How can we estimate the magnitude of this additional term, if we do not know anything else about the system except the probability density P and the average momentum ∇S? To estimate the magnitude of the momentum spread, we will assume that an exact uncertainty principle holds, in the sense that the strength of the momentum fluctuations at a given time is

inversely correlated with uncertainty in position at that time, where the uncertainty of position is characterized by P. Clearly, this assumption is an additional hypothesis that is *independent* of classical mechanics.

To make this assumption precise, consider the general case of an n-dimensional space and a one-parameter family of probability distributions (which we label with a parameter $k > 0$) at time t_0, related by a rescaling of variables

$$P(\boldsymbol{x}) \to P_k(\boldsymbol{x}) \equiv k^n P(k\boldsymbol{x}).$$

These transformations preserve the normalization,

$$\int P(\boldsymbol{x})\, \mathrm{d}^n x \to \int k^n P(k\boldsymbol{x})\, \mathrm{d}^n x = \int P(\boldsymbol{y})\, \mathrm{d}^n y$$

where we have introduced the change of variables $\boldsymbol{y} = k\boldsymbol{x}$. We also have

$$\nabla P(\boldsymbol{x}) \cdot \nabla P(\boldsymbol{x}) \to k^{2n+2} \nabla_y P(\boldsymbol{y}) \cdot \nabla_y P(\boldsymbol{y})$$
$$\boldsymbol{x} \cdot \nabla P(\boldsymbol{x}) \to k^n \boldsymbol{y} \cdot \nabla_y P(\boldsymbol{y}).$$

Under such a transformation, any direct measurement of position uncertainty δx such as the rms uncertainty Δx changes according to the rule

$$\delta x \to \delta x_k \equiv \frac{1}{k}\,(\delta x).$$

Thus probability densities with different values of k represent physical systems that *only differ in how well we know the location of the particle*, since the shape of the probability densities is the same except for the rescaling. The exact uncertainty principle that we want to make use of corresponds roughly to the assumption that such a scaling of position by a factor $1/k$ scales the momentum fluctuation by a factor k.

More precisely, the exact uncertainty principle is equivalent to the statement that *the momentum fluctuation ΔN is determined by the uncertainty in position, where the latter is characterized by the probability density P, and where*

$$\Delta N \to k \Delta N \tag{7}$$

under k transformations. Note that the uncertainty product $\delta x\, \Delta N$ is thus preserved under k transformations, for any direct measure of position uncertainty δx.

To apply the exact uncertainty principle, we assume that the Lagrangian formalism remains applicable to L. Hence the additional term in equation (6) must be a spacetime integral over a scalar function of $\boldsymbol{x}$, P and S and their derivatives. Moreover, since $(\Delta N)^2$ is determined solely by position uncertainty (where the latter is characterized by P), then this additional term is in fact independent of S. Finally, for causality to be preserved (i.e. the equations of motion require only P and S to be specified on an initial surface), second and higher order derivatives of P must be excluded[4]. Hence, the additional term in the Lagrangian (6) can be written in the form

$$\int (\Delta N)^2\, \mathrm{d}t = \int P f(\boldsymbol{x}, P, \boldsymbol{x} \cdot \nabla P, \nabla P \cdot \nabla P)\, \mathrm{d}^n x\, \mathrm{d}t. \tag{8}$$

[4] Requirements of causality do not exclude a term linear in $\nabla^2 P$, but since it can be shown that such a term does not lead to a different result we will not consider it here.

The exact uncertainty principle requires f to transform under k transformations as follows:

$$\int P(\boldsymbol{x})\, f\,[\boldsymbol{x},\, P(\boldsymbol{x}),\, \boldsymbol{x}\cdot\nabla P(\boldsymbol{x}),\, \nabla P\cdot\nabla P(\boldsymbol{x})]\,\mathrm{d}^n x\,\mathrm{d}t$$
$$\to \int P(\boldsymbol{y})\, f\left(k^{-1}\boldsymbol{y},\, k^n P(\boldsymbol{y}),\, k^n \boldsymbol{y}\cdot\nabla_y P(\boldsymbol{y}),\, k^{2n+2}\nabla_y P(\boldsymbol{y})\cdot\nabla_y P(\boldsymbol{y})\right)\mathrm{d}^n y\,\mathrm{d}t$$
$$\equiv k^2 \int P(\boldsymbol{y})\, f(\boldsymbol{y},\, P(\boldsymbol{y}),\, \boldsymbol{y}\cdot\nabla_y P(\boldsymbol{y}),\, \nabla_y P(\boldsymbol{y})\cdot\nabla_y P(\boldsymbol{y}))\,\mathrm{d}^n y\,\mathrm{d}t.$$

This leads to the homogeneity condition

$$f(k^{-1}\boldsymbol{x}, k^n u, k^n v, k^{2n+2} w) = k^2 f(\boldsymbol{x}, u, v, w) \tag{9}$$

where we have introduced the more compact notation

$$u = P \qquad v = \boldsymbol{x}\cdot\nabla P \qquad w = \nabla P\cdot\nabla P. \tag{10}$$

From this requirement we derive the first-order partial differential equation

$$-\sum_{i=1}^{n} x_i \frac{\partial f}{\partial x_i} + nu\frac{\partial f}{\partial u} + nv\frac{\partial f}{\partial v} + (2n+2)w\frac{\partial f}{\partial w} = 2f. \tag{11}$$

The problem of finding the general integral of such an equation is equivalent to the problem of finding the general integral of a system of ordinary differential equations [8], which in our case is given by

$$-\frac{\mathrm{d}x_1}{x_1} = \cdots = -\frac{\mathrm{d}x_n}{x_n} = \frac{\mathrm{d}u}{nu} = \frac{\mathrm{d}v}{nv} = \frac{\mathrm{d}w}{(2n+2)w} = \frac{\mathrm{d}f}{2f}.$$

This system of ordinary differential equations has $(n+3)$ independent integrals, which can be chosen as

$$u^{-1}w^{1/2}x_i = \text{const}$$
$$u^{-1}v = \text{const}$$
$$u^{2/n}\boldsymbol{x}\cdot\boldsymbol{x} = \text{const}$$
$$u^2 w^{-1} f = \text{const}.$$

and the solution of the first-order partial differential equation (11) is then of the general form

$$f = (u^{-2}w)\, g(u^{-1}w^{1/2}\boldsymbol{x},\, u^{-1}v,\, u^{2/n}\boldsymbol{x}\cdot\boldsymbol{x}) \tag{12}$$

where g is an arbitrary function.

3.3. Independent subsystems

To determine f completely, we need to fix the form of g in equation (12). We therefore introduce a natural *independence* condition, by the requirement that the Lagrangian L decomposes into additive subsystem contributions for the case of a system composed of independent subsystems. This is equivalent to the condition that the momentum fluctuations N_1 and N_2 are linearly uncorrelated for two such subsystems, and hence can equivalently be interpreted as a further randomness assumption for the momentum fluctuations.

To investigate the requirements imposed on f by the independence condition, it will be sufficient to consider the case where we have a system consisting of two uncorrelated particles of mass m that do not interact, one particle described by a set of coordinates $\boldsymbol{x}_1$ and the other by $\boldsymbol{x}_2$. Thus P is of the form

$$P(\boldsymbol{x}_1, \boldsymbol{x}_2) = P_1(\boldsymbol{x}_1)P_2(\boldsymbol{x}_2) \tag{13}$$

and hence from equations (6) and (8) the independence condition requires

$$Pf = P_1 P_2 (f_1 + f_2) \tag{14}$$

where subscripts 1 and 2 refer to subsystems 1 and 2, respectively.

Equation (13) immediately implies the relations

$$u = u_1 u_2$$
$$v' \equiv u^{-1} v = u_1^{-1} v_1 + u_2^{-1} v_2 = v_1' + v_2'$$
$$w' \equiv u^{-2} w = u_1^{-2} w_1 + u_2^{-2} w_2 = w_1' + w_2'$$

and hence equation (12) becomes

$$f = (w_1' + w_2') g\big(\sqrt{w_1' + w_2'}\boldsymbol{x}, v_1' + v_2', (u_1 u_2)^{2/n} \boldsymbol{x} \cdot \boldsymbol{x}\big)$$

where $\boldsymbol{x} = (\boldsymbol{x}_1, \boldsymbol{x}_2)$. From equation (14), this form of f must decompose into the sum of a function of u_1, v_1', w_1' and $\boldsymbol{x}_1$, and a function of u_2, v_2', w_2' and $\boldsymbol{x}_2$. Since the factor that multiplies g, and the second and third arguments of g, are such functions (with respect to w', v', and $\boldsymbol{x}$ respectively), these terms cannot be mixed by the functional form of g. It follows that g must be of the form

$$g(\boldsymbol{a}, b, c) = C + g_0(\boldsymbol{a}) + b g_1(\boldsymbol{a}) + c g_2(\boldsymbol{a})$$

where C is a constant, and the functions g_j satisfy the condition

$$g_j(\lambda \boldsymbol{a}) = \lambda^{-2} g_j(\boldsymbol{a}) \quad j = 0, 1, 2 \tag{15}$$

(to allow cancellation of the factor $w_1' + w_2'$ that multiplies g). Hence

$$f = C(w_1' + w_2') + g_0(\boldsymbol{x}_1, \boldsymbol{x}_2) + (v_1' + v_2') g_1(\boldsymbol{x}_1, \boldsymbol{x}_2) + (u_1 u_2)^{2/n} (\boldsymbol{x}_1 \cdot \boldsymbol{x}_1 + \boldsymbol{x}_2 \cdot \boldsymbol{x}_2) g_2(\boldsymbol{x}_1, \boldsymbol{x}_2).$$

The independence condition equation (14) places further conditions on the g_j. First, g_0 is required to be a sum of a function of $\boldsymbol{x}_1$ and a function of $\boldsymbol{x}_2$. Hence it only represents a classical additive potential term (that satisfies the homogeneity condition (15) above), and so can be ignored as having no nonclassical role (it can be absorbed into the classical potential V in the Lagrangian). Secondly, to avoid subsystem cross terms, g_1 must be constant. But the homogeneity condition (15) is then only satisfied by the choice $g_1 = 0$. Thirdly, cross terms in u_1 and u_2 can only be avoided by choosing $g_2 = 0$.

The form of f thus reduces to the first term, $C(w_1' + w_2')$. From equation (14) this term is to be identified with the sum of f_1 and f_2, thus yielding the final form

$$f = C w' = C \frac{1}{P^2} \nabla P \cdot \nabla P \tag{16}$$

for f, where C is a universal constant. Note from equation (8) that C must be positive.

3.4. Equations of motion

The modified Lagrangian follows from equations (6), (8) and (16) as

$$L = \int P \left\{ \frac{\partial S}{\partial t} + \frac{1}{2m} \nabla S \cdot \nabla S + \frac{C}{2m} \frac{1}{P^2} \nabla P \cdot \nabla P + V \right\} \mathrm{d}^n x \, \mathrm{d}t. \tag{17}$$

Fixed end-point variation with respect to S leads again to (3), while fixed end-point variation with respect to P leads to

$$\frac{\partial S}{\partial t} + \frac{1}{2m} \nabla S \cdot \nabla S + \frac{C}{2m} \left[\frac{1}{P^2} \nabla P \cdot \nabla P - \frac{2}{P} \nabla^2 P \right] + V = 0. \tag{18}$$

Equations (3) and (18) are identical to the Schrödinger equation

$$i\hbar\partial\psi/\partial t = -(\hbar^2/2m)\nabla^2\psi + V\psi$$

provided the wavefunction $\psi(\boldsymbol{x}, t)$ is written in terms of S and P by

$$\psi = \sqrt{P}\exp\left(i\frac{S}{\hbar}\right)$$

and the constant C is set equal to

$$C = \left(\frac{\hbar}{2}\right)^2.$$

Just *why* one would introduce the wavefunction ψ at all is considered in section 4 below.

Note that the classical limit of the Schrödinger theory is not the Hamilton–Jacobi equation for a classical particle, but equations (1) and (3) which describe a classical ensemble.

3.5. Exact uncertainty relation

The Schrödinger equation has been derived above using an exact uncertainty principle to fix the strength of random momentum fluctuation in terms of the uncertainty in position. Note that no specific measure of position uncertainty was assumed; it was required only that the momentum fluctuations scale inversely with position uncertainty under k transformations. However, having obtained a unique form, equation (16), for the function f in (8) we are now in a position to write down an exact uncertainty *relation* relating position and momentum uncertainties.

For simplicity we consider the case of one dimension ($n = 1$), and define

$$\delta x = \left[\int P\left(\frac{1}{P}\frac{\mathrm{d}P}{\mathrm{d}x}\right)^2 \mathrm{d}x\right]^{-1/2}.$$

For the case of a Gaussian probability density with rms uncertainty σ one has $\delta x = \sigma$. More generally, this measure has units of position, scales appropriately with x ($\delta y = \lambda\delta x$ for $y = \lambda x$) and vanishes in the limit that P approaches a delta function. Hence it represents a direct measure of uncertainty in position. From equations (8) and (16) one has

$$\delta x\,\Delta N = \sqrt{C} = \frac{\hbar}{2}. \tag{19}$$

Thus we have an *exact* uncertainty relation between position and momentum. A quantum-operator form of this relation has been derived elsewhere, in which ΔN is replaced by the rms deviation of a nonclassical momentum operator [9].

The usual Heisenberg uncertainty relation can be derived from the above exact uncertainty relation. From the Cramer–Rao inequality of statistical estimation theory [10] one has $\Delta x \geqslant \delta x$, while the randomness assumptions in equation (5) imply

$$(\Delta p)^2 = \mathrm{Var}(\mathrm{d}S/\mathrm{d}x + N) = \mathrm{Var}(\mathrm{d}S/\mathrm{d}x) + (\Delta N)^2 \geqslant (\Delta N)^2$$

and hence it follows immediately from equation (19) that $\Delta x\,\Delta p \geqslant \hbar/2$.

4. Hamiltonian formulation and wavefunction representation

4.1. Hamiltonian formulation

In the previous section, we derived an extension of the classical Lagrangian which yields equations of motion equivalent to the Schrödinger equation. The Lagrangian field formalism

was conveniently used because it is well known. However, one can in fact obtain equivalent results using the *Hamiltonian* form of field theory, with no essential differences in the assumptions and manipulations used.

The Hamiltonian formalism does provide one important advantage: the concept of canonical transformations. In the previous section, the wavefunction representation $\psi = \sqrt{P}\exp\left(\mathrm{i}\frac{S}{\hbar}\right)$ was simply 'magicked out of thin air', to obtain the Schrödinger equation written in terms of the wavefunction ψ instead of the hydrodynamical variables P and S. In contrast, in the Hamiltonian formalism this complex combination of P and S arises immediately from asking a natural question about canonical transformations.

The Hamiltonian form corresponding to Lagrangian (17) is given by

$$H = \int P\left\{\frac{1}{2m}\nabla S\cdot\nabla S + \frac{\hbar^2}{8m}\frac{1}{P^2}\nabla P\cdot\nabla P + V\right\}\mathrm{d}^n x \equiv \int \mathcal{H}\,\mathrm{d}^n x \tag{20}$$

and is derived similarly. The field P plays the role of a field coordinate and S the role of the momentum canonically conjugate to P. The equations of motion are given by [7]

$$\frac{\partial P}{\partial t} = \{P, H\} = \frac{\delta H}{\delta S}$$
$$\frac{\partial S}{\partial t} = \{S, H\} = -\frac{\delta H}{\delta P}$$

where the Poisson bracket of two functions F and G is defined by

$$\{F(P(\boldsymbol{x}), S(\boldsymbol{x})), G(P(\boldsymbol{x}'), S(\boldsymbol{x}'))\} = \int\left[\frac{\delta F(\boldsymbol{x})}{\delta P(\boldsymbol{x}'')}\frac{\delta G(\boldsymbol{x}')}{\delta S(\boldsymbol{x}'')} - \frac{\delta F(\boldsymbol{x})}{\delta S(\boldsymbol{x}'')}\frac{\delta G(\boldsymbol{x}')}{\delta P(\boldsymbol{x}'')}\right]\mathrm{d}^n x''. \tag{21}$$

To simplify the formulae, we will sometimes use the notation $P \equiv P(\boldsymbol{x})$, $P' \equiv P(\boldsymbol{x}')$, etc which allows us to write equation (21) in the concise form

$$\{F, G'\} = \int\left[\frac{\delta F}{\delta P''}\frac{\delta G'}{\delta S''} - \frac{\delta F}{\delta S''}\frac{\delta G'}{\delta P''}\right]\mathrm{d}^n x''.$$

From

$$\frac{\delta P}{\delta P'} = \frac{\delta S}{\delta S'} = \delta^n(\boldsymbol{x} - \boldsymbol{x}') \tag{22}$$

we derive the Poisson bracket of the canonically conjugate fields as

$$\{P, S'\} = \delta^n(\boldsymbol{x} - \boldsymbol{x}').$$

The equations of motion that correspond to H are

$$\frac{\partial P}{\partial t} = \frac{\delta H}{\delta S} = -\nabla\cdot\left(P\frac{1}{m}\nabla S\right)$$
$$\frac{\partial S}{\partial t} = -\frac{\delta H}{\delta P} = -\left[\frac{1}{2m}\nabla S\cdot\nabla S + \frac{\hbar^2}{8m}\left(\frac{1}{P^2}\nabla P\cdot\nabla P - \frac{2}{P}\nabla^2 P\right) + V\right].$$

These equations are of course identical to (3) and (18) which were derived using the Lagrangian formalism.

4.2. Wavefunctions and normal modes

The Hamiltonian form H has been expressed in (20) in terms of fields which represent important physical quantities: P has the physical interpretation of a position probability density and S that of an average momentum potential. However, H can be rewritten in terms of any pair of

fields ϕ and χ without changing the physical content provided they are related to P and S by a canonical transformation, i.e.

$$\{P, S'\} = \int \left[\frac{\delta P}{\delta \phi''} \frac{\delta S'}{\delta \chi''} - \frac{\delta P}{\delta \chi''} \frac{\delta S'}{\delta \phi''} \right] \mathrm{d}^n x'' = \{\phi, \chi'\}. \tag{23}$$

Of course, such a transformation is generally only of interest if the new fields have some particular physical significance.

One transformation of obvious physical interest, when it exists, is to two fields ϕ and χ which have uncoupled equations of motion. Such fields label two independent physical degrees of freedom in the system, and hence have fundamental physical significance as the 'normal modes' of the system. It is therefore natural to ask whether such a transformation exists for H, i.e. whether there is a one–one mapping

$$P = P(\phi, \chi) \qquad S = S(\phi, \chi)$$

such that the fields ϕ and χ are uncoupled. It will be seen that this question is sufficient to *derive* the wavefunction representation $\psi = \sqrt{P} \exp\left(\mathrm{i}\frac{S}{\hbar}\right)$ and its complex conjugate from the Hamiltonian H, as corresponding to the physical fields describing the 'normal modes' of the system.

To examine the question of whether there is a canonical transformation that will lead to uncoupled equations of motion for ϕ and χ we first need to establish the following lemma.

Lemma. *A necessary condition for two conjugate fields ϕ and χ to be uncoupled is that the corresponding Hamiltonian density $\mathcal{H}'$ has the form*

$$\mathcal{H}' = F(\boldsymbol{x}, \phi, \chi) + A_k(\boldsymbol{x}, \phi, \chi)\partial_k\phi + B_k(\boldsymbol{x}, \phi, \chi)\partial_k\chi + G_{jk}(\boldsymbol{x}, \phi, \chi)(\partial_j\phi)(\partial_k\chi)$$

where $k = 1, \ldots, n$, repeated indices are summed over, and ∂_k denotes the partial derivative with respect to x_k. Furthermore, the symmetric part of G_{jk} is independent of ϕ and χ, i.e.

$$G_{jk}(\boldsymbol{x}, \phi, \chi) + G_{kj}(\boldsymbol{x}, \phi, \chi) = 2G_{jk}(\boldsymbol{x})$$

where $G_{jk}(\boldsymbol{x})$ is symmetric with respect to j and k.

Proof. For a Hamiltonian

$$H' = \int \mathcal{H}'(\boldsymbol{x}, \phi, \chi, \partial_k\phi, \partial_k\chi)\, \mathrm{d}^n x$$

the equations of motion are given by

$$\frac{\partial\phi}{\partial t} = \frac{\partial\mathcal{H}'}{\partial\chi} - \frac{\partial^2\mathcal{H}'}{\partial x_k(\partial_k\chi)} - \frac{\partial^2\mathcal{H}'}{(\partial\phi)\,\partial(\partial_k\chi)}\partial_k\phi - \frac{\partial^2\mathcal{H}'}{(\partial\chi)\,\partial(\partial_k\chi)}\partial_k\chi - \frac{\partial^2\mathcal{H}'}{\partial(\partial_l\phi)\,\partial(\partial_k\chi)}\partial_{kl}\phi - \frac{\partial^2\mathcal{H}'}{\partial(\partial_l\chi)\,\partial(\partial_k\chi)}\partial_{kl}\chi.$$

A similar expression is obtained for $\frac{\partial\chi}{\partial t}$. Since we assume that ϕ evolves independently of χ, then in particular no second derivatives of χ can appear in the above equation of motion for ϕ, and similarly, no second derivatives of ϕ can appear in the corresponding equation of motion for χ. Hence $\mathcal{H}'$ must be linear in both $\partial_k\phi$ and $\partial_k\chi$, and so $\mathcal{H}'$ has the general form given in the statement of the lemma. Substituting this form into the equation of motion for ϕ gives

$$\frac{\partial\phi}{\partial t} = \frac{\partial F}{\partial\chi} - \partial_k B_k + \left(\frac{\partial A_k}{\partial\chi} - \frac{\partial B_k}{\partial\phi} - \partial_j G_{kj} \right) \partial_k\phi - \frac{\partial G_{jk}}{\partial\phi}(\partial_j\phi)(\partial_k\phi) - G_{jk}\partial_{kl}\phi$$

and a similar equation for $\frac{\partial \chi}{\partial t}$. Hence, since G_{jk} is the coefficient of $\partial_{kl}\phi$ and $\partial_{kl}\chi$ in the respective equations of motion, the fields are uncoupled only if the symmetric part of G_{jk} is independent of both ϕ and χ. □

If we now express the Hamiltonian density $\mathcal{H}$ (20) in terms of the new variables, we find

$$\mathcal{H} = P\left\{\frac{1}{2m}\left[\left(\frac{\partial S}{\partial \phi}\right)^2 + \left(\frac{\hbar}{2}\right)^2\left(\frac{\partial \ln P}{\partial \phi}\right)^2\right]\nabla\phi\cdot\nabla\phi + \frac{1}{2m}\left[\left(\frac{\partial S}{\partial \chi}\right)^2 + \left(\frac{\hbar}{2}\right)^2\left(\frac{\partial \ln P}{\partial \chi}\right)^2\right]\right.$$
$$\left.\times\,\nabla\chi\cdot\nabla\chi + \frac{1}{m}\left[\frac{\partial S}{\partial \phi}\frac{\partial S}{\partial \chi} + \left(\frac{\hbar}{2}\right)^2\frac{\partial \ln P}{\partial \phi}\frac{\partial \ln P}{\partial \chi}\right]\nabla\phi\cdot\nabla\chi + V\right\}.$$

It follows immediately from the lemma that the first two terms of $\mathcal{H}$ must vanish, implying

$$\frac{\partial S}{\partial \phi} = \mathrm{i}\alpha\frac{\hbar}{2}\frac{\partial \ln P}{\partial \phi} \qquad \frac{\partial S}{\partial \chi} = \mathrm{i}\beta\frac{\hbar}{2}\frac{\partial \ln P}{\partial \chi} \tag{24}$$

where $\alpha, \beta = \pm 1$. Since P and S are real, the normal modes are therefore complex fields. Substituting equations (24) into the third term of $\mathcal{H}$, the lemma further implies that

$$G_{jk}(\boldsymbol{x}) = P\left(\frac{\hbar}{2}\right)^2\left(\frac{1-\alpha\beta}{m}\right)\frac{\partial \ln P}{\partial \phi}\frac{\partial \ln P}{\partial \chi}\delta_{jk} = G\delta_{jk}$$

where G is a constant (the last equality follows since the second term has no explicit $\boldsymbol{x}$ dependence). Now, if $\alpha = \beta$, the Hamiltonian density reduces to $\mathcal{H} = P(\phi, \chi)V$, and the inverse transformation to the fields P and S then yields a Hamiltonian density proportional to V, which is inconsistent with the form of $\mathcal{H}$. Therefore

$$\alpha = -\beta \qquad 2P\left(\frac{\hbar}{2}\right)^2\frac{1}{m}\left[\frac{\partial \ln P}{\partial \phi}\frac{\partial \ln P}{\partial \chi}\right] = G. \tag{25}$$

From equations (24) and (25) the Hamiltonian density $\mathcal{H}$ in terms of ϕ and χ is

$$\mathcal{H} = G\nabla\phi\cdot\nabla\chi + P(\phi, \chi)V$$

and the equations of motion take the simple form

$$\frac{\partial \phi}{\partial t} = \frac{\partial P}{\partial \chi}V - G\nabla^2\phi$$
$$-\frac{\partial \chi}{\partial t} = \frac{\partial P}{\partial \phi}V - G\nabla^2\chi.$$

For these equations to be uncoupled P must be of the form $P = W + X\phi + Y\chi + Z\phi\chi$, which when substituted into (25) yields

$$P = \left(\frac{2}{\hbar}\right)^2\frac{m}{2}G\,(\phi + K)\,(\chi + L) \tag{26}$$

where K and L are constants (related to X, Y and Z). The general form of $S(\phi, \chi)$ is found by substitution of (26) in (24) with $\alpha = -\beta$, which leads to a pair of differential equations with solution

$$S = b + \mathrm{i}\alpha\frac{\hbar}{2}\ln\frac{\phi + K}{\chi + L} \tag{27}$$

where b is an arbitrary complex constant.

Equations (26) and (27) establish the functional forms of $P(\phi, \chi)$ and $S(\phi, \chi)$ that will permit uncoupled equations of motion for ϕ and χ. We now have to check that these functional forms lead to a canonical transformation. This requires

$$\begin{aligned}\{P, S'\} &= \int \left[\frac{\delta P}{\delta \phi''}\frac{\delta S'}{\delta \chi''} - \frac{\delta P}{\delta \chi''}\frac{\delta S'}{\delta \phi''}\right] \mathrm{d}^n x'' \\ &= -mG\left(\mathrm{i}\alpha\frac{2}{\hbar}\right)\delta^n(\boldsymbol{x} - \boldsymbol{x}') \\ &= \delta^n(\boldsymbol{x} - \boldsymbol{x}')\end{aligned}$$

and thus the value of G is fixed to be

$$G = \mathrm{i}\alpha\hbar/(2m).$$

Recalling that P and S are real (and using the property that P is positive), one can show that the inverse transformation follows from (26) and (27) as

$$\phi = a\sqrt{P}\exp(-\mathrm{i}\alpha S/\hbar) - K \tag{28}$$

$$\chi = \frac{\alpha\hbar}{\mathrm{i}a}\sqrt{P}\exp(\mathrm{i}\alpha S/\hbar) - L \tag{29}$$

where a is an arbitrary complex constant (related to b).

Thus, an essentially unique canonical transformation to uncoupled fields ϕ and χ indeed exists, given by equations (28) and (29). We recognize that these fields are, up to a scale factor and additive constant, the usual wavefunction $\psi = \sqrt{P}\exp\left(\mathrm{i}\frac{S}{\hbar}\right)$ and its complex conjugate, and hence the wavefunction has a fundamental physical significance as a 'normal mode' of the system. The corresponding Hamiltonian density $\mathcal{H}$ follows as

$$\begin{aligned}\mathcal{H} &= \frac{\mathrm{i}\alpha\hbar}{2m}\nabla\phi\cdot\nabla\chi + \frac{\mathrm{i}\alpha}{\hbar}V\,(\phi + K)\,(\chi + L) \\ &= \frac{\hbar^2}{2m}\,|\nabla\psi|^2 + V\,|\psi|^2\end{aligned}$$

for all choices of a, K and L, and leads directly to the Schrödinger equation and its conjugate.

We point out a quantization condition that follows from equations (27), (28) and (29). If $\Phi(\boldsymbol{x})$ is a single-valued complex function, $\ln\Phi$ is a multi-valued function which satisfies $\oint_C \mathrm{d}\ln\Phi = \pm\mathrm{i}2\pi n$, where n is an integer. If we make the assumption that the fields ϕ and χ describing the 'normal modes' of the system are single-valued functions, then

$$\oint_C \mathrm{d}S = -\mathrm{i}\alpha\frac{\hbar}{2}\oint_C \mathrm{d}(\ln\psi - \ln\psi^*) = \pm 2\pi\hbar n.$$

This is precisely the quantization condition that was introduced by Takabayasi as 'a new postulate' in his hydrodynamic interpretation of quantum mechanics [11]. This subsidiary condition is of course compatible with the equations of motion.

4.3. Expectation values

While the wavefunction and the corresponding wave equation have been obtained, these do not represent the full quantum formalism. For example, the nature of the assumptions about momentum fluctuations in section 3.1 provides recipes for calculating the first two moments of the momentum distribution in terms of integrals that can now be expressed in terms of the wavefunction, since

$$\langle \boldsymbol{p} \rangle = \int P \nabla S \, \mathrm{d}^n x = \frac{\hbar}{\mathrm{i}} \int \psi^* \nabla \psi \, \mathrm{d}^n x$$
$$\langle p^2 \rangle = \int P \left(\nabla S \cdot \nabla S + \left(\frac{\hbar}{2} \right)^2 \frac{1}{P^2} \nabla P \cdot \nabla P \right) \mathrm{d}^n x = \hbar^2 \int |\nabla \psi|^2 \, \mathrm{d}^n x.$$

However, it is not immediately clear how within this framework higher order moments are to be calculated, nor expectation values of functions of position and momentum. We briefly note here a possible approach to this problem, based on a symmetry in the representation of position and momentum displacements, which leads to the usual relations assumed in the Hilbert space formulation of quantum mechanics.

Under a position displacement T_a: $\boldsymbol{x} \to \boldsymbol{x} + \boldsymbol{a}$, the fields P and S transform as $P(\boldsymbol{x}) \to P(\boldsymbol{x} - \boldsymbol{a})$, $S(\boldsymbol{x}) \to S(\boldsymbol{x} - \boldsymbol{a})$. Hence in the wavefunction representation one has

$$T_a \colon \psi(\boldsymbol{x}) \to \psi(\boldsymbol{x} - \boldsymbol{a}). \tag{30}$$

Under a momentum displacement M_q: $\boldsymbol{p} \to \boldsymbol{p} + \boldsymbol{q}$, the position distribution (which is given by the field P) should be unaffected, while the average momentum must change by $\boldsymbol{q}$, $\nabla S \to \nabla S + \boldsymbol{q}$. Therefore, the fields P and S transform as $P(\boldsymbol{x}) \to P(\boldsymbol{x})$, $S(\boldsymbol{x}) \to S(\boldsymbol{x}) + \boldsymbol{q} \cdot \boldsymbol{x}$ (where an arbitrary additive constant added to S has been ignored, as it has no effect on the equations of motion). Hence in the wavefunction representation one has

$$M_q \colon \psi(\boldsymbol{x}) \to \exp(\mathrm{i}\boldsymbol{q} \cdot \boldsymbol{x}/\hbar)\psi(\boldsymbol{x}). \tag{31}$$

Comparing (30) and (31), one recognizes that the transformations T_a and M_q are Fourier-pairs. In particular, if one defines the Fourier transform of $\psi(\boldsymbol{x})$ by

$$\varphi(\boldsymbol{p}) = \frac{1}{(2\pi\sigma)^{-n/2}} \int \psi(\boldsymbol{x}) \exp(\mathrm{i}\boldsymbol{x} \cdot \boldsymbol{p}/\sigma) \, \mathrm{d}^n x$$

where σ is a constant with units of action, then one has

$$T_a \colon \varphi(\boldsymbol{p}) \to \exp(\mathrm{i}\boldsymbol{a} \cdot \boldsymbol{p}/\sigma)\varphi(\boldsymbol{p}) \qquad M_q \colon \varphi(\boldsymbol{p}) \to \varphi(\boldsymbol{p} - \sigma \boldsymbol{q}/\hbar).$$

Comparing with equations (30) and (31), there is a direct symmetry between ψ and φ under position and momentum translations, provided one sets $\sigma = \hbar$.

In light of this symmetry, it is natural to postulate that, in analogy to $P(\boldsymbol{x}) = |\psi(\boldsymbol{x})|^2$, the momentum probability density is given by $\tilde{P}(\boldsymbol{p}) = |\varphi(\boldsymbol{p})|^2$. Under this postulate one finds that

$$\langle f(\boldsymbol{p}) \rangle = \int \tilde{P}(\boldsymbol{p}) f(\boldsymbol{p}) \, \mathrm{d}^n p = \int \psi^*(\boldsymbol{x}) f\left(\frac{\hbar}{\mathrm{i}} \nabla \right) \psi(\boldsymbol{x}) \, \mathrm{d}^n x$$

which then leads to the natural generalization

$$\langle f(\boldsymbol{x}, \boldsymbol{p}) \rangle = \int \psi^*(\boldsymbol{x}) f\left(\boldsymbol{x}, \frac{\hbar}{\mathrm{i}} \nabla \right) \psi(\boldsymbol{x}) \, \mathrm{d}^n x \tag{32}$$

as per standard quantum theory (where in general an operator ordering must be specified for the expectation value to be well defined).

Finally, we point out another approach that is also natural within this framework. Since the equations of motion in the variables ψ and ψ^* are linear, it is natural to investigate the

group of canonical transformations that preserve the linearity of these equations. This leads us to consider the group of functional transformations of the form

$$\rho(\boldsymbol{y}) = \int K(\boldsymbol{x}, \boldsymbol{y})\psi(\boldsymbol{x})\,\mathrm{d}^n x$$

$$\rho^*(\boldsymbol{y}) = \int K^*(\boldsymbol{x}, \boldsymbol{y})\psi^*(\boldsymbol{x})\,\mathrm{d}^n x.$$

Using (22), a simple calculation leads to the following condition for the transformation to be canonical:

$$\{\rho, \rho^{*\prime}\} = \int \left[\frac{\delta\rho}{\delta\psi''}\frac{\delta\rho^{*\prime}}{\delta\psi^{*\prime\prime}} - \frac{\delta\rho}{\delta\psi^{*\prime\prime}}\frac{\delta\rho^{*\prime}}{\delta\psi''}\right]\mathrm{d}^n x''$$
$$= \int K(\boldsymbol{x}'', \boldsymbol{y})K^*(\boldsymbol{x}'', \boldsymbol{y}')\,\mathrm{d}^n x'' = \delta(\boldsymbol{y} - \boldsymbol{y}').$$

This is the condition for a transformation to be unitary. Arguments similar to those discussed above can then be used to single out the choice

$$K(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{(2\pi\hbar)^{-n/2}}\exp(\mathrm{i}\boldsymbol{x}\cdot\boldsymbol{y}/\hbar)$$

which corresponds to the transformation that leads to the momentum space representation.

5. Conclusions

We have shown that an exact uncertainty principle, formulated in the form that the strength of the momentum fluctuations is inversely correlated with the uncertainty in position, leads from the classical equations of motion to the Schrödinger equation. The assumptions that we used for this fall into three main categories: maximal randomness (equations (5) and (14)), an exact uncertainty principle (equation (7)) and causality (equation (8)).

The additional term in the Lagrangian is essentially the Fisher information, originally introduced by Fisher [12] as a measure of 'intrinsic accuracy' in statistical estimation theory. This Fisher information term was derived using an information theoretical approach in [13]. The connection between Fisher information and quantum mechanics has been developed further in [9], where it was shown that the Fisher information is proportional to the difference of a classical and quantum variance (thus providing a measure of nonclassicality) and to the rate of entropy increase under Gaussian diffusion (thus providing a measure of robustness). The operator formulation of the exact uncertainty relation in equation (19) is studied in detail in [14] including its extension to entangled systems. We point out that in all of these references the Fisher information is defined in the usual way, that is, as a functional of the probability distribution—and therefore, one should not confuse it with the quantity by the same name that appears in Frieden [15], which is essentially a generalized Fisher information defined for wavefunctions and proportional to the quantum kinetic energy.

It is worth noting that the approach here, based on exact uncertainty, is rather different from other approaches which assign physical meaning to fields P and S related to the wavefunction. For example, in the de Broglie–Bohm approach [16], there are *no* momentum fluctuations and the classical equations of motion for P and S are instead modified by adding a mass-dependent 'quantum potential', Q, to the classical potential term in the Hamilton–Jacobi equation. The form of this quantum potential is left unexplained and is interpreted as arising from the influence of an associated wave acting on the system. Similarly, while Bohm and Vigier generalize Bohm's original formalism to permit fluctuations of momentum

about ∇S, this is merely to ensure that an ensemble of such particles will quickly evolve to have a stable distribution given by the modulus-squared of the associated wave [17]. In contrast, in the exact uncertainty approach ∇S is an *average* momentum, the form of an additional kinetic energy term arising from random momentum fluctuations is *derived*, and no associated wave is assumed. The formal connection between the two approaches is the relation

$$\delta(L - L_C) = \int \mathrm{d}t\, \mathrm{d}^n x\, Q \delta P.$$

The exact uncertainty approach is also very different from the stochastic mechanics approach [18]. The latter postulates the existence of a classical stochastic process in configuration space, with a drift velocity assumed to be the gradient of some scalar, and defines an associated time-symmetric 'mean acceleration' $\boldsymbol{a}$ in terms of averages over both the stochastic process and a corresponding time-reversed process, which is postulated to obey Newton's law $m\boldsymbol{a} = -\nabla V$. In contrast, the exact uncertainty approach does not rely on a classical model of fluctuations, nor on a new definition of acceleration, nor on properties of stochastic processes running backwards in time. Indeed, as remarked in section 3.1, one may view the introduction of $\boldsymbol{N}$ as a means of effectively eliminating the notion of trajectories, differentiable or otherwise, from the classical hydrodynamical formulation of section 2. The formal connections between the approaches are

$$\nabla S = m\boldsymbol{u} \qquad (\Delta N)^2 = m^2 \langle \boldsymbol{v} \cdot \boldsymbol{v} \rangle$$

where $\boldsymbol{u} + \boldsymbol{v}$ and $\boldsymbol{u} - \boldsymbol{v}$ are the drift velocities of the forward-in-time and backward-in-time processes, respectively. It should be noted that $\langle \boldsymbol{u} \cdot \boldsymbol{v} \rangle \neq 0$, and hence, noting equation (5), one cannot identify $m\boldsymbol{v}$ with the random momentum fluctuation $\boldsymbol{N}$.

In [13] it was suggested that the Fisher information term represented an 'epistemological' contribution to the action, which in the context of the present analysis can be interpreted as reflecting a lack of detailed knowledge of nonclassical momentum fluctuations. In our approach we do not attempt to provide a 'realistic' model of such fluctuations, which would at any rate require a whole new (and nonlocal) theory that goes beyond quantum mechanics. Our approach to understanding quantum mechanics is therefore different from other descriptions based on the postulate of an underlying stochastic process, such as stochastic mechanics [18]. What our analysis primarily offers is a new way of viewing the uncertainty principle as *the* key concept in quantum mechanics. While it is true that no one before quantum mechanics would think of taking an uncertainty principle as a fundamental principle, our analysis is valuable in that it enforces the importance of the uncertainty principle in distinguishing quantum mechanics from classical mechanics—in a sense, it says that the uncertainty principle is *the* fundamental element that is needed for the transition to quantum mechanics.

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