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# Disorder-induced quantum-to-classical transition, or how the world becomes classical

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**Abstract.** Decoherence theory explains how quantum mechanics gives rise to classical mechanics through the entanglement of a quantum system's evolution with the degrees of freedom of the environment. The present article explores another pathway from the quantum to the classical behaviour. We consider a spinless particle interacting with a disordered landscape of potential energy. The matter-wave evolution is handled within time-dependent quantum statistical mechanics, in which the wave function is replaced by a Wigner function defined in position-momentum space. Upon zooming out to scales exceeding the correlation length of the disorder, it is found that the description only involves the state populations as defined in classical statistical physics. Quantum coherence effects are significant only over smaller spatial scales, where they give rise to a noise superimposing on the classical description. The waning of coherence, which reflects the emergence of classicality, is due to the multiple scattering of matter waves; and the framework may be viewed as a stochastic wave mechanics.

## 1 The quantum-to-classical transition in decoherence theory

For a long time, it was believed that quantum mechanics only holds at the microscopic level. The emergence of classicality in quantum theory has been a long-standing enigma. A clue was offered by decoherence theory initiated in the 1970s and 1980s in the works of Zeh and Zurek [1–5]. One could then understand, within the framework of quantum theory, why the macroworld appears to be classical. For instance, a macroscopic object is found in an approximate position of its centre of mass, but never in a Schrödinger-cat-like superposition of two or more macroscopically distinct positions. Explaining such an effective superselection rule was one motivation of decoherence theory. Besides, the derivation of classical concepts in a purely quantum framework removes many oddities of the Copenhagen interpretation. The new theory rests upon the unavoidable coupling of the quantum system to the environment hosting it. The latter, for instance a huge number of air molecules and/or photons, scatters the guest system, the dynamics of which is entangled with that of the many-degree-of-freedom environment. This strongly affects the measurement of variables attached to the system itself. Even though, classically speaking, the influence of the environment on the system (for instance, the damping of its momentum) is negligible, interference effects with respect to certain physical quantities (especially position) become prohibitively difficult to observe in most cases. Consider two states of a particle,  $\psi_1$  and  $\psi_2$ , such as Gaussian wave packets of well-defined centroids. They may superpose to give a new

state, namely  $2^{-1/2}(\psi_1 + \psi_2)$  if the overlap is negligible, of state operator  $2^{-1}[|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2| + |\psi_1\rangle\langle\psi_2| + |\psi_2\rangle\langle\psi_1|]$ , at zero time. The cross terms embody the system's ability to exhibit interference effects. Owing to environmental influences, such a superposition state is not stable over time, and it decays into a statistical mixture  $2^{-1}[|\psi_1\rangle\langle\psi_1|_t + |\psi_2\rangle\langle\psi_2|_t]$  at a long enough time  $t > 0$ . The coherences, defined as the off-diagonal elements of the matrix of the state operator [6, 7], are destroyed, hence the name ‘decoherence’. Decoherence theory determines the basis with respect to which off-diagonal elements disappear as  $t \rightarrow +\infty$ , and the typical time scale of their disappearance. It is the interaction Hamiltonian that primarily determines the basis and the time scale, together with the system's Hamiltonian. As the interaction is often dependent on the position variable, a Schrödinger-cat-like superposition of macroscopically distant wave packets  $\psi_1$  and  $\psi_2$  rapidly decoheres into a classical mixture, whereby the interference effect is effectively suppressed. The formalism of decoherence theory rests upon the fact that the environmental degrees of freedom are unobserved in most practical cases, owing to their huge number and/or uncontrollable nature. By tracing out those degrees of freedom, a reduced state operator is obtained. That operator is the repository of the information allowing to predict (statistically) the behaviour of the system embedded in its environment.

This paper investigates another approach to the quantum-to-classical transition. The system studied herein is a spinless particle and the environment hosting it is very simple. It is a static potential-energy landscape of a disordered nature. By ‘disordered’ we mean a

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random scalar field which may have many instantiations (‘realisations’) distributed according to a probability law. The behaviour of the guest particle will be obtained by averaging over all realisations of the energyscape. Our goal is to recover the classical-mechanical behaviour of the guest particle subjected to a non-random potential-energy field besides the random field. We will examine how quantum mechanics turns into classical-statistical mechanics. It is only possible to recover statistical physics, rather than Newton’s deterministic dynamics, because the information encoded in Schrödinger’s state vector  $\psi$  or von Neumann’s state operator  $|\psi\rangle\langle\psi|$  is inherently statistical. Quotation from Einstein and Infeld [8]: ‘Quantum physics formulates laws governing crowds and not individuals. Not properties but probabilities are described, not laws disclosing the future of systems are formulated, but laws governing the changes in time of the probabilities and relating to great congregations of individuals’. Likewise, Schrödinger wrote: ‘We never experiment with just one electron or atom or (small) molecule. In thought-experiments we sometimes assume that we do; this invariably entails ridiculous consequences’ [9].

The paper unfolds as shown in figure 1. Section 2 starts out from Schrödinger’s formulation of quantum dynamics and section 3 specifies the quantum states of the spinless particle. Section 4 reformulates wave mechanics in position-momentum space where the wave function or the state operator is replaced by its Wigner transform. In section 5, the disordered environment is specified as a random energyscape. Wave mechanics in such an environment is studied in section 6. The transition to classical behaviour in Boltzmann’s statistical formulation is the subject of section 7. Section 8 comes back to decoherence theory and closes the paper. Appendix A provides details about the multiple-scale expansion sorting out the large-scale behaviour from the small-scale one. In appendix B, the change due to a non-static environment is sketched out, and this is tied to the issue of thermalization by the environment.

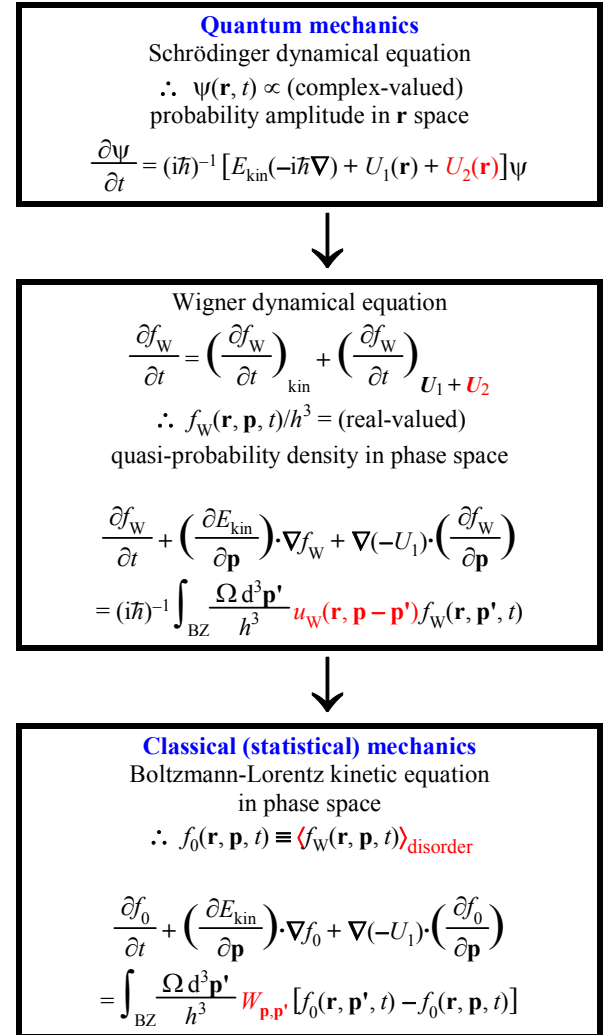
## 2 The issue: Quantum particle in a disordered environment

The present paper deals with the quantum-mechanical motion of a particle hosted in an environment which is modelled in the simplest way as a disordered static energyscape. More specifically, we are considering a spinless particle of mass  $m$  acted upon by a force derived from an external potential energy  $U_1(\mathbf{r})$  where  $\mathbf{r}$  is the position. The Hamiltonian operator is

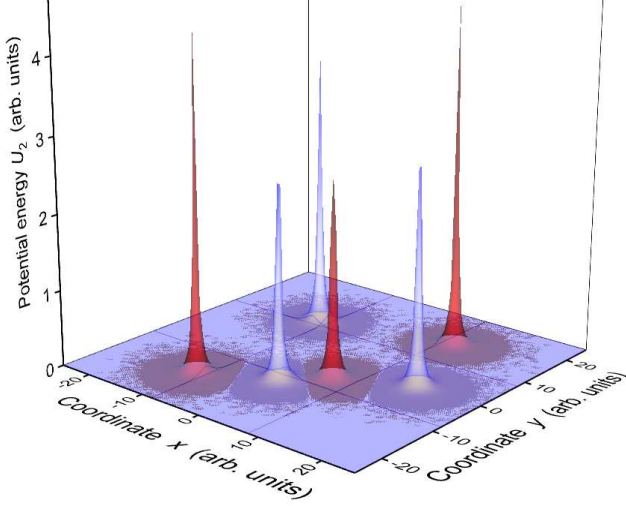
$$H = \frac{(-i\hbar\nabla)^2}{2m} + U_1(\mathbf{r}) + U_2(\mathbf{r}), \quad (1)$$

where  $\hbar = h/2\pi$  is the reduced Planck constant and  $\nabla \equiv \partial/\partial\mathbf{r}$  is the gradient operator. While  $U_1(\mathbf{r})$  is a given function of position known with certainty,  $U_2(\mathbf{r})$  is known only statistically. Mathematically speaking  $U_1$  ( $U_2$ ) is a deterministic (probabilistic) function of  $\mathbf{r}$ . For definiteness, the environment as modelled by  $U_2$  may be thought of as a set of fixed scatterers without internal

degrees of freedom, haphazardly distributed throughout a volume  $\Omega$ . This is pictured in figure 2 which shows two instantiations of the random field  $U_2$ . In the example of an electron in a weakly ionised gas, the scatterers are the neutral atoms or molecules of the gas, which in a first approximation are taken as infinitely heavy and therefore stay at rest. Both fields  $U_1$  and  $U_2$  are time-independent (static); but eventually this assumption can be relaxed. There are two other differences between the two fields: (i)  $U_1$  is taken to be smooth whereas  $U_2$  exhibits small-scale irregularities, or loosely speaking disorder; and (ii) this disordered potential is taken to be weak, as will be specified in section 5.



**Fig. 1.** Organization chart of the article, where the notations of the physical quantities involved will be introduced along the paper. The starting point is Schrödinger’s differential equation governing the complex amplitude of a probability density, i.e. the matter-wave field  $\psi$  of a spinless particle. Its Wigner transform  $f_w$  is  $h^3$  times a quasi-probability density in phase space which is governed by an integro-differential equation. Both the Schrödinger and Wigner equations describe quantum dynamics endowed with phase coherence. The ending point of the article is Boltzmann’s classical-statistical description which makes use of true (phaseless) probabilities.



**Fig. 2.** Random potential-energy field  $U_2(x, y)$  in two dimensions  $x$  and  $y$ . The field shown is a sum of three Yukawa potentials of identical strength and range. The potentials only differ in their central positions. Two instantiations (‘realisations’) of the random field are shown in the figure.

### 3 The quantum states of a particle in a box

The mathematical set-up of the quantum states is simpler in a finite volume such as a cubic box of side  $L = \Omega^{-1/3}$  [10]. With cyclic (Born-von Kármán) boundary conditions, the momentum  $\mathbf{p}$  of a plane wave  $b_{\mathbf{p}}(\mathbf{r}) = \exp(i\mathbf{p} \cdot \mathbf{r}/\hbar)/\Omega^{1/2}$  takes discrete values. In one dimension they are  $p_n = n(h/L)$  with  $n = 0, \pm 1, \pm 2 \dots$ . Cyclic boundary conditions allow for a steady particle flow through the volume with a probability-current density (to be defined below)  $\mathbf{J} = \Omega^{-1}\mathbf{p}/m$ . As two neighbouring values of  $p_n$  differ by  $h/L$ , the momentum-space volume per state is  $(h/L)^3 = h^3/\Omega$  in three dimensions. It is mathematically easier to restrict  $n$  to  $N_c$  values, i.e.  $-N_c/2 < n \leq +N_c/2$ , and eventually let  $N_c \rightarrow \infty$ . The quantum states make up a Hilbert space of finite dimension  $N_c$ . The momentum space has a volume  $N_c(h^3/\Omega)$  in three dimensions.

The momentum representation is connected, via a unitary transformation, to the complementary (i.e. mutually exclusive) position representation. The latter has a basis set [11]

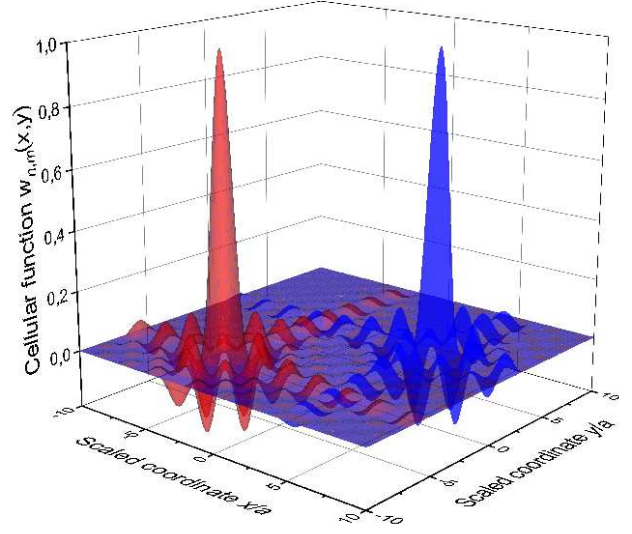
$$w_{\mathbf{l}}(\mathbf{r}) = \frac{1}{\sqrt{N_c}} \sum_{\mathbf{p}} \exp\left(\frac{i\mathbf{p} \cdot \mathbf{l}}{\hbar}\right) b_{\mathbf{p}}(\mathbf{r}), \quad (2)$$

where  $w_{\mathbf{l}}(\mathbf{r})$  is a ‘cellular function’ localized about position  $\mathbf{l}$ . There are  $N_c$  such positions which make up a ‘ghost lattice’ in the box. In one dimension, the positions of the ghost lattice sites  $\mathbf{l}$  are  $x_n = na$ , where  $a$  is  $L/N_c$  and  $n$  takes  $N_c$  values. The calculation yields

$$w_n(x) = \frac{1}{N_c a^{1/2}} \frac{\sin[\pi(x - x_n)/a]}{\sin[\pi(x - x_n)/L]} \approx \frac{1}{a^{1/2}} \frac{\sin[\pi(x - x_n)/a]}{\pi(x - x_n)/a} \quad \text{if } N_c \gg 1. \quad (3)$$

This function peaks at the discrete position  $x_n$ . Two cellular functions are shown in figure 3. Accordingly, the

momentum space is the fundamental Brillouin zone (times  $\hbar$ ), henceforth denoted by BZ, in the parlance of the physics of the crystalline solid state.



**Fig. 3.** Cellular functions  $w_{n,m}$  complementary to the discrete plane waves, in two dimensions  $x$  and  $y$ . Two functions are shown in the figure, namely  $w_{5,2}$  and  $w_{-3,-6}$ , centred at  $\{x_n = 5a, y_m = 2a\}$  and  $\{x_n = -3a, y_m = -6a\}$  respectively. The cellular functions make up an orthonormal basis set of the Hilbert space. In the continuum limit  $a \rightarrow 0$ , the cellular function  $w_{n,m}$  tends to  $\delta(x - x_n)\delta(y - y_m)$ .

The case of an unbounded continuum is recovered by letting  $\Omega \rightarrow \infty$  and  $N_c \rightarrow \infty$  [10, 12]. Table 1 shows that, in this double limit, a Darboux sum is replaced by a Leibniz integral and a Kronecker symbol goes over to a Dirac delta function. As noted by Messiah [10] and expressed by the notation  $\approx$  in Table 1, this procedure is not mathematically rigorous, but it provides the physically pertinent results.

**Table 1.** Discrete vs continuum description.

Darboux sum	$\leftrightarrow$	Leibniz integral
$\sum_{\mathbf{r}} \frac{\Omega}{N_c} F(\mathbf{r}) \approx \int_{\Omega} F(\mathbf{r}) d^3\mathbf{r}$		
$\sum_{\mathbf{p}} \frac{h^3}{\Omega} G(\mathbf{p}) \approx \int_{\text{BZ}} G(\mathbf{p}) d^3\mathbf{p}$		
Kronecker symbol	$\leftrightarrow$	Dirac function
$\delta_{\mathbf{r},\mathbf{r}'} \approx \frac{\Omega}{N_c} \delta(\mathbf{r} - \mathbf{r}')$		
$\delta_{\mathbf{p},\mathbf{p}'} \approx \frac{h^3}{\Omega} \delta(\mathbf{p} - \mathbf{p}')$		

A warning is in order. Cyclic boundary conditions are associated with a torus topology in which Ehrenfest’s

first relation does *not* hold for a plane wave because the expectation value of position is independent of time while that of velocity does not vanish, namely

$$\frac{d}{dt}(b_p|r|b_p) = 0 \text{ while } \left(b_p \left| \frac{-i\hbar\nabla}{m} \right| b_p\right) = \frac{\mathbf{p}}{m} \neq 0. \quad (4)$$

In this paper round brackets  $(|)$  denote the scalar product in the Hilbert space of states.

## 4 Wigner's formulation of wave mechanics in phase space

The dynamics of the particle is governed by Schrödinger's wave equation, namely

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi, \quad (5)$$

where  $\psi(\mathbf{r}, t)$  is a complex-valued function. Its squared modulus is the particle's probability of presence per unit volume at position  $\mathbf{r}$  and time  $t$ . Its argument  $\phi(\mathbf{r}, t)$  provides the probability-current density  $\mathbf{J}(\mathbf{r}, t) = |\psi|^2 \hbar \nabla \phi / m$  appearing in the local conservation equation,

$$\frac{\partial |\psi|^2}{\partial t} + \text{div } \mathbf{J} = 0. \quad (6)$$

From the matter-wave field  $\psi(\mathbf{r})$  at a given time, one can build a Wigner transform  $f_W(\mathbf{r}, \mathbf{p})$  in phase space at the same time. The phrase 'phase space' is used herein to mean the Cartesian product  $\Omega \times \text{BZ}$  whose volume is  $N_c h^3$ . Juste like  $\mathbf{r}$  in  $\psi(\mathbf{r})$ ,  $\mathbf{r}$  and  $\mathbf{p}$  in  $f_W(\mathbf{r}, \mathbf{p})$  are not quantum operators but classical variables, namely the position of a geometric point and  $\hbar$  times the reciprocal (Fourier) variable. In keeping with the cyclic boundary conditions and following the guidelines of [13], we shall consider all functions of  $\mathbf{r}$ , such as the wave function  $\psi$  or the Wigner function  $f_W$  to be introduced below, as restrictions to  $\Omega$  of periodic functions on the unbounded position space, with period  $L$  in one dimension. Then, we can write  $\psi$  as a Fourier series,

$$\psi(\mathbf{r}) = \sum_{\mathbf{p}} \hat{\psi}(\mathbf{p}) \exp\left(\frac{i\mathbf{p}\cdot\mathbf{r}}{\hbar}\right), \quad (7)$$

where  $\mathbf{p}$  is a quantized momentum, and

$$\hat{\psi}(\mathbf{p}) \equiv \int_{\Omega} \psi(\mathbf{r}) \exp\left(-\frac{i\mathbf{p}\cdot\mathbf{r}}{\hbar}\right) \frac{d^3\mathbf{r}}{\Omega} \quad (8)$$

has the same physical dimension as  $\psi$ . On restricting the summation over  $\mathbf{p}$  to  $N_c$  values, the equality (7) becomes approximate, but it is expected to become accurate in the limit  $N_c \rightarrow \infty$ . In the continuum limit (see Table 1), the equality (7) is replaced by

$$\psi(\mathbf{r}) \approx \int_{\text{BZ}} \hat{\psi}(\mathbf{p}) \exp\left(\frac{i\mathbf{p}\cdot\mathbf{r}}{\hbar}\right) \frac{\Omega d^3\mathbf{p}}{h^3}. \quad (9)$$

Likewise, we consider all functions of  $\mathbf{p}$ , such as  $E_{\text{kin}}(\mathbf{p})$  or the Wigner function  $f_W(\mathbf{r}, \mathbf{p})$ , as restrictions to the BZ of periodic functions on the unbounded momentum space, with period  $h/a$  in one dimension. The Wigner function is given in Table 2 where the definitions only hold in the limits of large  $\Omega$  and BZ. Note that, in Table 2, the integrand is periodic in  $\mathbf{s}$  with period  $L$  in one dimension (respectively, periodic in  $\mathbf{q}$  with period  $h/a$ ) so that no boundary terms are produced upon integration by parts.

Several definitions of  $f_W$  exist in the literature [7, 11, 13, 14]; the one chosen in this paper is dimensionless. Just as there is one quantum state, there is one Wigner function. The  $\mathbf{r}$ -to- $\mathbf{p}$  duality is evinced in the two equally valid formulae for  $f_W$  in Table 2. The advantage of the discretized finite box of section 3 is now apparent. While the use of delta-peaked wave functions is common practice in Schrödinger's wave mechanics, it is troublesome in Wigner's formulation because then a squared delta function can arise in the Wigner transform. A similar trouble is met with unbounded plane waves such that  $\hat{\psi}$  is a delta function of momentum.

**Table 2.** Definition of the Wigner function  $f_W$  from the wave function  $\psi$  in either the position or the momentum representation.

Wave function	Wigner function $f_W(\mathbf{r}, \mathbf{p})$
$\psi(\mathbf{r})$	$\int_{\Omega} \psi\left(\mathbf{r} + \frac{\mathbf{s}}{2}\right) \psi^*\left(\mathbf{r} - \frac{\mathbf{s}}{2}\right) \exp\left(-\frac{i\mathbf{p}\cdot\mathbf{s}}{\hbar}\right) d^3\mathbf{s}$
$\hat{\psi}(\mathbf{p})$	$\int_{\text{BZ}} \Omega \hat{\psi}\left(\mathbf{p} + \frac{\mathbf{q}}{2}\right) \hat{\psi}^*\left(\mathbf{p} - \frac{\mathbf{q}}{2}\right) \exp\left(\frac{i\mathbf{q}\cdot\mathbf{r}}{\hbar}\right) \frac{\Omega d^3\mathbf{q}}{h^3}$

The function  $f_W$  is real-valued. It has some, but not all, attributes of a probability distribution in phase space. The function provides the marginal distributions in position and in momentum, namely

$$\int_{\text{BZ}} f_W(\mathbf{r}, \mathbf{p}) \frac{d^3\mathbf{p}}{h^3} = |\psi(\mathbf{r})|^2, \quad (10)$$

$$\int_{\Omega} f_W(\mathbf{r}, \mathbf{p}) d^3\mathbf{r} = |\Omega \hat{\psi}(\mathbf{p})|^2, \quad (11)$$

whence

$$\iint_{\Omega \times \text{BZ}} f_W(\mathbf{r}, \mathbf{p}) \frac{d^3\mathbf{r} d^3\mathbf{p}}{h^3} = 1. \quad (12)$$

However,  $f_W(\mathbf{r}, \mathbf{p}) d^3\mathbf{r} d^3\mathbf{p} / h^3$  cannot be thought of as the probability of finding the particle in the volume  $d^3\mathbf{r} d^3\mathbf{p}$ . For example,  $f_W$  can take non-zero values at positions  $\mathbf{r}$  (momenta  $\mathbf{p}$ ) where  $|\psi(\mathbf{r})|^2$  ( $|\hat{\psi}(\mathbf{p})|^2$ ) vanishes. This happens in particular prior to the overlapping of two Gaussian wave packets which are about to meet together and interfere. The Wigner function takes significant values midway between the two packets, where  $\psi(\mathbf{r})$  vanishes and no particle can be detected [7, 14]. Where  $\psi(\mathbf{r})$  vanishes, relation (10) implies that  $f_W(\mathbf{r}, \mathbf{p})$  takes both positive and negative values. It is said that  $f_W(\mathbf{r}, \mathbf{p}) / h^3$  is a *quasi*-probability density in phase space. Given a subvolume  $\varpi$  of  $\Omega \times \text{BZ}$  where  $f_W < 0$ , the integral

$$\iint_{\varpi} f_W(\mathbf{r}, \mathbf{p}) \frac{d^3\mathbf{r} d^3\mathbf{p}}{h^3} \quad (13)$$

over the complementary subvolume  $\varpi'$ , such that  $\varpi \cup \varpi' = \Omega \times \text{BZ}$ , will exceed unity. Likewise, if  $f_W$  exceeds unity in one or more Planck cells  $h^3$ , then because of (12) it will take negative values somewhere else. Because (13) may lie outside the range 0–1, it is a *quasi*-probability.

Thus, the function  $f_W$  should be understood as a mathematical tool which fully specifies the state of the particle, just as the state operator  $|\psi\rangle\langle\psi|$  also known as the probability density operator in quantum statistical mechanics. In particular, the Wigner function enables one to calculate the expectation value, denoted by an overbar, of observables such as  $E_{\text{kin}}(\mathbf{p}) \equiv \mathbf{p}^2/2m$  or  $U(\mathbf{r})$ , in the manner of classical statistical mechanics, namely

$$\overline{E_{\text{kin}}} = \iint_{\Omega \times \text{BZ}} E_{\text{kin}}(\mathbf{p}) f_W(\mathbf{r}, \mathbf{p}) \frac{d^3\mathbf{r} d^3\mathbf{p}}{h^3}, \quad (14)$$

$$\overline{U} = \iint_{\Omega \times \text{BZ}} U(\mathbf{r}) f_W(\mathbf{r}, \mathbf{p}) \frac{d^3\mathbf{r} d^3\mathbf{p}}{h^3}. \quad (15)$$

The Wigner function also provides the probability current density according to the familiar formula,

$$\mathbf{J} = \int_{\text{BZ}} \left( \frac{\partial E_{\text{kin}}}{\partial \mathbf{p}} \right) f_W(\mathbf{r}, \mathbf{p}) \frac{d^3\mathbf{p}}{h^3}, \quad (16)$$

where  $\partial E_{\text{kin}}/\partial \mathbf{p}$  is the group velocity of the matter wave.

How does the Wigner function  $f_W(\mathbf{r}, \mathbf{p}, t)$  change in time? Just as  $\partial\psi/\partial t$  is a sum of kinetic- and potential-energy contributions in Schrödinger's formulation of wave mechanics, here one can write

$$\frac{\partial f_W}{\partial t} = \left( \frac{\partial f_W}{\partial t} \right)_{\text{kin}} + \left( \frac{\partial f_W}{\partial t} \right)_{\text{pot}}. \quad (17)$$

The kinetic-energy contribution is calculated as

$$\left( \frac{\partial f_W}{\partial t} \right)_{\text{kin}} = - \left( \frac{\partial E_{\text{kin}}}{\partial \mathbf{p}} \right) \cdot \nabla f_W. \quad (18)$$

The pattern is simple because third- and higher-order derivatives of  $E_{\text{kin}}(\mathbf{p})$  vanish; otherwise, see [15, 16]. The potential-energy contribution is calculated as

$$\left( \frac{\partial f_W}{\partial t} \right)_{\text{pot}} = \frac{1}{i\hbar} \int_{\text{BZ}} \frac{\Omega d^3\mathbf{p}'}{h^3} u_W(\mathbf{r}, \mathbf{p} - \mathbf{p}') f_W(\mathbf{r}, \mathbf{p}', t), \quad (19)$$

where

$$u_W(\mathbf{r}, \mathbf{q}) \equiv \int_{\Omega} \left[ U(\mathbf{r} + \frac{\mathbf{s}}{2}) - U(\mathbf{r} - \frac{\mathbf{s}}{2}) \right] \exp\left(-\frac{i\mathbf{q}\cdot\mathbf{s}}{\hbar}\right) \frac{d^3\mathbf{s}}{\Omega} \quad (20)$$

and  $U \equiv U_1 + U_2$ . The dynamical equation obeyed by the Wigner function is thus

$$\frac{\partial f_W}{\partial t} + \left( \frac{\partial E_{\text{kin}}}{\partial \mathbf{p}} \right) \cdot \nabla f_W = \frac{1}{i\hbar} \int_{\text{BZ}} \frac{\Omega d^3\mathbf{p}'}{h^3} u_W(\mathbf{r}, \mathbf{p} - \mathbf{p}') f_W(\mathbf{r}, \mathbf{p}', t). \quad (21)$$

Alternatively, the right-hand side may be written in terms of the Fourier transform  $\hat{U}(\mathbf{q})$  of  $U(\mathbf{r})$ ,

$$\left( \frac{\partial f_W}{\partial t} \right)_{\text{pot}} = \frac{i}{\hbar} \int_{\text{BZ}} \frac{\Omega d^3\mathbf{q}}{h^3} \hat{U}(\mathbf{q}) \left[ f_W(\mathbf{r}, \mathbf{p} + \frac{\mathbf{q}}{2}) - f_W(\mathbf{r}, \mathbf{p} - \frac{\mathbf{q}}{2}) \right] \exp\left(\frac{i\mathbf{q}\cdot\mathbf{r}}{\hbar}\right). \quad (22)$$

By integration upon momentum, the right-hand side of (21) does not contribute and we arrive at (6) given (10) and (16).

If  $U_2$  is absent and  $U_1$  is smooth enough to allow neglect of its third- and higher-order derivatives, the associated  $u_W$  is  $L(\partial U_1/\partial x) \delta(q)$  in one dimension. Then, the potential-energy contribution reduces to a differential term, namely  $\nabla U_1 \cdot (\partial f_W/\partial \mathbf{p})$  in three dimensions. The rate of change of  $f_W$  due to the potential energy becomes local

in the force  $\nabla(-U_1)$  (this occurs in particular with a quadratic potential) and  $f_W$  obeys Liouville's equation of classical physics,

$$\frac{\partial f_W}{\partial t} + \left( \frac{\partial E_{\text{kin}}}{\partial \mathbf{p}} \right) \cdot \nabla f_W + \nabla(-U_1) \cdot \left( \frac{\partial f_W}{\partial \mathbf{p}} \right) = 0. \quad (23)$$

But it should be kept in mind that  $f_W/h^3$  is only a *quasi*-probability density. If its integral over a subvolume of phase space is negative or lies above unity at  $t = 0$ , then at a later time this non-classical feature will show up in another subvolume. This comes about because the range of  $f_W$  is preserved during the evolution, as can be seen by rewriting (23) as

$$f_W(\mathbf{r}, \mathbf{p}, t + dt) = f_W\left(\mathbf{r} - \left(\frac{\partial E_{\text{kin}}}{\partial \mathbf{p}}\right) dt, \mathbf{p} - \nabla(-U_1) dt, t\right). \quad (24)$$

In many problems, the knowledge of the system cannot be specified as a pure state (*reine Fall*). Instead of one wave function  $\psi$ , one has to consider several wave functions  $\psi_i$  with weights  $w_i \geq 0$  such that  $\sum_i w_i = 1$ . The weights have to be specified at a given instant such as  $t = 0$ . The state of the system is then called a statistical mixture and it is embodied in the state operator  $\sum_i w_i |\psi_i\rangle\langle\psi_i|$ . This straightforwardly carries over to the Wigner-function formalism, where the pure-state  $f_W$  is replaced by a weighted sum  $\sum_i w_i f_{W,i}$ . Because the weights do not depend on time, the Wigner function of the mixture obeys the same dynamical equation as  $f_W$ .

The next section is devoted to the mathematical specification of the environment, and how it affects the particle's behaviour according to classical physics. Its effect in quantum physics is dealt with in section 6.

## 5 The disordered environment as a static energyscape

In this work the real-valued function  $U_2$  is a random scalar field specified at every location by its mean,  $\langle U_2(\mathbf{r}) \rangle$ , and an unbiased fluctuation,  $u(\mathbf{r})$ , that is to say

$$U_2(\mathbf{r}) \equiv \langle U_2(\mathbf{r}) \rangle + u(\mathbf{r}). \quad (25)$$

The brackets  $\langle \dots \rangle$  denote the averaging over all instantiations ('realisations') of the energyscape. Averaging is an operation which associates with a random variable a non-random or 'sure' number. A possible  $U_2(\mathbf{r})$  in two dimensions is pictured in figure 2; the static function  $U_2(\mathbf{r})$  may be thought of as a spacewise noise. The random field has a covariance  $C_U \equiv \langle u(\mathbf{r}) u(\mathbf{r} + \mathbf{s}) \rangle$ . The field is taken to be homogeneous (translationally invariant), i.e.  $\langle U_2 \rangle$  and  $C_U$  do not depend on  $\mathbf{r}$ . We further assume isotropy (rotational invariance), i.e.  $C_U$  is a function of the modulus  $|\mathbf{s}|$  only. The function  $C_U$  is characterized by the variance of the fluctuation, namely  $u_0^2 \equiv C_U(\mathbf{s} = 0)$ , and its typical decay length, denoted by  $l_c$  and called the correlation length. The *Zitterkraft* (stochastic force) exerted by the field is  $\mathbf{Z}(\mathbf{r}) \equiv \nabla(-U_2)$ . Homogeneity entails a vanishing  $\langle \mathbf{Z}(\mathbf{r}) \rangle$ , i.e. the *Zitterkraft* is unbiased. It is characterized by a covariance matrix which is derived from the covariance of the random potential energy,

$$\langle Z_i(\mathbf{r}) Z_j(\mathbf{r} + \mathbf{s}) \rangle = - \left( \frac{\partial^2 C_{ij}}{\partial s_i \partial s_j} \right), \quad i, j = x, y, z. \quad (26)$$

As an example, consider that  $U_2(\mathbf{r})$  is due to  $N_s$  identical scatterers, of individual potential energy  $v(\mathbf{p})$ , haphazardly interspersed in the volume  $\Omega$ . In this example,

$$U_2(\mathbf{r}) = \sum_{j=1 \dots N_s} v(\mathbf{r} - \mathbf{R}_j). \quad (27)$$

This is called a Poisson random field in the mathematical literature. Its randomness lies in the position  $\mathbf{R}_j$  of each scatterer  $j = 1 \dots N_s$ . The probability of finding  $\mathbf{R}_j$  in a volume  $d^3\mathbf{R}_j$  is  $d^3\mathbf{R}_j/\Omega$ , it being assumed that the number density of scatterers  $n_s \equiv N_s/\Omega$  is low. An analytically workable example is the Yukawa potential,

$$v(\mathbf{p}) = v_0 \left( \frac{\rho_0}{\rho} \right) \exp\left(-\frac{\rho}{\rho_0}\right), \quad (28)$$

where  $|v_0|$  and  $\rho_0$  respectively assess the strength and range of the potential. In figure 2,  $N_s = 3$  and the coordinates have been scaled by  $\rho_0$ . In this example,  $\langle U_2 \rangle = 2\pi n_s \rho_0^3 v_0$  where  $n_s \rho_0^3$  is the number of scatterers in a volume  $\rho_0^3$ . Taking this number to be much less than unity makes  $\langle U_2 \rangle$  negligible. The covariance of this energyscape is calculated to be exponential [17]

$$C_U(\mathbf{s}) = u_0^2 \exp\left(-\frac{s}{l_c}\right), \quad (29)$$

where

$$l_c = \rho_0, \quad (30)$$

$$u_0 = \sqrt{2\pi n_s \rho_0^3} |v_0|. \quad (31)$$

A weak disorder is obtained either in the weak-coupling ( $v_0 \rightarrow 0$ ) or the low-density ( $n_s \rightarrow 0$ ) limit [18]. The covariance matrix of the force is

$$\langle Z_i(\mathbf{r}) Z_j(\mathbf{r} + \mathbf{s}) \rangle = \left( \frac{u_0}{l_c} \right)^2 \frac{\exp(-s/l_c)}{s/l_c} \left[ \delta_{ij} - \left( \frac{s}{l_c} + 1 \right) \frac{s_i s_j}{s^2} \right], \quad i, j = x, y, z. \quad (32)$$

Since  $(u_0/l_c)^2 = 2\pi n_s \rho_0^3 (v_0/\rho_0)^2$ , the typical Zitterkraft  $u_0/l_c$  is smaller than the typical force  $|v_0|/\rho_0$  of a single Yukawa scatterer by a factor  $(2\pi n_s \rho_0^3)^{1/2}$ .

Classically speaking the Zitterkraft scatters particles in a chance-like manner. The average momentum  $\langle \mathbf{p} \rangle$  of an ensemble of particles which start out with the same initial momentum is damped. The modulus  $p$ , however, is unchanged as scattering is elastic. In classical kinetic theory, the rate of momentum—or velocity—relaxation is

$$\frac{1}{\tau_v} = \frac{p}{m} n_s \sigma_v, \quad (33)$$

where  $\sigma_v$ , called the velocity-relaxation scattering cross section off the potential  $v(\mathbf{p})$ , includes velocity persistence in a scattering event. The velocity-persistence ratio  $c$  is defined as the average direction-cosine of the velocities before and after the event. For scattering by a Yukawa potential, at vanishing kinetic energies  $p^2/2m$  the differential cross section becomes independent of the scattering angle so that  $c \approx 0$ . At increasing energies, the differential cross section falls off increasingly rapidly as a function of the scattering angle. Once  $p \gg p_0 \equiv \hbar/\rho_0$ , only a forward peak of angular width  $\approx \hbar/p\rho_0$  is left so that the collision becomes ineffective and  $c \rightarrow 1$ . In the

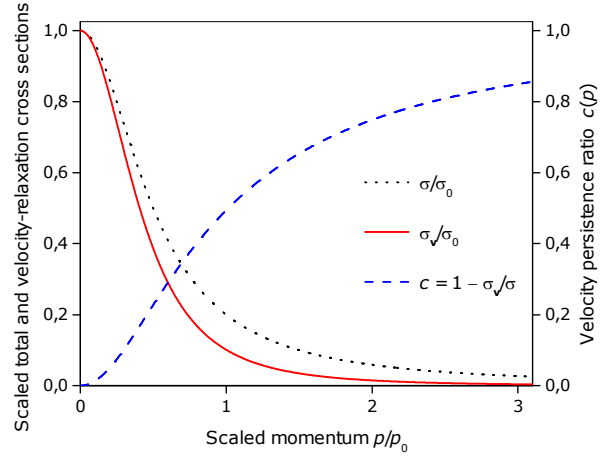
first Born approximation of quantum scattering theory [19], it is calculated that

$$\sigma_v(p) = 2\sigma_0 \left( \frac{p_0}{2p} \right)^4 \left\{ \ln \left[ 1 + \left( \frac{2p}{p_0} \right)^2 \right] - \left[ 1 + \left( \frac{p_0}{2p} \right)^2 \right]^{-1} \right\}, \quad (34)$$

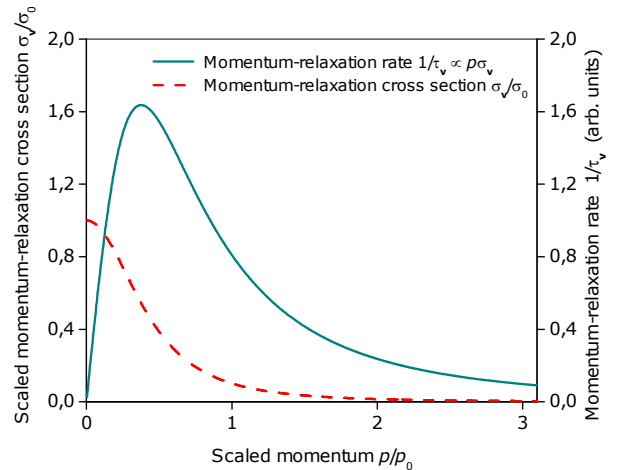
where

$$\sigma_0 \equiv 4\pi\rho_0^2 \left( \frac{2mv_0}{p_0^2} \right)^2 \quad (35)$$

is its value as  $p \rightarrow 0$ . The function  $\sigma_v$  is plotted against momentum  $p$  in figure 4 along with  $c(p)$ . It is seen that  $\sigma_v(p)$  takes its highest value  $\sigma_0$  as  $p$  vanishes. The momentum-relaxation rate  $1/\tau_v$  is plotted against the momentum in figure 5. The rate takes its highest value  $\approx n_s \sigma_0 p_0/2m$  as  $p \approx p_0/2$ ; that is to say the de Broglie wavelength of the matter wave,  $\hbar/p$ , is on a par with the range  $\rho_0$  of the Yukawa potential.



**Fig. 4.** The total scattering cross section ( $\sigma$ ) and velocity-relaxation scattering cross section ( $\sigma_v$ ) of the Yukawa potential  $v(\mathbf{p})$  are plotted as functions of the momentum  $p$ . The momentum scale  $p_0$  is  $\hbar/\rho_0$ , where  $\rho_0$  is the range of  $v(\mathbf{p})$ . The cross sections have been scaled by the value  $\sigma_0$  at a vanishing energy. Also shown is the ratio of velocity persistence  $c(p)$ , or average direction-cosine of the scattering angle  $(\mathbf{p}, \mathbf{p}')$ , as a function of  $p = p'$ .



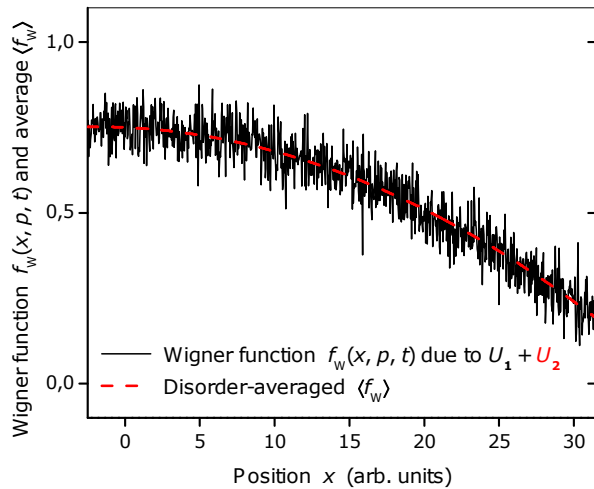
**Fig. 5.** The rate of momentum relaxation ( $1/\tau_v$ ) is plotted as a function of the scaled momentum together with the momentum-relaxation scattering cross section ( $\sigma_v$ ) of the

Yukawa potential. The former peaks at about  $p_0/2$ , where  $\hbar/p_0$  is the range of the potential.

Often the quantum scattering cross section is quite different from the classical one. This is why frequently classical-physics models are built which make use of the quantum cross section or a phenomenological one. In those models, it is considered that in multiple scattering the probability current densities of matter waves add up incoherently, just like in optics the intensities of light beams reflected by several obstacles add up without interfering. Whereas single scattering is handled quantum-mechanically i.e. coherently, coherence effects are ignored in multiple scattering. The next section investigates the motion of a particle through a disordered set of obstacles within the Wigner formalism where coherence is fully accounted for.

## 6 Wave mechanics in a disordered environment

We have to do with a matter wave propagating through an energyscape which, as a stochastic field, can have many realisations. Given an initial condition  $\psi(\mathbf{r}, t=0)$ , a matter wave has a unique history determined by the peculiar realisation of  $U_2(\mathbf{r})$ . Each one gives rise to a matter-wave field  $\psi(\mathbf{r}, t>0)$  or Wigner transform thereof. Thereby  $\psi$  and  $f_W$  themselves are stochastic quantities. We have to consider a statistical ensemble of particles, and we are primarily interested in the average  $\langle f_W \rangle$  over all realisations of  $U_2$ . The fluctuating  $U_2$  will entail a fluctuating Wigner function  $f_W$ . If the fluctuation  $u(\mathbf{r})$  is weak, then a realisation of  $f_W$  will be close to the average  $\langle f_W \rangle$ . This is sketched in figure 6. The fact that covariance is short-ranged implies that two contiguous volumes  $l_c^3$  are statistically independent. Thereby each one is the seat of a realisation of the random variable; and the spatial average over a large volume is identical with the average over a large number of realisations, that is to say an ensemble average [16].



**Fig. 6.** Typical position dependence of the Wigner function  $f_W(x, p, t)$  in one space dimension  $x$  at given  $p$  and  $t$ . The small-scale fluctuation of the Wigner function arises from the

spatially fluctuating potential energy  $u(x) = U_2(x) - \langle U_2 \rangle$  (not shown in the figure). The fluctuation  $u(x)$  is small, i.e.  $\langle u(x)^2 \rangle^{1/2} \ll E_{\text{typ}}$ , and values  $u(x)$  and  $u(x')$  are uncorrelated over a distance  $|x - x'| \gg l_c$ .

If the weakness of the fluctuation can be assessed by a dimensionless parameter  $\varepsilon$ , we may attempt to express  $f_W - \langle f_W \rangle$  as an expansion in powers of  $\varepsilon$  or equivalently  $\varepsilon^{1/2}$ , namely

$$f_W = f_0 + \varepsilon^{1/2} f_1 + \varepsilon f_2 + O(\varepsilon^{3/2}). \quad (36)$$

In this expression,  $f_0 \equiv \langle f_W \rangle$  is independent of the realisation of the fluctuation  $u(\mathbf{r})$  while  $f_1, f_2 \dots$  do depend on the realisation. By construction of the expansion,  $\langle f_1 \rangle, \langle f_2 \rangle \dots$  vanish<sup>1</sup>. To find out a small dimensionless parameter  $\varepsilon$ , we know of two small physical parameters, namely the strength  $u_0$  of the fluctuation and its characteristic length  $l_c$ . The former is taken to be small against the typical energy scale of  $f_W \approx \langle f_W \rangle$ , hereafter denoted by  $E_{\text{typ}}$  and estimated as  $\overline{E_{\text{kin}}}$  such as given by (14). The length  $l_c$  is taken to be much shorter than the scale over which  $\langle f_W \rangle$  undergoes a significant variation. That scale, denoted by  $L$  (usually not identical with the  $L$  of section 3), depends on the applied force  $\nabla(-U_1)$  or, in the absence thereof, the box side  $\Omega^{-1/3}$ . Here  $L$  will be defined in connection with  $u_0$  [16, 21]. Over a length  $l_c$ , energy  $U_2$  varies by about  $+u_0$  or  $-u_0$  with equal probabilities. Over a length  $L \gg l_c$  consisting of  $L/l_c$  segments  $l_c$ , the root-mean-square variation of  $U_2$  is  $u_0(L/l_c)^{1/2}$ . A significant variation will ensue in the matter-wave field or its average Wigner transform, if  $u_0(L/l_c)^{1/2}$  is on a par with the typical energy scale  $E_{\text{typ}}$  of  $f_W$ . Thereby we let

$$\varepsilon^{1/2} \equiv \left( \frac{l_c}{L} \right)^{1/2} = \frac{u_0}{E_{\text{typ}}}. \quad (37)$$

This yields  $L = l_c(E_{\text{typ}}/u_0)^2$ . For  $u_0$  much smaller than  $E_{\text{typ}}$ , a length  $L$  much larger than  $l_c$  is needed for the average Wigner function of the matter wave to be significantly affected by the small but numerous kicks. The main correction  $f_1$  to  $f_0$  is expected to scale as the relative fluctuation in  $U_2$ , namely  $\varepsilon^{1/2}$ ; and (36) is also an expansion in powers of the perturbation strength  $u_0$ .

As a function of position,  $f_W$  will vary over both the long scale  $L$  and the short scale  $l_c$ . This state of affairs is reminiscent of the dynamics of a damped harmonic oscillator, the position function  $f$  of which varies over both the scale of the reduced period  $1/\omega$  (owing to the elastic force) and the scale of the decay time  $\tau$  (owing to the damping force). Provided that  $1/\omega \ll \tau$ , it is mathematically convenient to consider that the instantaneous oscillation  $f$  formally depends on two time variables, a ‘fast’ one  $t'$  and a ‘slow’ one  $t = \varepsilon t'$ , with  $\varepsilon$  standing here for the small dimensionless parameter  $(\omega\tau)^{-1}$  [20]. Accordingly, the time derivative of  $f(t, t')$  is  $\partial f / \partial t + \varepsilon^{-1}(\partial f / \partial t')$ , and the second contribution dominates. In a similar way, in the present issue  $f_W(\mathbf{r}, \mathbf{r}')$  will be

<sup>1</sup> Actually it is not possible to make  $\langle f_1 \rangle, \langle f_2 \rangle \dots$  simultaneously vanish if the expansion is limited to a finite order. Here we take  $\langle f_1 \rangle = 0$ , and dropping the second-order term  $\langle f_2 \rangle$  serves as a closure relation of the expansion [20].

envisaged as a function of two formally independent position variables,  $\mathbf{r}'$  and  $\mathbf{r} = \varepsilon \mathbf{r}'$  where  $\varepsilon$  is the ratio  $l_c/L$  of the characteristic variation lengths, besides the variables  $\mathbf{p}$  and  $t$ . The gradient of  $f_w$  is  $\nabla f_w + \varepsilon^{-1} \nabla' f_w$  where  $\nabla' \equiv \partial/\partial \mathbf{r}'$ . The deterministic potential energy is taken as a function  $U_1(\mathbf{r})$  of the slow variable while the random fluctuation  $u(\mathbf{r}')$  is a function of the fast variable. Omitting the  $\mathbf{p}$  and  $t$  dependencies for a simpler notation, the expansion (36) of  $f_w$  is recast as<sup>2</sup>

$$f_w(\mathbf{r}, \mathbf{r}') = f_0(\mathbf{r}, \mathbf{r}') + \varepsilon^{1/2} f_1(\mathbf{r}, \mathbf{r}') + \varepsilon^1 f_2(\mathbf{r}, \mathbf{r}') + O(\varepsilon^{1/2}). \quad (38)$$

It will be shown that the dominant term  $f_0 = \langle f_w \rangle$  only depends on the slow variable  $\mathbf{r}$ , in keeping with the fact that  $f_0$  does not depend on the peculiar realisation of the fluctuation  $u(\mathbf{r}')$ . Contrariwise the other terms  $f_1, f_2 \dots$  do vary over the small scale of the fluctuation. For the expansion to be a solution of the Wigner dynamical equation of section 4, the zero-order term will have to satisfy a certain equation. A closed-form equation not involving the higher-order terms is obtained in appendix A and it is discussed in the next section.

## 7 Classical statistical mechanics recovered

With the local force term included and letting  $\mathbf{v}(\mathbf{p}) \equiv \partial E_{\text{kin}}/\partial \mathbf{p}$ , the function  $f_0$  is governed by a linear Boltzmann kinetic equation of the Lorentz type [22] (see appendix A), namely

$$\frac{\partial f_0}{\partial t} + \mathbf{v}(\mathbf{p}) \cdot \nabla f_0 + \nabla(-U_1) \cdot \left( \frac{\partial f_0}{\partial \mathbf{p}} \right) = \int_{\text{BZ}} \frac{W_{\mathbf{p}, \mathbf{p}'} d^3 \mathbf{p}'}{h^3} [f_0(\mathbf{p}') - f_0(\mathbf{p})], \quad (39)$$

where

$$W_{\mathbf{p}, \mathbf{p}'} \equiv \frac{2\pi}{\hbar} \int_{\Omega} C_U(\mathbf{s}) \exp\left(\frac{i(\mathbf{p} - \mathbf{p}') \cdot \mathbf{s}}{\hbar}\right) \frac{d^3 \mathbf{s}}{\Omega} \delta(E(\mathbf{p}') - E(\mathbf{p})). \quad (40)$$

We can see that  $\langle f_w \rangle = f_0$  obeys a closed-form equation involving the covariance of the random potential-energy field instead of the full probability law governing the random field itself. If  $u$  in  $C_U(\mathbf{s})$  is written as a Poisson sum (27) of  $N_s$  identical potentials  $v(\mathbf{p})$  shifted at random with respect to one another, then in (40) we have to do with a random sum of  $N_s$  independent phasors. The Verdet-Rayleigh theorem gives [23]

$$\int_{\Omega} \langle u(\mathbf{R}) u(\mathbf{R} + \mathbf{s}) \rangle \exp\left(\frac{i(\mathbf{p} - \mathbf{p}') \cdot \mathbf{s}}{\hbar}\right) \frac{d^3 \mathbf{s}}{\Omega} = N_s \left| \int_{\Omega} v(\mathbf{p}) \exp\left(\frac{i(\mathbf{p} - \mathbf{p}') \cdot \mathbf{p}}{\hbar}\right) \frac{d^3 \mathbf{p}}{\Omega} \right|^2. \quad (41)$$

The right-hand side involves a matrix element of the particle-scatterer interaction potential reminiscent of the first Born approximation of scattering theory. Equation (39) is the Liouville equation (23) supplemented with a

Lorentz-type scattering term on the right-hand side, in which  $W_{\mathbf{p}, \mathbf{p}'} d^3 \mathbf{p}'/\hbar^3$  is the transition probability per unit time that a particle of momentum  $\mathbf{p}$  gets scattered to momentum  $\mathbf{p}'$ . Equations (40–41) mean that, if the scatterers are arranged independently, the total scattering is proportional to the number  $N_s$  of scatterers.

We can see that  $W_{\mathbf{p}, \mathbf{p}'}$  is given by first-order perturbation theory as originally worked out by Dirac [24] and called the second golden rule by Fermi [25]. That golden rule plays a major role also in decoherence theory [1]; and it continues to arouse a number of comments [26, 27]. We remark that strict energy conservation, as expressed by the delta function of energy in (40), is obtained here without assuming long-lived plane waves. The time-energy uncertainty relation invoked in textbooks [10] is unnecessary. Even for a high scattering rate causing short-lived and energy-broadened states, expression (40–41) of  $W_{\mathbf{p}, \mathbf{p}'}$  is valid if used in (39)<sup>3</sup>. A similar conclusion had been reached in a different way in the case of a particle colliding inelastically [28].

The present paper deals with a weak disorder; the opposite case of a strong disorder is shown in Table 3. The golden rule does not hold for a strong  $U_2$  which cannot be handled perturbatively owing to the non-existence of delocalized energy eigenstates of  $H$  (plane waves); and then localization in Anderson's sense arises [29]. In a weak disorder, a particle may be seen to propagate as a plane wave, the lifetime of which is finite owing to scattering events.

**Table 3.** Weak vs strong disordered energyscape.

<b>Weak disorder</b> $u_0 \rightarrow 0$	<b>Strong disorder</b> $u_0 \rightarrow \infty$
<i>Fermi's golden rule</i> perturbative treatment is possible	<i>Anderson's localization</i> propagative states $\exp(i\mathbf{p} \cdot \mathbf{r}/\hbar)$ cannot be zero-order solutions

With (39–40) we have recovered classical non-equilibrium statistical physics, save for two points:

- (i) the classical scattering cross section is replaced by the quantum one in the first Born approximation;
- (ii) the unknown  $f_0$  is the disorder average of a *quasi*-probability density.

The first point should not come as a surprise: the size of atoms (bound states of electrons, as opposed to

<sup>2</sup> The general scheme of a multiple-scale expansion involves an infinite ladder of scales [20], while this expansion of  $f_w$  is limited to two length scales.

<sup>3</sup> In textbook derivations of the golden rule, a pseudo-problem arises from arbitrarily picking out an initial time  $t_0$  in addition to the current time  $t$ . In a rate-equation description, no duration  $\Delta t = t - t_0$  and no energy uncertainty  $\hbar/\Delta t$  arise. Accordingly,  $W_{\mathbf{p}, \mathbf{p}'}$  reflects a tendency or propensity in line with a probabilistic description of the phenomenon.

continuum states) is given by Bohr's radius  $a_0$  which involves the non-classical constant  $\hbar$ . For  $\hbar \rightarrow 0$ ,  $a_0$  vanishes and the discontinuous structure of matter does not arise. The emergence of classicality has to do with the second point. The function  $f_W$  enfolds the information allowing to calculate the expectation values of most observables as if  $f_W$  were a probability density in phase space. Its classicality is conditional upon

$$0 \leq \iint_{\varpi} f_W(\mathbf{r}, \mathbf{p}) \frac{d^3\mathbf{r} d^3\mathbf{p}}{h^3} \leq 1, \quad (42)$$

whatever the subvolume  $\varpi$  of  $\Omega \times \text{BZ}$ , that is to say quasi-probabilities reduce to probabilities. On replacing  $f_W$  by an approximation  $f_0$  which ignores fine-grained details on a scale  $l_c$ , the range of values spanned by the function is reduced and condition (42) is easier to satisfy. Then,  $f_0$  admits of a classical interpretation. If (42) is *not* satisfied at  $t = 0$ , the dynamics will be non-classical at short times. But the Boltzmann-Lorentz evolution of  $f_0$  combines advection in phase space, on the left-hand side of (39) which preserves the range of values of  $f_0$  as implied by (24), with scattering, on the right-hand side of (39) which shrinks that range to one single value at long times as isoenergetic scatterings tend to distribute the values of  $\mathbf{p}$  equally over the energy shell  $E_{\text{kin}}(\mathbf{p}) = E$  [16]. Thereby the approximation  $f_0$  to  $f_W$  will eventually satisfy condition (42) and it will become interpretable as the occupancy of a classical state defined as a pair  $(\mathbf{r}, \mathbf{p})$  i.e. a point in phase space.

An important limitation is in order, however. Classical physics allows for occupancies  $f_0$  such that both  $\mathbf{r}$  and  $\mathbf{p}$  are defined with arbitrarily sharp accuracy. This cannot arise in the present description because  $f_W$  is bounded by a Cauchy-Schwarz inequality  $|f_W| \leq 8$ ; see also [7]. This feature outlives the  $\varepsilon \rightarrow 0$  limit of  $f_W$  in (38). Therefore, not all features of classical physics are recovered in the  $\varepsilon \rightarrow 0$  limit.

In this study the particle is elastically bounced off a static energyscape, which embodies a set of infinitely heavy scatterers. The perfect Lorentz limit of kinetic theory ensues. Appendix B discusses the modification brought about when scatterers are not infinitely heavy; and this is tied to the distinct issue of thermalization by the environment.

## 8 Closing summary

This paper has made use of the Wigner function, instead of the state vector or von Neumann's state operator, to describe the quantum state of a simple system. The Wigner function is a tool which allows one to calculate the expectation values of most major observables as did the phase-space occupation function in classical statistical physics. Actually, however,  $f_W/h^3$  is a density of quasi-probability in phase space, whose integral over a subvolume of phase space may lie outside the range 0–1. A strongly non-classical dynamics is typified by a large positive quasi-probability being almost cancelled by a negative quasi-probability to give the normalization (12) to unity. On the contrary, in nearly classical dynamics, the integral of  $f_W/h^3$  over any subvolume lies within 0–1

or so. A sufficient condition to achieve this is a smooth variation of the potential energy, besides the initial condition  $0 \leq f_W \leq 1$  at  $t = 0$ . *A contrario*, a fast spatial variation of the deterministic potential energy  $U_1$  usually entails non-classical values of  $f_W$ , as actually occurs in a resonant tunnelling diode where the particle is an electron and  $U_1$  is the fast-wiggling applied electrostatic energy [30].

A non-classical behaviour also occurs in a disordered potential energy  $U_2$ , but then it is liable to zoom out to scales exceeding the correlation length of the disorder. Averaging  $f_W$  over a correlation volume  $l_c^3$  shrinks the range of  $\langle f_W \rangle$  which may then fall within the 0–1 interval. To the lowest order in the disorder strength, it is found that  $\langle f_W \rangle$  satisfies a closed-form linear Boltzmann equation of the Lorentz type. That kinetic equation contains a scattering term which further shrinks the range of values of  $\langle f_W \rangle$ . One classical feature is out of reach, however, namely an arbitrarily sharp function of  $(\mathbf{r}, \mathbf{p})$  forbidden by Heisenberg's indeterminacy principle.

The Wigner representation treats position and momentum on the same foot; this is at odds with decoherence theory where position is often the preferred observable which becomes effectively superselected. The dynamical theory of decoherence involves a time scale  $\tau_{\text{dec}}$  much shorter than the characteristic damping time  $\tau_v$  of classical physics. In the present study no time scale is involved because the environment is a non-dynamical entity. Coherent i.e. non-classical effects are present in the correction  $f_1$  to the classical behaviour embodied in  $f_0$ . The coherence correction  $f_1$ , so to speak a quantum noise, is given by (A.7) in appendix A. It depends on the peculiar realisation of the disorder, and it varies over the scale  $l_c$ . This length is akin to the spatial coherence length in optics. Let us compare the matter-wave coherence length with the momentum-damping length of the random energyscape. The latter length is the mean free path  $\lambda(p) = v(p)\tau_v(p)$ . An upper bound of the ratio  $l_c/\lambda(p)$  is  $2\pi n_s p_0^3 (2mv_0/p_0^2)^2$  or, in terms of the stochastic energyscape,

$$\frac{l_c}{\lambda(p)} \leq \left( \frac{u_0}{E_0} \right)^2, \quad (43)$$

where  $E_0$  stands for  $(\hbar/l_c)^2/2m$ . The waning of the phase coherence takes precedence over damping if  $u_0 < E_0$ . This inequality may be viewed as a condition on the root-mean-square amplitude of disorder  $u_0$  being less than  $E_0$  at a given  $l_c$ , or as a condition on the correlation length of disorder  $l_c$  being smaller than  $\hbar/(2mu_0)^{1/2}$  at a given  $u_0$ . In the present approach, a classical behaviour is not obtained dynamically after a time exceeding a *decoherence time* scale. Instead, this behaviour comes out by zooming out to spatial scales exceeding a *coherence length* equal to the correlation length of the static disordered environment. Classical physics emerges (subject to some limitations) as a coarse-grained description of the quantum reality.

I am indebted to Jean-Claude Serge Lévy (Université de Paris–Denis Diderot) for inviting me to participate in the Eighth Complexity-Disorder Meeting.

## Appendix A

### Multiple-scale expansion of the Wigner dynamical equation

Plugging the expansion (38) into the dynamical equation (21–22) results in

$$\frac{1}{\varepsilon} \mathbf{v} \cdot \nabla' f_0 + \frac{1}{\sqrt{\varepsilon}} \mathbf{v} \cdot \nabla' f_1 + \varepsilon^0 \left( \frac{\partial f_0}{\partial t} + \mathbf{v} \cdot \nabla f_0 + \mathbf{v} \cdot \nabla' f_2 \right) + O(\sqrt{\varepsilon}) = \left( \frac{\partial f_0}{\partial t} \right)_u + \sqrt{\varepsilon} \left( \frac{\partial f_1}{\partial t} \right)_u, \quad (\text{A.1})$$

where the  $\nabla U_1$  contribution is omitted. The right-hand side of (A.1),

$$\left( \frac{\partial f}{\partial t} \right)_u \equiv \frac{i}{\hbar} \int_{\text{BZ}} \frac{\Omega \mathbf{d}^3 \mathbf{q}}{h^3} \hat{u}(\mathbf{q}) \left[ f(\mathbf{r}, \mathbf{r}', \mathbf{p} + \frac{\mathbf{q}}{2}) - f(\mathbf{r}, \mathbf{r}', \mathbf{p} - \frac{\mathbf{q}}{2}) \right] \exp\left(\frac{i\mathbf{q} \cdot \mathbf{r}'}{\hbar}\right), \quad (\text{A.2})$$

is the rate of change of  $f \approx f_0 + \sqrt{\varepsilon} f_1$  due to the Zitterkraft. We note the scaling

$$\left( \frac{\partial}{\partial t} \right)_u \propto Z \propto \frac{1}{\sqrt{\varepsilon}}. \quad (\text{A.3})$$

Equating terms of like powers on the two sides of (A.1) yields a recursive chain of equations,

$$O(\varepsilon^{-1}) \quad \mathbf{v} \cdot \nabla' f_0 = 0, \quad (\text{A.4})$$

$$O(\varepsilon^{-1/2}) \quad \mathbf{v} \cdot \nabla' f_1 = \left( \frac{\partial f_0}{\partial t} \right)_u, \quad (\text{A.5})$$

$$O(\varepsilon^0) \quad \frac{\partial f_0}{\partial t} + \mathbf{v} \cdot \nabla f_0 + \mathbf{v} \cdot \nabla' f_2 = \left( \frac{\partial f_1}{\partial t} \right)_u. \quad (\text{A.6})$$

At the leading order ( $\varepsilon^{-1}$ ), we find that  $f_0(\mathbf{r}, \mathbf{r}')$  does not depend on the fast variable, so that it will be denoted by  $f_0(\mathbf{r})$ . In other words, in  $f_0$  short-scale details of  $f_W$  are dismissed upon zooming out to scales exceeding  $l_c$ . The next-order ( $\varepsilon^{-1/2}$ ) equation may be solved in the distributional sense upon Fourier transformation of  $f_0$  and  $f_1$  in the variable  $\mathbf{r}'$ ,

$$f_1(\mathbf{r}, \mathbf{r}') = \left( \int_{\text{BZ}} \frac{\Omega \mathbf{d}^3 \mathbf{q}}{h^3} \hat{u}(\mathbf{q}) \frac{f_0(\mathbf{r}, \mathbf{p} + \frac{\mathbf{q}}{2}) - f_0(\mathbf{r}, \mathbf{p} - \frac{\mathbf{q}}{2})}{-i\eta + \mathbf{q} \cdot \mathbf{v}(\mathbf{p})} \times \exp\left(\frac{i\mathbf{q} \cdot \mathbf{r}'}{\hbar}\right) \right)_{\eta \rightarrow 0}. \quad (\text{A.7})$$

Finally, at order  $\varepsilon^0$ , disorder averaging yields  $\langle f_0 \rangle = f_0$  and  $\langle \nabla' f_2 \rangle = \nabla' \langle f_2 \rangle$  is neglected, whence

$$\frac{\partial f_0}{\partial t} + \mathbf{v} \cdot \nabla f_0 = \left\langle \left( \frac{\partial f_1}{\partial t} \right)_u \right\rangle. \quad (\text{A.8})$$

Now  $f_1$  is known from  $f_0$  according to (A.7). Thereby a closed-form equation on the zero-order function  $f_0$  is obtained. The calculation of the right-hand side of (A.8), which involves the Fourier transform  $\hat{C}_U(\mathbf{q})$  of  $C_U(\mathbf{s})$ , is given elsewhere [16, 31]. Equation (39–40) ensues.

## Appendix B

### Non-static energyscape and thermalization

In the perfect Lorentz limit considered in section 7, energy is exactly conserved in a scattering event, which is to say that the energy-relaxation time  $\tau_E$  is infinite.

Now, if a motionless scatterer has a mass  $m_e$  largely exceeding  $m$ , an  $m$ - $m_e$  scattering event causes a small recoil of  $m_e$  whereby the guest particle imparts kinetic energy to the environment hosting it. In this imperfect Lorentz model ( $1 \ll m_e/m < \infty$ ), scattering events are slightly inelastic; and the energy-relaxation time  $\tau_E(p) \propto m_e/m$  is not infinite although it largely exceeds the momentum-relaxation time  $\tau_v(p)$ . The latter assesses the friction undergone by the particle, i.e. the damping of the ensemble-averaged velocity. If the heavy scatterers are not motionless but thermally agitated at a well-defined and stable temperature  $T_e$ , they tend to bring the guest particle's momentum distribution to a thermal-equilibrium one at the temperature  $T_e$ . In other words, the scatterers act, with respect to the guest particle, as a thermostat<sup>4</sup>. It is possible to extend the present treatment to a random time-varying environment, as was done by Henkel [32], and then the particle can undergo inelastic scattering events. To the lowest order in  $u$ , in the golden rule the delta function  $\delta(E - E')$  becomes  $\delta(E \pm \hbar\omega(\mathbf{q}) - E')$  where  $\hbar\omega(\mathbf{q})$  is the energy quantum of a vibrational mode of the environment. Thermalisation, however, does not arise unless the time-varying field is quantized [16].

The opposite limit of a heavy guest particle knocked about in a host medium of light scatterers ( $m_e \ll m$ ) is called a Brownian particle; one also speaks of a Rayleigh particle [33–35]. This is shown in Table 4. The particle interchanges energy with the environment when bouncing off the light scatterers. This allows for the thermalisation of the guest particle at the temperature  $T_e$  of the environment. The mathematical proof of this statement is simple because the scattering operator of Brownian motion is differential instead of integral as occurs in the Lorentz case, and it is given here.

**Table 4.** Light particle ( $m \ll m_e$ ) governed by the Lorentz integro-differential equation contrasted with heavy (Brownian) particle ( $m \gg m_e$ ) governed by the Klein-Kramers differential equation.

<b>Lorentz particle</b> $m \ll$ mass of environmental scatterers	<b>Brown particle</b> $m \gg$ mass of environmental scatterers
Large change of $\mathbf{p}$ per scattering event	Small change of $\mathbf{p}$ per scattering event
<i>Integral</i> scattering operator (Lorentz 1905)	<i>Differential</i> scattering operator (Klein 1922, Kramers 1940)

<sup>4</sup> There is no interaction between guest particles which would mediate energy, which is the usual thermalisation mechanism in a molecular gas.

In classical statistical physics, the Brownian particle's phase-space occupation  $f(\mathbf{r}, \mathbf{p}, t)$  obeys the Klein-Kramers kinetic equation [36–39],

$$\frac{\partial f}{\partial t} + \mathbf{v}(\mathbf{p}) \cdot \nabla f + \nabla(-U_1) \cdot \left( \frac{\partial f}{\partial \mathbf{p}} \right) = \gamma \operatorname{div}_{\mathbf{p}} \left[ \mathbf{p}f + mkT_e \left( \frac{\partial f}{\partial \mathbf{p}} \right) \right]. \quad (\text{B.1})$$

The scattering term on the right-hand side is differential, instead of integral, in  $\mathbf{p}$  because momentum is infinitesimally changed in a scattering event with an environmental particle of mass  $m_e \ll m$ . In the scattering term,  $T_e$  denotes the temperature of the environmental particles, assumed to be in thermal equilibrium (this demands that  $T_e$  be homogeneous), and  $\gamma$  is the rate of momentum relaxation in force-free motion ( $U_1 = 0$ ). The rate  $\gamma$  is expressible in terms of the  $m$ - $m_e$  differential scattering cross section [38]. Unlike the momentum-dependent rate  $1/\tau_v(p)$  of section 5, here  $\gamma$  is an average over the thermal distribution of momenta of the environmental particles. The mean kinetic energy  $u(\mathbf{r}, t)$  of the guest particle is given by

$$nu = \int E_{\text{kin}}(\mathbf{p}) f(\mathbf{r}, \mathbf{p}, t) \frac{d^3 \mathbf{p}}{h^3} \quad (\text{B.2})$$

where  $n$  is the particle density,

$$n(\mathbf{r}, t) \equiv \int f(\mathbf{r}, \mathbf{p}, t) \frac{d^3 \mathbf{p}}{h^3}. \quad (\text{B.3})$$

Likewise, the energy-current density (reckoned in watt per  $\text{m}^2$  in SI unit) is given, in the absence of  $U_1(\mathbf{r})$ , by

$$\mathbf{j}_U(\mathbf{r}, t) \equiv \int E_{\text{kin}}(\mathbf{p}) \mathbf{v}(\mathbf{p}) f(\mathbf{r}, \mathbf{p}, t) \frac{d^3 \mathbf{p}}{h^3}. \quad (\text{B.4})$$

From the Klein-Kramers equation (B.1), we can derive a Maxwell equation of change of the energy [40, 41]. Multiplying the kinetic equation by  $E_{\text{kin}}(\mathbf{p})$  and integrating over momentum yield

$$\frac{\partial(nu)}{\partial t} + \operatorname{div} \mathbf{j}_U = -\gamma \int \mathbf{v}(\mathbf{p}) \cdot \left[ \mathbf{p}f + mkT_e \left( \frac{\partial f}{\partial \mathbf{p}} \right) \right] \frac{d^3 \mathbf{p}}{h^3}, \quad (\text{B.5})$$

where the right-hand side has been integrated by parts. Given that  $\mathbf{p} \cdot (\partial f / \partial \mathbf{p}) = \operatorname{div}_{\mathbf{p}}(\mathbf{p}f) - 3f$ , we finally obtain

$$\frac{\partial(nu)}{\partial t} + \operatorname{div} \mathbf{j}_U = -2\gamma n \left( u - \frac{3}{2} kT_e \right). \quad (\text{B.6})$$

This is a local energy-balance equation in which the source term, on the right-hand side, is the net rate of energy change per unit volume. Now  $u$  is  $3kT/2$  for a thermal-equilibrium momentum distribution of the guest particle at temperature  $T$ . Thus, the net rate of energy change is positive if the environmental bath has a temperature  $T_e$  higher than the guest particle's temperature  $T$  so that the bath heats up that particle. On the contrary, a particle which is 'hotter' than the environment, i.e. such that  $u > 3kT_e/2$ , will be cooled down until it eventually gets thermalized at the bath's temperature. To finish with, we note from (B.6) that the rate of energy variation of the Brown particle is twice the rate  $\gamma$  of momentum variation, in stark contrast with the Lorentz particle for which the rate  $1/\tau_E$  is much less than  $1/\tau_v$  [35].

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