A maximum entropy approach to wave mechanics

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ABSTRACT.

We employ the maximum entropy principle, in the context of statistical inference by impersonal physical interactions, together with the experimental position-momentum uncertainty phenomenon to construct the general wave mechanical static state of a single, interacting mass particle with no internal degrees of freedom. Subsequently, using Newtonian mechanics, this physically transparent entropic approach allows us to derive the corresponding wave mechanical expectation values and the equation of motion, i.e., the Schrödinger equation.

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1. Introduction

Since the advent of modern wave mechanics and Schrödinger's seminal papers [1] in 1920s, the origins of the theory have been a subject of much discussion and many approaches have been proposed over the past century, including Ref. [2] where a particular form of the uncertainty principle is assumed in order to derive the Schrödinger equation, that is, the fundamental equation that governs probabilistic states, i.e., wave functions. This uncertainty approach to wave mechanics is quite compelling as it allows to extend classical mechanics based on a single non-classical assumption, originally found as a matrix relation by Heisenberg [3]. In this article the experimental uncertainty phenomenon, together with the maximum entropy principle [4] are used to construct the general wave mechanical static state of a single, interacting mass particle with no internal degrees of freedom. Subsequently, Newtonian mechanics provides additional physical constraints to morph the probabilistic ensemble, hence to obtain the corresponding physical quantities and finally the dynamical representation, i.e., the Schrödinger equation.

2. The wave mechanical model

The well-known single or many slit electron diffraction experiment illustrates a non-classical phenomenon as individual electrons form a diffraction pattern as a collective behaviour [5; 6]. Therefore, electrons, like other point-like particles with small mass, behave statistically: every identical particle is observed at a random location but many observations form a probability distribution that is similar to the optical phenomenon where photons form an intensity pattern that can be explained by wave interference and Huygens' principle. Let us also recall that any wave motion can transfer not only energy, that is proportional to the square of its amplitude, but also momentum that is inversely proportional to its wavelength, and the wave form may also be a localized wave packet, along with its group velocity, when multiple simple waves are superposed. Thus, we are persuaded to conclude that the motion of a mass particle is wave-like and it does not travel along a classical path. Classically the state of motion of a mass particle is represented by its position $\mathbf{x}$ and momentum $\mathbf{p}$, and furthermore we can consider classical statistical mechanics where the state is a probabilistic variable. The observed wave interference pattern visibly implies that statistical mechanics is inadequate, but we may still assume that this peculiar distribution of microstates $(\mathbf{x}, \mathbf{p})$ obeys some wave physical rules and also the universal principle under which the information entropy of a physical system tends to be maximized [4]. Here the rather elusive concept of entropy is understood as a measure of uncertainty implied by a probability distribution, and every external interaction contributes to this objective state of knowledge, i.e., the global prior distribution about the physical reality, cf. Refs. [10; 18].

Let us examine the idealized single slit electron diffraction experiment where electrons arrive from far away with a definite momentum. When the slit is made more narrow, i.e., the location of those electrons that move through the slit become more accurate, we can observe that the direction of motion becomes more uncertain, i.e., the momentum spreads. Thus, we are strongly motivated to define the kinematic system of a single particle as a joint distribution of $\mathbf{x}$ and $\mathbf{p}$, and the statistical behaviour is understood as a new symmetry principle, but here we do not try to describe the reality behind the result of a single measurement of $\mathbf{x}$ or $\mathbf{p}$. Now we can state Heisenberg's uncertainty principle: *If the position/momentum in the system of a particle localises, then the momentum/position becomes more spread out*, cf. Refs. [3; 5; 17]. The time-independent reciprocity between $\mathbf{x}$ and $\mathbf{p}$, and intensity of related waves, suggest that there exists an invertible transformation that scales two weight amplitudes in a reciprocal manner, and the characteristical wave phenomenon motivates to seek a linear transformation. This approach should include both interference of probabilities and uncertainty (diffraction). In the spirit of the maximum entropy principle [4], we begin by forming unbiased estimations of the both distributions that model the time-independent random process and reciprocality. Our initial model is a symmetric spectral density estimation of two wave forms on the real line:

$$\psi(\mathbf{x}) = \sum_{\mathbf{p}\in\mathbb{R}\times\{0,0\}} \phi(\mathbf{p}) u_{\mathbf{p}}(\mathbf{x}) \text{ with the observable intensity } \sum_{\mathbf{x}\in\mathbb{R}\times\{0,0\}} \|\psi(\mathbf{x})\|^2 = 1, \tag{2.1}$$

$$\phi(\mathbf{p}) = \sum_{\mathbf{x}\in\mathbb{R}\times\{0,0\}} \psi(\mathbf{x}) v_{\mathbf{x}}(\mathbf{p}) \text{ with the observable intensity } \sum_{\mathbf{p}\in\mathbb{R}\times\{0,0\}} \|\phi(\mathbf{p})\|^2 = 1, \tag{2.2}$$

where ψ and ϕ are sums of weighted modes and the intensities $\|\psi\|^2$ and $\|\phi\|^2$ give respectively the position and momentum distributions. The common linear vector norm $\|\cdot\|$ is assumed to be induced by a suitable inner product, and the both intensity terms $\|\psi\|^2$ and $\|\phi\|^2$ may become sharply localized with unit value since the sum (2.1) or (2.2) may have only one non-zero term if we imagine an extremely narrow or wide slit. The intensity $\|\psi\|^2$ at the slit may seem constant, but nevertheless it is based on the smooth wave ψ in such a way that ϕ has a finite dispersion. This flat-topped shape at the slit indicates that the perpendicularly incoming wave is planar, thus we may assume that $u_{\mathbf{p}}(\mathbf{x}) = u(\mathbf{p}\cdot\mathbf{x})$ and $v_{\mathbf{x}}(\mathbf{p}) = v(\mathbf{p}\cdot\mathbf{x})$. Furthermore, the observed intensity $\|\phi(\mathbf{p})\|^2$ should not change under a constant shift of the slit, i.e., $\psi(\mathbf{x}) \to \psi(\mathbf{x}+\mathbf{x}_0)$, and this suggests that $v(\mathbf{p}\cdot(\mathbf{x}+\mathbf{x}_0)) = v(\mathbf{p}\cdot\mathbf{x})\delta(\mathbf{p}\cdot\mathbf{x}_0)$ and thus $\|\delta(\mathbf{p}\cdot\mathbf{x}_0)\phi(\mathbf{p})\| = \|\phi(\mathbf{p})\|$, where δ acts like a phase factor. The waves ψ and ϕ are also reciprocal, i.e., if $\psi(\mathbf{x})$ vanishes outside of a narrow interval $\Delta\mathbf{x}$, then $\phi(\mathbf{p})$ is non-zero on a large interval $\Delta\mathbf{p}$, and vice versa.

From now on we consider a generalized three-dimensional aperture that confines our wave ψ. We may assume that there exists a unitary linear transformation between the probabilistic "weight vectors" $\{\psi(\mathbf{x})\}_{\mathbb{R}^3}$ and $\{\phi(\mathbf{p})\}_{\mathbb{R}^3}$ that both have unit norm, and thus the both Eqs. (2.1) and (2.2) can be interpreted as an inner product of an orthonormal row vector and a probabilistic column vector, where the row elements are phase factors. Eventually, we assume that the state of motion of a mass particle is represented by the following sums over weighted plane waves, where the smooth functions ψ and ϕ are denoted as *wave functions*:

$$\psi(\mathbf{x}) = \int_{\mathbb{R}^3} \phi(\mathbf{p}) u(\mathbf{p}\cdot\mathbf{x}) d^3p \quad \text{and} \quad \phi(\mathbf{p}) = \int_{\mathbb{R}^3} \psi(\mathbf{x}) v(\mathbf{p}\cdot\mathbf{x}) d^3x. \tag{2.3}$$

From harmonic analysis, and also from the theory of optical diffraction [6], we may infer that a suitable method to connect the wave functions ψ and ϕ is a unitary Fourier transform, where the transformation pair contains both the spectrums and intensities of two random variables.[2] In Fourier theory, a vector of $\mathbf{x}$ in the infinite-dimensional vector space $L^2(\mathbb{R}^3;\mathbb{C})$ is projected onto an orthonormal basis made of vectors $\exp(i\mathbf{k}\cdot\mathbf{x})/(2\pi)^{3/2}$ or vectors $\exp(-i\mathbf{k}\cdot\mathbf{x})/(2\pi)^{3/2}$. Since both the position and momentum of a physical particle are finite, we have $\psi, \phi \to 0$ as $|\mathbf{x}|, |\mathbf{p}| \to \infty$, and therefore we can assume that $\psi, \phi \in L^2(\mathbb{R}^3;\mathbb{C})$. Consequently, ψ has the Fourier transform $\hat{\psi}$ and ϕ has the inverse Fourier transform $\check{\phi}$ as follows, see Refs. [7; 8]:

$$\psi(\mathbf{x}) = \frac{1}{\sqrt{2\pi}^3} \int_{\mathbb{R}^3} \hat{\psi}(\mathbf{k}) \exp(i\mathbf{k}\cdot\mathbf{x}) d^3k \quad \text{and} \quad \phi(\mathbf{p}) = \frac{1}{\sqrt{2\pi}^3} \int_{\mathbb{R}^3} \check{\phi}(\mathbf{q}) \exp(-i\mathbf{q}\cdot\mathbf{p}) d^3q. \tag{2.4}$$

Next we employ the natural L^2-norm to the probabilistic weights and thus the spectral densities become probability distributions. Here the intensity in each mode adds independently like in the length of an infinite-dimensional Cartesian vector. Due to Plancherel's theorem, we have

$$\int_{\mathbb{R}^3} |\psi(\mathbf{x})|^2 d^3x = \int_{\mathbb{R}^3} \left|\hat{\psi}(\mathbf{k})\right|^2 d^3k = 1 \quad \text{and} \quad \int_{\mathbb{R}^3} |\phi(\mathbf{p})|^2 d^3p = \int_{\mathbb{R}^3} \left|\check{\phi}(\mathbf{q})\right|^2 d^3q = 1. \tag{2.5}$$

[2] The choice of complex basis is due to its mathematical simplicity and the fact that we are only interested of intensities, but we can always use Euler's formula and choose a real two dimensional basis and thus represent the intensity as a sum of two squares, i.e., $|\psi_1 + i\psi_2|^2 = \psi_1^2 + \psi_2^2$. From an algebraic point of view, the Fourier transform behaves like a change of basis matrix, and the unitarity allows to connect two probabilistic vectors. Fourier methods are also at play in the closely related, dispersion theory-based work of Heisenberg [25; 26].

The wave functions ψ and ϕ can be connected if we do a substitution $\mathbf{p} := C\mathbf{k}$, where $C > 0$ is some experimental constant that has the dimension of [length $\times$ momentum] = [time $\times$ energy]. If we also substitute $\phi(\mathbf{p}) := \hat{\psi}(\mathbf{k})/C^{3/2}$, the probability condition remains unchanged:

$$\int_{\mathbb{R}^3} |\phi(\mathbf{p})|^2 \, d^3p = \int_{\mathbb{R}^3} \left|\hat{\psi}(\mathbf{k})/C^{3/2}\right|^2 C^3 \, d^3k = \int_{\mathbb{R}^3} \left|\hat{\psi}(\mathbf{k})\right|^2 d^3k = \int_{\mathbb{R}^3} |\psi(\mathbf{x})|^2 \, d^3x.$$

It turns out that the appropriate constant C is the reduced *Planck's constant* $\hbar = h/2\pi$ and its magnitude determines the waviness of a system; see the *de Broglie wavelength* in Refs. [5; 9]. Now we have replaced the concepts of determinism and point-like particles, and have adopted the phenomenological wave model to describe the maximally unbiased kinematical information:

$$\psi(\mathbf{x}) = \frac{1}{\sqrt{2\pi\hbar}^3} \int_{\mathbb{R}^3} \phi(\mathbf{p}) \exp(i\mathbf{p}\cdot\mathbf{x}/\hbar) d^3p, \tag{2.6}$$

$$\phi(\mathbf{p}) = \frac{1}{\sqrt{2\pi\hbar}^3} \int_{\mathbb{R}^3} \psi(\mathbf{x}) \exp(-i\mathbf{p}\cdot\mathbf{x}/\hbar) d^3x, \tag{2.7}$$

where $|\psi(\mathbf{x})|^2$ and $|\phi(\mathbf{p})|^2$ correspond respectively to the position and momentum distributions.

In a sense, the kinematic state of motion is a weighted sum over all possibilities, but here we do not assume that any of these possible states is the state of reality like in classical mechanics. Moreover, it is impossible to localize both probability distributions $|\psi|^2$ and $|\phi|^2$ simultaneously. To this end, we need to have a model for measuring statistical uncertainty or indeterminacy:[3]

If f belongs to $L^2(\mathbb{R}^3;\mathbb{C})$ and $\int_{\mathbb{R}^3} |f(\mathbf{x})|^2 \, d^3x = 1$, then the standard deviation of random variable $\mathbf{x} \in \mathbb{R}^3$ with probability density function $|f|^2$ about expected value $\mathbf{a} \in \mathbb{R}^3$ is

$$\triangle_{\mathbf{a}}(f) := \sqrt{\int_{\mathbb{R}^3} |\mathbf{x}-\mathbf{a}|^2 \, |f(\mathbf{x})|^2 \, d^3x}. \tag{2.8}$$

It is clear that $\triangle_{\mathbf{a}}(f)$ is a statistical measure of how much $|f|^2$ is localized around $\mathbf{a} \in \mathbb{R}^3$. Therefore, $\triangle_{\mathbf{x}'}(\psi)$ is the standard deviation of position distribution and $\triangle_{\mathbf{p}'}(\phi)$ is the standard deviation of momentum distribution, where $\mathbf{x}'$ and $\mathbf{p}'$ are the corresponding expectation values. After a change of variable, we note that $\triangle_{\mathbf{p}'}(\phi) = \hbar\triangle_{\mathbf{p}'/\hbar}(\hat{\psi}) = \hbar\triangle_{\mathbf{k}'}(\hat{\psi})$. Now we can introduce the mathematical Heisenberg's uncertainty principle (or inequality), see Refs. [7; 8]:

If f and every component of ∇f belong to $L^2(\mathbb{R}^3;\mathbb{C})$ and $\int_{\mathbb{R}^3} |f(\mathbf{x})|^2 \, d^3x = 1$, then

$$\triangle_{\mathbf{a}}(f)\triangle_{\mathbf{b}}(\hat{f}) \geq \frac{3}{2}, \quad \textit{for } \mathbf{a},\mathbf{b} \in \mathbb{R}^3. \tag{2.9}$$

We will find out below that the above condition $\nabla\psi \in L^2(\mathbb{R}^3)$ implies that the expectation value of momentum remains finite, as required. In what follows, we have the well-known formulation of Heisenberg's uncertainty principle that in the classical sense is a statistical result for an infinite ensemble of identically prepared particles, i.e., particles with identical wave functions. That is, let us consider a very large ensemble of identically prepared particles, and if we measure position of one half of the particles and momentum of the other half, as accurately as possible, then our (more or less objective) knowledge of particle's kinematic state is fundamentally limited by the positive – and in principle sharp – lower bound:

$$\triangle_{\mathbf{x}'}(\psi)\triangle_{\mathbf{p}'}(\phi) \geq \frac{3}{2}\hbar, \quad \text{for } \mathbf{x}',\mathbf{p}' \in \mathbb{R}^3. \tag{2.10}$$

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[3] The standard deviation is a natural measure of statistical uncertainty. However, let us note that in the framework of information theory, both the Fisher and Shannon information measures can be used to produce meaningful uncertainty relations due to ψ and ϕ, see Ref. [15]. But in any case, the wave mechanical uncertainty or indeterminacy is objective due to the collective nature of the assumed global prior probability distribution.

Due to Heisenberg's uncertainty principle, there are no sharp values for both dynamical variables $\mathbf{x}$ and $\mathbf{p}$ simultaneously. On the other hand, classically both position and momentum are always sharply single-valued observable quantities, e.g., a classical (ideal or projective) high energy measurement of position equals the complete information and hence $|\psi|^2$ will vanish outside the observed location $\mathbf{x}_0$. At the very same time, the momentum appears everywhere in the momentum space, i.e., it has become completely indefinite. Furthermore, if a physical interaction with the external environment changes the objective property of information content of a system, then every distribution is updated without delay in order to preserve the probability condition, i.e., the sum of probabilities remains unity, cf. Bayesian inference and Refs. [10; 18].

The peculiar fact that there is no definite value for the position of a particle allows to prevent the hydrogen atom from collapsing, an inevitable and paradoxal consequence of electrostatic forces in classical physics as the electron spirals into the nucleus and the atomic system releases an infinite amount of energy. The uncertainty principle allows a form of steady state equilibrium between the electron and nucleus, where the massive nucleus of a practically definite location is actively localizing the electron by interaction that carries energy; the information content of the state of motion induces an entropic pressure that counters the electric force that, in turn, accumulates information. This illustrates the objective or ontological nature of wave functions.

Having the pair of global prior amplitudes ψ and ϕ allows to consider the expectation value of a generic observable physical quantity $O(\mathbf{x}, \mathbf{p})$ in the non-relativistic regime. In particular, the position $\mathbf{x}$ of a particle, real valued potential energy $V(\mathbf{x})$ and corresponding external force $\mathbf{F}(\mathbf{x})$ acting on a particle have the following well-known expectation values:

$$\mathbb{E}_\psi(\mathbf{x}) = \int_{\mathbb{R}^3} \mathbf{x}\,|\psi(\mathbf{x})|^2\, d^3x = \int_{\mathbb{R}^3} [\mathbf{x}\psi(\mathbf{x})]\,\overline{\psi(\mathbf{x})}\, d^3x, \tag{2.11}$$

$$\mathbb{E}_\psi(V) = \int_{\mathbb{R}^3} V(\mathbf{x})\,|\psi(\mathbf{x})|^2\, d^3x = \int_{\mathbb{R}^3} [V(\mathbf{x})\psi(\mathbf{x})]\,\overline{\psi(\mathbf{x})}\, d^3x, \tag{2.12}$$

$$\mathbb{E}_\psi(\mathbf{F}) = \mathbb{E}_\psi(-\nabla V) = \int_{\mathbb{R}^3} [-\nabla V(\mathbf{x})\psi(\mathbf{x})]\,\overline{\psi(\mathbf{x})}\, d^3x. \tag{2.13}$$

Furthermore, as it is well-known, the expectation values of momentum $\mathbf{p}$, kinetic energy $T(\mathbf{p})$ and total energy $E(\mathbf{x}, \mathbf{p})$ can be represented in the position space, when we apply the Fourier transform of derivative and Plancherel's theorem:

$$\mathbb{E}_\phi(\mathbf{p}) = \int_{\mathbb{R}^3} \mathbf{p}\,|\phi(\mathbf{p})|^2\, d^3p = \int_{\mathbb{R}^3} [\mathbf{p}\phi(\mathbf{p})]\,\overline{\phi(\mathbf{p})}\, d^3p = \int_{\mathbb{R}^3} [-i\hbar\nabla\psi(\mathbf{x})]\,\overline{\psi(\mathbf{x})}\, d^3x = \mathbb{E}_\psi(\mathbf{p}), \tag{2.14}$$

$$\mathbb{E}_\phi(T) = \int_{\mathbb{R}^3} \frac{\mathbf{p}^2}{2m}\,|\phi(\mathbf{p})|^2\, d^3p = \int_{\mathbb{R}^3} \left[-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x})\right]\overline{\psi(\mathbf{x})}\, d^3x = \mathbb{E}_\psi(T), \tag{2.15}$$

$$\mathbb{E}_\psi(E) = \int_{\mathbb{R}^3} \left[-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x}) + V(\mathbf{x})\psi(\mathbf{x})\right]\overline{\psi(\mathbf{x})}\, d^3x. \tag{2.16}$$

In classical mechanics the angular momentum for a point-like mass particle with respect to the origin is $\mathbf{L} = \mathbf{x} \times \mathbf{p}$ and its componentwise representation is $L_1 = x_2p_3 - x_3p_2$, $L_2 = x_3p_1 - x_1p_3$ and $L_3 = x_1p_2 - x_2p_1$. For example, if we first consider term x_1p_2, then we need to consider the inverse Fourier transform of $p_2\phi(\mathbf{p})$ and multiply both sides by x_1. Thus, we have

$$\frac{1}{\sqrt{2\pi\hbar}^3}\int_{\mathbb{R}^3} (x_1p_2 - x_2p_1)\phi(\mathbf{p})\exp(i\mathbf{p}\cdot\mathbf{x}/\hbar)d^3p = -i\hbar\left(x_1\frac{\partial}{\partial x_2} - x_2\frac{\partial}{\partial x_1}\right)\psi(\mathbf{x}),$$

and by applying Plancherel's theorem:

$$\mathbb{E}_\phi(\mathbf{L}) = \int_{\mathbb{R}^3} (\mathbf{x}\times\mathbf{p})\,|\phi(\mathbf{p})|^2\, d^3p = \int_{\mathbb{R}^3} [(-i\hbar\mathbf{x}\times\nabla)\,\psi(\mathbf{x})]\,\overline{\psi(\mathbf{x})}\, d^3x = \mathbb{E}_\psi(\mathbf{L}). \tag{2.17}$$

Together with interference experiments, the hydrogen atom is a paradigm in wave mechanics. Let us consider Eq. (2.16) and the Coulomb potential $V(\mathbf{x}) \sim -|\mathbf{x}|^{-1}$ of the hydrogen atom. If we study the spectral theory for self-adjoint operators in $L^2(\mathbb{R}^3;\mathbb{C})$, we notice that $\mathbb{E}_\psi(E)$ can be decomposed into a weighted sum over the eigenvalues of $(V-\nabla^2)\psi = E\psi$, where[4] we have omitted the constants, and the eigenvalues agree with the observed atomic spectra [5; 7]. Since the eigenvectors ψ_n are bounded by the Coulomb potential well, i.e., $E_n < 0$, the set of eigenvalues $\{E_n\}$ is discrete. Equations (2.11-17) suggest that every observable quantity $O(\mathbf{x},\mathbf{p})$ corresponds to a linear self-adjoint operator $\hat{O}$ of $L^2(\mathbb{R}^3;\mathbb{C})$. This ensures that the eigenvectors of $\hat{O}$ span an orthonormal eigenbasis in $L^2(\mathbb{R}^3;\mathbb{C})$ and thus allow to represent the expectation value as a weighted sum over the corresponding real eigenvalues, i.e., $\mathbb{E}_\psi(O) = \langle\psi,\hat{O}\psi\rangle$, where $\psi = \sum_n c_n\psi_n$, $\hat{O}\psi_n = O_n\psi_n$, $\sum_n |c_n|^2 = 1$ and $\langle\cdot,\cdot\rangle$ is the inner product of $L^2(\mathbb{R}^3;\mathbb{C})$ [5; 7]. Consequently, every observable physical quantity is associated with a probability distribution and every physical interaction that changes the distribution is considered as a *measurement*. In particular, a classical measurement of O distinguishes only one of the possible independent and classically exclusive states, i.e., one of the eigenvectors of $\hat{O}$ that becomes the updated state and the result is the corresponding eigenvalue. If two observables share a common eigenvector, it is possible to have sharp measurements simultaneously. We must also demand that a physical expectation value is finite and thus we infer from the Schwarz's inequality that the domain of $\hat{O}$ is componentwise a subspace of $L^2(\mathbb{R}^3;\mathbb{C})$ where the expectation value integral exists, i.e.,

$$\mathfrak{D}(\hat{O}) := \left\{\psi \in L^2(\mathbb{R}^3;\mathbb{C}) \ : \ \hat{O}\psi \in L^2(\mathbb{R}^3;\mathbb{C})\right\} \subset L^2(\mathbb{R}^3;\mathbb{C}). \tag{2.18}$$

Here we assume that $\mathfrak{D}(\hat{O})$ is dense in $L^2(\mathbb{R}^3;\mathbb{C})$ in order to consider every physical system. The analysis of densely defined self-adjoint operators in Eqs. (2.11-17) can be found in Ref. [7].

Next we consider a dynamical state of motion, i.e., the wave function is of the form $\psi(\mathbf{x},t)$. Here we may assume that expectation values obey Newton's equations of motion:

$$m\frac{d}{dt}\mathbb{E}_\psi(\mathbf{x}) = \mathbb{E}_\psi(\mathbf{p}), \tag{2.19}$$

$$\frac{d}{dt}\mathbb{E}_\psi(\mathbf{p}) = \mathbb{E}_\psi(\mathbf{F}). \tag{2.20}$$

The correct dynamical model must also provide the conservation of probability, i.e.,

$$\frac{d}{dt}\int_{\mathbb{R}^3} |\psi(\mathbf{x},t)|^2\, d^3x = 0, \tag{2.21}$$

where the numerical value of integral is unity, independently of time $t \geq 0$. When we try to solve $\psi(\mathbf{x},t)$ from the previous integral equations the task is not trivial, but fortunately we have a clue how to proceed, see *Ehrenfest's theorem* in Refs. [5; 11] and see also Ref. [13]. Since we consider a physical particle, that is described by its wave function, it is natural that the expectation values of position, momentum, kinetic energy, potential energy and force exist, i.e., all the following terms ψ, $\mathbf{x}\psi$, $\nabla\psi$, $\nabla^2\psi$, V, $V\psi$ and $\nabla V\psi$ are continuous and vanish as $|\mathbf{x}| \to \infty$. Moreover, the previous integrals demand a suitable expression for the continuous and bounded[5] time derivative $\partial_t\psi$. With all these regularity conditions, let us now begin with the expectation value of force and use partial integration when trying to solve the time evolution:

$$\begin{aligned}\frac{d}{dt}\mathbb{E}_\psi(\mathbf{p}) &= \int_{\mathbb{R}^3} \frac{\partial}{\partial t}\left((-i\hbar\nabla\psi)\,\overline{\psi}\right) d^3x = \int_{\mathbb{R}^3}\left(-i\hbar\frac{\partial\overline{\psi}}{\partial t}\nabla\psi - i\hbar\overline{\psi}\frac{\partial}{\partial t}(\nabla\psi)\right) d^3x \\ &= \int_{\mathbb{R}^3}\left(-i\hbar\frac{\partial\overline{\psi}}{\partial t}\nabla\psi - i\hbar\overline{\psi}\nabla\left(\frac{\partial\psi}{\partial t}\right)\right) d^3x = \int_{\mathbb{R}^3}\left(-i\hbar\frac{\partial\overline{\psi}}{\partial t}\nabla\psi + i\hbar\frac{\partial\psi}{\partial t}\nabla\overline{\psi}\right) d^3x.\end{aligned}$$

[4]In his notebooks, Schrödinger derived this equation from the Helmholtz equation and Planck–de Broglie relations by considering the atom as a vibrating system [28, p. 269], but the published work is in Ref. [1].

[5]A physical process, that continuously updates the suitably stored information content, is not instant.

On the other hand, in aiming to obtain a corresponding form, we have

$$\mathbb{E}_\psi(\mathbf{F}) = \int_{\mathbb{R}^3} -\nabla V\, |\psi|^2\, d^3x = \int_{\mathbb{R}^3} V\nabla\, |\psi|^2\, d^3x = \int_{\mathbb{R}^3} \left(V\overline{\psi}\nabla\psi + V\psi\nabla\overline{\psi}\right) d^3x.$$

Now the equality holds in Eq. (2.20) if $\partial_t\psi = -iV\psi/\hbar$ that represents the potential energy. The previous choice for $\partial_t\psi$ is not unique, but here we follow equations with physical meaning. Next we consider the expectation value of momentum vector:

$$m\frac{d}{dt}\mathbb{E}_\psi(\mathbf{x}) = \int_{\mathbb{R}^3} m\frac{\partial}{\partial t}\left(\mathbf{x}\,|\psi|^2\right) d^3x = \int_{\mathbb{R}^3}\left(m\mathbf{x}\psi\frac{\partial\overline{\psi}}{\partial t} + m\mathbf{x}\overline{\psi}\frac{\partial\psi}{\partial t}\right) d^3x.$$

On the other hand, we have

$$\begin{aligned}
\mathbb{E}_\psi(\mathbf{p}) &= \int_{\mathbb{R}^3} \left(-i\hbar\nabla\psi\right)\overline{\psi}\, d^3x \\
&= \frac{i\hbar}{2}\int_{\mathbb{R}^3}\left(-\overline{\psi}\nabla\psi - \overline{\psi}\nabla\psi\right) d^3x + \frac{i\hbar}{2}\sum_{j=1}^{3}\mathbf{e}_j\int_{\mathbb{R}^3}\nabla\cdot\left(x_j\overline{\psi}\nabla\psi - x_j\psi\nabla\overline{\psi}\right) d^3x \\
&= \frac{i\hbar}{2}\int_{\mathbb{R}^3}\left(\psi\nabla\overline{\psi} - \overline{\psi}\nabla\psi\right) d^3x \\
&+ \frac{i\hbar}{2}\sum_{j=1}^{3}\mathbf{e}_j\int_{\mathbb{R}^3}\left(x_j\nabla\overline{\psi}\cdot\nabla\psi + \overline{\psi}\mathbf{e}_j\cdot\nabla\psi + x_j\overline{\psi}\nabla^2\psi\right) d^3x \\
&- \frac{i\hbar}{2}\sum_{j=1}^{3}\mathbf{e}_j\int_{\mathbb{R}^3}\left(x_j\nabla\psi\cdot\nabla\overline{\psi} + \psi\mathbf{e}_j\cdot\nabla\overline{\psi} + x_j\psi\nabla^2\overline{\psi}\right) d^3x \\
&= \sum_{j=1}^{3}\mathbf{e}_j\int_{\mathbb{R}^3}\left(\frac{i\hbar}{2}x_j\overline{\psi}\nabla^2\psi - \frac{i\hbar}{2}x_j\psi\nabla^2\overline{\psi}\right) d^3x \\
&= \int_{\mathbb{R}^3}\left(\frac{i\hbar}{2}\mathbf{x}\overline{\psi}\nabla^2\psi - \frac{i\hbar}{2}\mathbf{x}\psi\nabla^2\overline{\psi}\right) d^3x.
\end{aligned}$$

Again, the equality in Eq. (2.19) holds if $\partial_t\psi = i\hbar\nabla^2\psi/2m$ that represents the kinetic energy. The additional integrals of divergence are zero due to Gauss' theorem since the integrands vanish outside of a sufficiently large sphere in $\mathbb{R}^3$. Furthermore, if the time evolution of an energy state is independent of kinetic energy, then the expectation value of position is independent of time. Indeed, if $\partial_t\psi = -iV\psi/\hbar$, then

$$\frac{d}{dt}\mathbb{E}_\psi(\mathbf{x}) = \int_{\mathbb{R}^3}\left(\mathbf{x}\psi\frac{\partial\overline{\psi}}{\partial t} + \mathbf{x}\overline{\psi}\frac{\partial\psi}{\partial t}\right) d^3x = \int_{\mathbb{R}^3}\left(\mathbf{x}\psi\frac{i}{\hbar}V\overline{\psi} - \mathbf{x}\overline{\psi}\frac{i}{\hbar}V\psi\right) d^3x = 0.$$

On the other hand, if the time evolution of an energy state is independent of potential energy, then the expectation value of momentum is independent of time; if $\partial_t\psi = i\hbar\nabla^2\psi/2m$, then by Green's second identity and vanishing boundary conditions, we have

$$\begin{aligned}
\frac{d}{dt}\mathbb{E}_\psi(\mathbf{p}) &= \sum_{j=1}^{3}\mathbf{e}_j\int_{\mathbb{R}^3}\left(-i\hbar\frac{\partial\overline{\psi}}{\partial t}\frac{\partial\psi}{\partial x_j} - i\hbar\overline{\psi}\frac{\partial}{\partial t}\frac{\partial\psi}{\partial x_j}\right) d^3x \\
&= \sum_{j=1}^{3}\mathbf{e}_j\int_{\mathbb{R}^3}\left(-i\hbar\frac{\partial\overline{\psi}}{\partial t}\frac{\partial\psi}{\partial x_j} - i\hbar\overline{\psi}\frac{\partial}{\partial x_j}\frac{\partial\psi}{\partial t}\right) d^3x \\
&= \frac{\hbar^2}{2m}\sum_{j=1}^{3}\mathbf{e}_j\int_{\mathbb{R}^3}\left(-\frac{\partial\psi}{\partial x_j}\nabla^2\overline{\psi} + \overline{\psi}\nabla^2\left(\frac{\partial\psi}{\partial x_j}\right)\right) d^3x = 0.
\end{aligned}$$

Now we have demonstrated that the choice $\partial_t\psi = i\hbar\nabla^2\psi/2m - iV\psi/\hbar$ satisfies the both Eqs. (2.19) and (2.20). Our choice also satisfies the conservation of probability in Eq. (2.21), i.e.,

$$\frac{d}{dt}\int_{\mathbb{R}^3}|\psi|^2\,d^3x = \int_{\mathbb{R}^3}\left(\overline{\psi}\frac{\partial\psi}{\partial t} + \psi\frac{\partial\overline{\psi}}{\partial t}\right)d^3x = \frac{i\hbar}{2m}\int_{\mathbb{R}^3}\left(\overline{\psi}\nabla^2\psi - \psi\nabla^2\overline{\psi}\right)d^3x = 0.$$

To sum up, we have arrived to the fundamental result of dynamical states of motion:

$$i\hbar\frac{\partial\psi}{\partial t}(\mathbf{x},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x},t) + V(\mathbf{x},t)\psi(\mathbf{x},t), \text{ for } (\mathbf{x},t)\in\mathbb{R}^3\times[0,\infty[. \tag{2.22}$$

This is the *Schrödinger equation* (of motion) that describes system's time evolution when a mass particle interacts with an external potential [1; 5], where Heisenberg's uncertainty principle manifests itself as follows: a binding force localizes the particle (the compression of ψ) but then the momentum becomes more uncertain (the spread of ϕ) and thus the kinetic energy increases. In the sense of maximum entropy, ψ is the most probable state that satisfies not only Eq. (2.10) but also the total energy relation during its time evolution, that is

$$\mathbb{E}_\psi(E) - \mathbb{E}_\psi(T) - \mathbb{E}_\psi(V) = \int_{\mathbb{R}^3}\left[i\hbar\frac{\partial\psi}{\partial t} + \frac{\hbar^2}{2m}\nabla^2\psi - V\psi\right]\overline{\psi}\,d^3x = 0. \tag{2.23}$$

By our assumption, a wave function is the global prior amplitude to any act of measurement that can influence the objective information content, and this maximally unbiased information describes how the kinematic state is localized. On the other hand, we do know that our smooth wave model only approximates the underlying randomness, as seen in the electron diffraction.[6] That is, Eq. (2.22) is of the first order in time and thus the initial condition $\psi(\mathbf{x},t_0)$ determines the time evolution and every solution $\psi(\mathbf{x},t)$ evolves both continuously and deterministically. In particular, a classical measurement of position corresponds to the complete information and the associated physical process behind the Bayesian update causes a very rapid consentration of $|\psi|^2$ around the observed location $\mathbf{x}_0$, and – in practical terms – a new initial state $\psi(\mathbf{x},t_0)$ emerges that evolves according to the Schrödinger equation. The fundamental equation (2.22) is also linear, building a far-reaching connection with Huygens' principle that describes wave propagation and allows to explain interference-like observations at microscopic level.

The energy of a physical system tends to disperse spontaneously, i.e., the macrostate becomes more homogeneous. In wave mechanics, the coupled position and momentum distributions are spread out around the average values and an entropic force, that manifests itself through wave dispersion, drives the joint distribution towards the maximum randomness within all the macroscopic constraints. Incidentally, the compression of ψ creates a form of an internal kinetic energy which increase reflects the work done by the external environment in gaining positional information via physical interactions. Conversely, the spread of ψ is an entropy driven process that erases information by dissipating kinetic energy into the environment, cf. Ref. [12].

In this physical model, a classical path $(\mathbf{x}(t),\mathbf{p}(t))$ is replaced by a wave function $\psi(\mathbf{x},t)$. To this end, we have the expectation value of a generic observable $O(\mathbf{x},\mathbf{p},t)$ and the related list of operators that correspond to physical quantities in classical mechanics:

$$\mathbb{E}_\psi(O) = \langle\psi,\hat{O}\psi\rangle = \int_{\mathbb{R}^3}\overline{\psi(\mathbf{x},t)}\hat{O}\psi(\mathbf{x},t)d^3x. \tag{2.24}$$

$$\hat{\mathbf{x}} = \mathbf{x}, \quad \hat{\mathbf{p}} = -i\hbar\nabla, \quad \hat{\mathbf{L}} = -\,i\hbar\mathbf{x}\times\nabla \quad \text{and} \quad \hat{\mathbf{F}} = -\nabla V(\mathbf{x},t). \tag{2.25}$$

$$\hat{T} = -\frac{\hbar^2}{2m}\nabla^2, \quad \hat{V} = V(\mathbf{x},t) \quad \text{and} \quad \hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x},t). \tag{2.26}$$

[6] Following John Wheeler [24], bits and clicks are far more fundamental than continuous models.

3. Conclusions

Entropy can be understood as a measure of randomness, uncertainty or missing information content of a system. E. T. Jaynes introduced the information theoretical maximum entropy principle to derive the least biased estimate possible on a given information in the framework of statistical physics [4], i.e., the most probable statistical distribution of microstates is the least biased estimate that is consistent with all the macroscopic constraints that determine the particular physical model. Our task is to maximize a suitable entropy functional or to otherwise obtain the least biased estimate and this should correspond to the most probable distribution of microstates $(\mathbf{x}, \mathbf{p})$ before an act of measurement. Here we have obtained the non-relativistic wave mechanical model of a single, interacting mass particle with no internal degrees of freedom by using the maximum entropy principle as a philosophical basis of modeling, together with the constraints that arise from the non-classical uncertainty principle and classical statistical theory. There are also other probability estimation based approaches in the literature, but they differ from our quite straightforward presentation that is an amalgamation of many known results: Heisenberg's uncertainty principle and its representation through de Broglie's relation and the Heisenberg–Weyl inequality, Copenhagen interpretation with Bayesianism, Dirac–von Neumann axioms, Born's conditions and Ehrenfest's theorem. The analogous works are built upon various models, be them epistemic or ontic, that contain statistical constraints for dynamical variables, see e.g., Refs. [2; 13-23] and refs. therein, that are related to the uncertainty principle.

In the famous article [3], Heisenberg addressed his desire to derive the laws of wave mechanics (rather, his own *matrix mechanics* [25; 26] that is an equivalent formulation of wave mechanics) directly from the physical foundations, e.g., from the uncertainty principle. He also supported an epistemic view in his book [27], where he argued that the observer has only the function of registering processes, and that an observation is an irreversible process and the irreversibility, i.e., the mathematical state reduction, is a consequence of observer's incomplete knowledge. Here we have demonstrated that both the superposition and uncertainty principles are decisive ingredients of the wave mechanical model. Along these lines, the outcome of a measurement has no definite causal explanation, i.e., every attempt to investigate the system changes the prior distribution, which then spoils the whole idea. On the other hand, the theory is complete in the sense that there is a fundamental limit what can be known about the probabilistic one particle system, a characterization that bears no unobservable metaphysical assumptions.

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