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Wigner formalism for a particle on an infinite lattice: dynamics and spin

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Abstract

PAPER

The recently proposed Wigner function for a particle in an infinite lattice (Hinarejos M, Bañuls M C and Pérez A 2012 *New J. Phys.* **14** 103009) is extended here to include an internal degree of freedom as spin. This extension is made by introducing a Wigner matrix. The formalism is developed to account for dynamical processes, with or without decoherence. We show explicit solutions for the case of Hamiltonian evolution under a position-dependent potential, and for evolution governed by a master equation under some simple models of decoherence, for which the Wigner matrix formalism is well suited. Discrete processes are also discussed. Finally, we discuss the possibility of introducing a negativity concept for the Wigner function in the case where the spin degree of freedom is included.

1. Introduction

Since its introduction, the Wigner function (WF) [1] has played an important role in physics. Quantum mechanics can be entirely formulated using this tool, thereby providing an alternative description of quantum phenomena and their dynamics. Also, from a more experimental perspective, the WF has proven instrumental for tomographic reconstruction of the states prepared in the lab. Therefore the WF is completely equivalent to the standard quantum mechanical formalism. Nevertheless, the particular features of the phase space description make it advantageous in some situations, such as recognizing the quantum features of states or dealing with decoherence scenarios. In the WF, interference effects manifest in a clear way [2–5]. Another interesting property that manifests in the visualization of the WF of some states is the appearance of negative values over the phase space. This fact has been considered as a direct manifestation of the WF [9] has also found applications to a wide variety of problems, including general relativistic kinetic theory and statistical mechanics [10, 11], nuclear matter at high densities and temperatures [12], electrons in magnetic fields [13, 14], the quark-gluon plasma [15], and neutrino propagation in astrophysical or cosmological scenarios [16, 17].

The applications mentioned above make use of a WF defined in continuous space. It is nevertheless also possible to introduce a sensible WF for systems on a discrete space. The definition for the case of a finite dimensional Hilbert space can be traced back to Stratonovich and Agarwal [18, 19] (see also [20]), who introduced a spherical, continuous phase space for a spin particle. A possible generalization was proposed by Wootters in 1987 [21] for prime dimensional systems, and later generalized to any power of primes in [22]. A different construction was followed in [23–25] that could cope with any dimension of the Hilbert space at the expense of enlarging the size of the phase space grid (see [26, 27] for a review). The discrete WF for a finite-dimensional system is furthermore related to quantum information problems [7, 25, 27–31].

If the discrete Hilbert space is infinite dimensional, a different extension of the WF is required. In [32], we proposed a definition of the WF that can be used for such systems, having the correct marginal properties and with the advantage that a closed form can be obtained in some cases, such as the Gaussian states. Note that, in contrast to the continuous case where the axiomatic definition of the WF uniquely determines its functional

form [33], in the discrete case different definitions that respect the mathematical conditions enumerated above are possible. (See also [34, 35] for alternative, related definitions, motivated by the study of the angle and angular momentum phase space.)

Many of the problems where the continuous WF has been applied concern particles with spin, or with spinor descriptions of quantum fields. To use the phase space formalism in this scenario, a generalization has to be introduced that combines the spin and spatial degrees of freedom (dof). One of the most common prescriptions in the literature is the use of a matrix-valued WF [36], where the spinor or spin indices give rise to various matrix elements. Indeed, other possibilities exist, such as introducing a phase space for the spin degrees of freedom, which correspond to another discrete, finite-dimensional Hilbert space and construct a real valued WF for the Cartesian product of spin and space phase spaces. In the matrix-valued WF, the treatment of space and spin dof is not symmetric. The spatial part is described in terms of a phase space, while the spin is unchanged. Although the treatment is asymmetric, this description has some advantages when dealing with a particle subject to a spin-dependent force, since some effects like the spin precession, or motion that depends on the spin component, are better visualized with respect to a fixed spin basis. Examples of this description are the analysis of the Stern-Gerlach experiment [37], the study of entangled vibronic quantum states of a trapped atom [36], or the reconstruction of the full entangled quantum state for the cyclotron and spin degrees of freedom of an electron in a Penning trap [38].

In this paper, we have extended the definition of the WF introduced in [32] to incorporate the spin of a particle, using the Wigner matrix (WM) formalism for the spin degrees of freedom, and we illustrate the consequences of this definition by analyzing some simple physical situations, such as states involving spatial and spin entanglement or dynamical evolution, as they appear for a particle subject to a spin-dependent force.

The rest of this paper is organized as follows. In section 2, we introduce a definition for the WM that incorporates the spin of the particle, and we summarize the main properties that are satisfied by this object. To illustrate the structure of this representation, we consider some simple cases in section 3. Section 4 contains the main results of our paper, concerning the dynamics obeyed by the WM under the influence of an interacting Hamiltonian that may or may not depend on the spin. First, we study the time evolution in continuous time by deriving the equation of motion for the WM and solving this equation in some simple cases. The situation without spin allows us to consider the special case of a particle on a lattice interacting with a linear potential. We also investigate the interaction that appears for a spin-dependent force to visualize the main differences with the spinless case. Finally, we study the effect of decoherence for the system under consideration. In section 4, we also show how one can use the WM to investigate the dynamics that appear in some discrete-time problems, and we consider the particular example of the quantum walk. As before, we show the effect that decoherence may have on such problems.

One of the advantages of a WF description of continuous variable systems is the access to a negativity that measures the nonclassicality of states. Although the relation of the negativity to nonclassicality is well established, this quantity does not correspond to a physical observable. With a more general definition as the WM and the occurrence of (nonclassical) spin degrees of freedom, we may wonder if there is a generalized negativity quantity and whether it retains some physical information. This is discussed in section 5. Section 6 presents our main conclusions. The derivation of some formulae has been relegated to the appendix to make our presentation more transparent.

2. Particle with spin on a one-dimensional lattice

We are interested in the phase space description of a spin 1/2 particle that is allowed to move on an infinite onedimensional (1D) lattice. A paradigmatic example is the quantum walk on the line, where a particle moves along the sites of a 1D lattice. In its discrete-time version [39], the direction of motion is dictated by the state of an extra two-dimensional Hilbert space (the *coin*), that can correspond to the internal spin of the moving particle. In fact, during the process, the spatial and internal states become entangled even if the initial state was separable, thus clarifying the need for a joint description of both degrees of freedom. Another example is the study of spindependent transport properties of single atoms in a 1D optical lattice [40].

We will start with the definition of the WF for a (spinless) particle on a 1D lattice already introduced in [32]. We consider a lattice with sites $\{na/n \in \mathbb{Z}\}$, where *a* is the lattice spacing. To these sites, one can associate a basis $\{|n\rangle\}$, with $n \in \mathbb{Z}$. By a Fourier transformation, we define a quasi-momentum basis, $|q\rangle = \sqrt{\frac{a}{2\pi}} \sum_{n} e^{iqna} |n\rangle$, which can be restricted to the first Brillouin zone, $q \in [-\frac{\pi}{a}, \frac{\pi}{a}]$. The phase space is defined by points (m, k), where $m \in \mathbb{Z}$, whereas *k* is continuous and periodic, taking values in $[-\pi, \pi]$. With these notations, we define the WF as

$$W(m,k) \equiv \operatorname{tr}[\rho A(m,k)] = \frac{1}{2\pi} \sum_{n} \langle n | \rho | m - n \rangle e^{-i(2n-m)k},$$
(1)

where ρ is the density operator corresponding to the state of the system, and $A(m, k) = \frac{1}{2\pi}\sum_{n}|m-n\rangle\langle n|e^{-i(2n-m)k}$ are the phase point operators for the lattice. It can be checked that the above definition fulfills the necessary requirements to be considered a valid WF. We refer the reader to the above reference for more information about the properties obeyed by (1).

We will now incorporate the additional degree of freedom arising from the spin of the particle. As discussed in the Introduction, there are different approaches in the literature to describe finite-dimensional Hilbert spaces, such as the spin of a particle. One can combine both degrees of freedom (spin and lattice) by a tensor multiplication of the corresponding point operators, as done in [41] for angular momentum and spin states.

As discussed in the introduction, here we opt for a prescription with ample acceptance in the continuous applications, namely a matrix-valued WF. A similar choice has been used in relativistic and nonrelativistic setups with continuous spatial dof. Among the latter, we mention the study of the Stern–Gerlach experiment [37], the analysis of entangled vibronic quantum states of a trapped atom [36], or the reconstruction of the full entangled quantum state for the cyclotron and spin degrees of freedom of an electron in a Penning trap [38]. The WF defined in this way combines the following properties:

- It keeps a close analogy with the definition of the relativistic WF [9–11], thus allowing one to describe the transition from the relativistic to the non relativistic regime.

- It appears as a simple and convenient choice to describe the spin motion in some particular cases, like the Stern–Gerlach experiment in continuous space [37] or the dynamics of a spin 1/2 particle on a lattice under the effect of a spin-dependent force, as described in section 4.

We consider the Hilbert space, $\mathcal{H} = \mathcal{H}_l \bigotimes \mathcal{H}_s$, where \mathcal{H}_l stands for the motion on the lattice and \mathcal{H}_s describes the spin states. The composed Hilbert space is spanned by the basis { $|n, \alpha\rangle \equiv |n\rangle \bigotimes |\alpha\rangle$ }, with $n \in \mathbb{Z}$ and $|\alpha\rangle/\alpha = 0$, 1 designating the eigenvectors of the σ_z Pauli matrix; these states might also correspond to the computational basis of a qubit, or to the levels of a two-level system. According to the above discussion, we propose the following definition for the WM

$$W_{\alpha\beta}(m,k) \equiv \frac{1}{2\pi} \sum_{n} \langle n, \alpha | \rho | m - n, \beta \rangle e^{-i(2n-m)k}.$$
 (2)

We then have a set of four functions, $W_{\alpha\beta}(m, k), \alpha, \beta = 0, 1$, forming a 2 × 2 matrix. Each function, as before, is defined on the phase space of points (m, k), with $m \in \mathbb{Z}$, and k takes values in $[-\pi, \pi]$. A similar definition can be made for any operator, \mathcal{O} , acting on \mathcal{H} :

$$W_{\alpha\beta}^{\mathcal{O}}(m,k) \equiv \frac{1}{2\pi} \sum_{n} \langle n, \alpha | \mathcal{O} | m - n, \beta \rangle e^{-i(2n-m)k}.$$
(3)

Unlike the spatial variables, where the relationship with phase space points is nontrivial, there is a direct correspondence between spin indices in the state of the system and indices in the matrix WF. This implies that operations on the spin space, such as rotations, change of basis, or interactions with a spin-dependent force, as studied below, become more transparent using the matrix WF than any other kind of representation for the spin. Moreover, the definition equation (2) keeps a closer analogy, for pure states, to the relativistic WF used in quantum field theory. For such states, one has $\rho = |\Psi\rangle \langle \Psi|$, and we can write

$$W_{\alpha\beta}(m,k) \equiv \frac{1}{2\pi} \sum_{n} \Psi_{\alpha}(n) \Psi_{\beta}^{*}(m-n) \mathrm{e}^{-\mathrm{i}(2n-m)k}$$
⁽⁴⁾

with $\Psi_{\alpha}(n) \equiv \langle n, \alpha | \Psi \rangle$. In the continuum limit, the functions $\Psi_{\alpha}(n)$ can be interpreted as the components of a Pauli spinor or a Dirac spinor. In this case, equation (4) can be related to the relativistic WF already mentioned in the Introduction.

Some of the properties discussed in [32] can be easily generalized for the matrix WF.

(1) We have

$$W_{\beta\alpha}(m,k) = W^*_{\alpha\beta}(m,k), \tag{5}$$

which implies that the matrix WF is Hermitian. The normalization condition becomes

$$\sum_{\alpha} \sum_{m} \int_{-\pi}^{+\pi} \mathrm{d}k W_{\alpha\alpha}(m, k) = 1.$$
⁽⁶⁾

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(2) Also,

$$W_{\alpha\beta}(m, k \pm \pi) = (-1)^m W_{\alpha\beta}(m, k).$$
⁽⁷⁾

(3) Given two operators C, D and their corresponding Wigner matrices, $W_{\alpha\beta}^{C}(m, k), W_{\alpha\beta}^{D}(m, k)$, one has

$$2\pi \sum_{\alpha,\beta} \sum_{m=-\infty}^{\infty} \int_{-\pi}^{+\pi} dk W^{C}_{\alpha\beta}(m,k) W^{D}_{\beta\alpha}(m,k) = \operatorname{tr}(CD).$$
(8)

(4) A complete knowledge of the WF can be used to reconstruct the density operator, ρ :

$$\langle \alpha | \rho | \beta \rangle = 2\pi \sum_{m} \int_{-\pi}^{+\pi} dk W_{\alpha\beta}(m, k) A(m, k).$$
⁽⁹⁾

(5) The marginal distributions of (2) are related to matrix elements of the density operator

$$\sum_{m=-\infty}^{+\infty} W_{\alpha\beta}(m,k) = \frac{1}{a} \left\langle \frac{k}{a}, \alpha |\rho| \frac{k}{a}, \beta \right\rangle, \tag{10}$$

and

$$\int_{-\pi}^{+\pi} \mathrm{d}k W_{\alpha\beta}(m,k) = \sum_{n} \delta_{m,2n} \langle n, \alpha | \rho | n, \beta \rangle.$$
(11)

As already discussed in [32], these equations reflect the distinction between the coordinates of the phase space points, $m \in \mathbb{Z}, k \in [-\pi, \pi]$, and the position and quasimomentum bases, n, q. The k coordinate is adimensional and does not directly represent a momentum value, but is connected to q = k/a. The *spatial* label m in phase-space is only connected to a discrete position, s, for even values m = 2s, while the odd values of m are analogous to the odd half-integer phase space grid points in [24, 25].

3. Particular cases

To obtain some insight into the characteristics of the matrix WF in equation (2), we will give the explicit form it takes for some particular cases.

Product state

We start by considering a product state of spatial and spin degrees of freedom

$$\rho = \rho_L \bigotimes \rho_S,\tag{12}$$

where ρ_L represents a general state on the lattice and ρ_S is an arbitrary spin state. In this case, we readily obtain

$$W_{\alpha\beta}(m,k) = W_L(m,k) \left\langle \alpha \left| \rho_S \right| \beta \right\rangle, \tag{13}$$

with

$$W_L(m, k) \equiv \frac{1}{2\pi} \sum_n \left\langle n \left| \rho_L \right| \, m - n \right\rangle e^{-i(2n-m)k}.$$
⁽¹⁴⁾

• Superposition of two deltas

Let us consider the WM for the state formed by a superposition of two localized states at lattice sites $|n_1\rangle$ and $|n_2\rangle$ with $n_1 \neq n_2 \in \mathbb{Z}$

$$|\Psi_{2\delta}\rangle = \frac{1}{\sqrt{1+|\alpha|^2}} \Big(|n_1\rangle|0\rangle + \alpha |n_2\rangle|1\rangle\Big),\tag{15}$$

where α is an arbitrary complex number that represents the relative weight of the state, $|n_2\rangle$. For $\alpha = 1$, we obtain a Schrodinger-cat state. The corresponding WF can be easily calculated. Written in matrix form in the above spin basis,

$$W(m, k) = \frac{1}{2\pi \left(1 + |\alpha|^2\right)} \begin{pmatrix} \delta_{m,2n_1} & \alpha^* e^{-ik(n_1 - n_2)} \delta_{m,n_1 + n_2} \\ \alpha e^{ik(n_1 - n_2)} \delta_{m,n_1 + n_2} & |\alpha|^2 \delta_{m,2n_2} \end{pmatrix}$$
(16)

In this case, the WM is zero everywhere except for three particular values of the space-like phase coordinate, $m = 2n_1, 2n_2, n_1 + n_2$. It is interesting to compare the structure provided by equation (16) with the corresponding superposition of two localized states without spin [32], given by

$$|\Psi_{2\delta}^{\text{no spin}}\rangle = \frac{1}{\sqrt{1+|\alpha|^2}} \Big(|n_1\rangle + \alpha |n_2\rangle\Big).$$
(17)

In that case, the WF is a scalar function

$$W_{2\delta}^{\text{no spin}}(m, k) = \frac{1}{2\pi \left(1 + |\alpha|^2\right)} \left\{ \delta_{m,2n_1} + |\alpha|^2 \delta_{m,2n_2} + 2 |\alpha| \delta_{m,n_1+n_2} \cos \left[\Delta n \ k + \phi\right] \right\},$$
(18)

where ϕ is the phase of the complex coefficient, α , and $\Delta n = n_2 - n_1$. One observes that the different terms in (18) appear distributed on different matrix positions in equation (16). In particular, the out-of-diagonal term in (16) corresponds to the interference, oscillating term in (18). This term plays an interesting role related to the nonpositivity of the WF. We will return to this point later.

• Superposition of two Gaussian states

The superposition of two discretized pure Gaussian states with orthogonal spin components is another interesting state for which the WM defined in this work can be computed analytically. Such a state is defined as

$$|\Psi_{2G}\rangle = \frac{1}{\sqrt{2}\mathcal{N}} \sum_{n} \left\{ e^{-\frac{(n-a)^2}{2\sigma^2}} |0\rangle + e^{-\frac{(n-b)^2}{2\sigma^2}} |1\rangle \right\} |n\rangle, \tag{19}$$

for arbitrary $a, b \in \mathbb{Z}, \sigma \in \mathbb{R}^+$. For this state, the WF can be expressed as a matrix in the same $\{|0\rangle, |1\rangle\}$ basis

$$W(m, k) = \frac{1}{2} \begin{pmatrix} W_a(m, k) & W_{ab}(m, k) \\ W_{ab}^{\star}(m, k) & W_b(m, k) \end{pmatrix}$$
(20)

where

$$W_{l}(m, k) = \frac{1}{2\pi N^{2}} e^{-\frac{l^{2} + (m-l)^{2}}{2\sigma^{2}}} e^{ikm} \theta_{3} \left(k + \frac{im}{2\sigma^{2}}, e^{-\frac{1}{\sigma^{2}}} \right), \quad l = a, b$$
(21)

$$W_{ab}(m, k) = \frac{1}{2\pi N^2} e^{-\frac{a^2 + (m-b)^2}{2\sigma^2}} e^{ikm} \theta_3 \left(k + \frac{i(m-b+a)}{2\sigma^2}, e^{-\frac{1}{\sigma^2}}\right)$$
(22)

with $\mathcal{N} = \sqrt{\theta_3(0, e^{-\frac{1}{\sigma^2}})}$ as the normalization constant. The Jacobi theta function, $\theta_3(z, q)$, is defined as $\theta_3(z, q) \equiv \sum_n q^{n^2} e^{2izn}$ for complex arguments q, z, with |q| < 1 [42]. As in the previous example, we find an important difference with the WF for the case without spin [32], since the components in the scalar function appear to be distributed here as the components of the matrix WF. In the limit $a = -b \gg \sigma$ with $\sigma \to 0$, we recover the result for the two deltas (16) corresponding to the case $n_1 = -n_2 = a$ and $\alpha = 1$.

Figure 1 shows the four components of the WM for a two-Gaussian state, as given by equations (20)–(22). One can immediately observe on each component the presence of a secondary image that reflects the property of equation (7). In [32], we discussed with some detail, for the spinless case, the peculiarities related to this duplicate.

4. Dynamics

The WF formalism can be used not only to allow for a description of a given state, but also to analyze its dynamics and to visualize it in phase space. Our purpose is to study the motion of a particle on a lattice in terms of the corresponding WF. We start from the simplest case, which corresponds to the spinless particle, and then move to a more general situation where the particle interacts with a spin-dependent term. The time evolution will be first considered within continuous time, a situation that can be applied to most problems in physics, and can be described by the Schrodinger equation.



4.1. Continuous time

4.1.1. Particle without spin

Let us consider a spinless particle moving on a lattice under the influence of a potential, *V*, that depends on the lattice site. We concentrate on the following Hamiltonian

$$H = J(T_{+} + T_{-}) + V,$$
(23)

which appears as a consequence of the tight-binding approximation in crystals, where the parameter, *J*, is a characteristic of the system that is related to the hoping probability of an electron to the nearest neighbor, and the displacement operators, T_{\pm} , are defined by $T_{\pm} |n\rangle = |n \pm 1\rangle$. Notice that the Hamiltonian (23) can also be considered as a discretized version of

$$H_{\rm cont} = -\frac{\nabla^2}{2M} + V(x) \tag{24}$$

(with *M* being the mass of the particle) if one defines $J = -\frac{1}{2Mq^2}$.

The wave function can be written as $\psi(n, t)$, with t begin the time, so that the Schrödinger equation³ reads

$$i\frac{\partial}{\partial t}\psi(n,t) = J[\psi(n+1,t) + \psi(n-1,t) - 2\psi(n,t)] + V_n\psi(n,t),$$
(25)

with $V_n \equiv \langle n | V | n \rangle$. The last term inside the brackets in equation (1) can be easily reabsorbed into the definition of the coefficients, V_n . (It can be also understood as a term proportional to the identity in the Hamiltonian, thus contributing only as a position-independent phase as time evolves.) Therefore, we omit that term.

It is straightforward to derive an evolution equation satisfied by the WF for the above problem. We begin with the von Neumann equation for the density operator

³ We work in units such that $\hbar = 1$.

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$$\frac{\partial}{\partial t}\rho(t) = -i[H,\rho(t)].$$
(26)

Making use of (1), one arrives at

$$\frac{\partial}{\partial t} W(m, k, t) = 2J \sin k [W(m+1, k, t) - W(m-1, k, t)] - \frac{i}{2\pi} \sum_{l} e^{-i(2l-m)k} (V_{l} - V_{m-l}) \times \langle l|\rho(t)|m-l\rangle,$$
(27)

where we have explicitly shown the time dependence of ρ and W(m, k) for the sake of clarity.

Let us consider V(x) to be is a continuous and infinitely derivable function. In this case, one can obtain a closed form of the above expression for the WF, as shown in the appendix. As a result, one arrives at the following expression

$$\frac{\partial}{\partial t}W(m, k, t) = 2J \sin k \left[W(m+1, k, t) - W(m-1, k, t)\right] + \sum_{s=0}^{\infty} \frac{(-1)^s a^{2s+1}}{2^{2s}(2s+1)!} \frac{d^{2s+1}V(x)}{dx^{2s+1}} \bigg|_{x=ma/2} \frac{\partial^{2s+1}W(m, k, t)}{\partial k^{2s+1}}.$$
(28)

Note that equation (28) also holds for the WM (2) if we introduce the spin of the particle by simply replacing $W(m, k, t) \longrightarrow W_{\alpha\beta}(m, k, t)$, since none of the spatial operations in this equation can affect the spin indices.

Before we go on, we will consider the continuous limit $(a \rightarrow 0)$ of equation (28). In this limit, our WF has to be replaced by the corresponding function, $W_c(x, q, t)$, following the prescription [32]

$$W(m, k, t)_{a \to 0} \frac{1}{2} W_c \left(x = \frac{ma}{2}, q = \frac{k}{a}, t \right).$$
 (29)

By replacing $J = -\frac{1}{2Ma^2}$ and substituting (29) into (28), and taking the limit $(a \rightarrow 0)$, one obtains the equation

$$\frac{\partial}{\partial t}W_{c}(x, q, t) + \frac{q}{M}\frac{\partial}{\partial x}W_{c}(x, q, t) = \sum_{s=0}^{\infty} \frac{(-1)^{s}}{2^{2s}(2s+1)!} \left. \frac{d^{2s+1}V(x)}{dx^{2s+1}} \right|_{x=ma/2} \frac{\partial^{2s+1}W_{c}(x, q, t)}{\partial q^{2s+1}}.$$
(30)

Equation (30) is the equation of motion for the WF under the effect of an external potential, V(x), in continuous space, where *q* represents the momentum of the particle (ranging from $-\infty \text{ to }\infty$). (See, for example [4].)

As an interesting particular case, we will study the case of a linear potential (i.e., $V(x) = \lambda x$), with λ a real constant. Equation (28) adopts a simple form

$$\frac{\partial}{\partial t}W(m,k,t) = 2J\sin k \left[W(m+1,k,t) - W(m-1,k,t)\right] + \lambda a \frac{\partial}{\partial k}W(m,k,t).$$
(31)

To solve this equation, we perform a Fourier transformation on the variable *m* by introducing the function

$$\tilde{W}(q, k, t) \equiv \frac{1}{\sqrt{2\pi}} \sum_{m} e^{iqm} W(m, k, t), \qquad (32)$$

with the new variable, q, taking values on the interval, $[-\pi, \pi]$. With the help of this function, we can rewrite equation (32) as

$$\frac{\partial}{\partial t}\tilde{W}(q,\,k,\,t) = -4iJ\,\sin k\,\sin q\tilde{W}(q,\,k,\,t) + \lambda a\frac{\partial}{\partial k}\tilde{W}(q,\,k,\,t).$$
(33)

The change of function

$$\tilde{W}(q, k, t) \equiv e^{-\frac{4iJ\cos k\sin q}{\lambda a}} f(q, k, t)$$
(34)

leads to the following equation for f(q, k, t):

$$\frac{\partial}{\partial t}f(q, k, t) = \lambda a \frac{\partial}{\partial k}f(q, k, t),$$
(35)

which implies that f(q, k, t) must be of the form $f(q, k, t) = g(q, k + \lambda at)$, with g(q, k) being an unknown function that can be determined by the initial (t=0) condition in equation (34), giving

$$g(q,k) = e^{\frac{4if\cos k\sin q}{\lambda a}} \tilde{W}(q,k,0).$$
(36)

We finally obtain, after some algebra

$$\tilde{W}(q, k, t) = \exp\left[-8i\frac{J}{\lambda a}\sin\left(k + \frac{\lambda at}{2}\right)\sin\left(\frac{\lambda at}{2}\right)\sin q\right]\tilde{W}(q, k + \lambda at, 0).$$
(37)

To derive an expression for the WF, we need the inverse relation of equation (32), given by

$$W(m, k, t) = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} dq e^{-iqm} \tilde{W}(q, k, t),$$
(38)

and we make use of the formula [43]

$$J_n(z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dq e^{-inq} e^{iz \sin q},$$
(39)

where $n \in \mathbb{Z}$, $z \in \mathbb{C}$, and $J_n(z)$ are the Bessel functions of the first kind. After substituting equation (37) into (38), we arrive at the final expression

$$W(m, k, t) = \sum_{l} J_{m-l} \left[-8 \frac{J}{\lambda a} \sin\left(k + \frac{\lambda at}{2}\right) \sin\frac{\lambda at}{2} \right] W(l, k + \lambda at, 0).$$
(40)

Note that in the latter equation, the argument $k + \lambda at$ is to be understood as modulo 2π . Using this fact, one can readily obtain that the above solution exhibits a time periodicity

$$W\left(m, \, k, \, t + \frac{2\pi}{\lambda a}\right) = W\left(m, \, k, \, t\right),\tag{41}$$

which corresponds to the well-known phenomenon of Bloch oscillations that can be observed for electrons confined in a periodic potential (the lattice) subject to a constant force, such as a constant electric field. The corresponding frequency, $\omega_B = |\lambda| a$, is precisely what is expected for our linear potential, $V(x) = \lambda x$.

Directly related to the above treatment, it appears quite natural to attempt a parallelism with a situation that describes the dynamics of a particle under the effect of a constant gravitational field, $V(x) = m_g gx$, where m_g is the gravitational mass and g, the acceleration of gravity. Note that for the following discussion to make sense, one should design a physical system that is described by this potential, and that equation (25) can be considered as a discretized approximation to (24), with $J = -\frac{1}{2Ma^2}$. We will return to this discussion later.

We find it convenient to use the symbol m_i instead of M to represent the *inertial mass* and to recover the Planck constant. We observe that the argument of the Bessel functions in equation (40) depends upon the combination

$$-\frac{J}{\lambda a} = \frac{\hbar^2}{2m_i m_g g a^3} \equiv \frac{1}{\left(k_g a\right)^3},\tag{42}$$

where $k_g \equiv \left(\frac{2m_i m_g g}{\hbar^2}\right)^{1/3}$ is a characteristic wave vector that modulates the spatial dependence of energy eigenstates in a gravitational field in continuous space [44]. As the authors of this work discuss, this is one of the possible effects for quantum particles under the effect of gravity, where various combinations of (powers of) m_g and m_i may appear depending on the problem under consideration, thus enabling us to measure these two quantities independently.

The dynamics on the lattice we just considered offers a similar perspective. The time evolution in equation (40) is governed by the product $k_g a$, which involves the lattice spacing as a new parameter, thus allowing an extra degree of freedom in the design of experiments, if they are performed on a lattice instead of in continuous space. However, one has to be careful about this point: only if the design of the experiment is such that *J* and *V*(*x*) correspond to the above hypothesis the previous discussion make sense.

To illustrate the behavior of the WF, in figure 2 we plotted several snapshots obtained by evolving an initial Gaussian state of the form (21). The time evolution is governed by equation (40). One observes several features on this plot. First, the position of the maximum shows oscillations for the variable m, as corresponding to the Bloch oscillations discussed above, while variable k evolves linearly and periodically with time. During the evolution, the WF also experiences a distortion that is similar to the one observed in continuous space [44]. One also observes the presence of a secondary image, which manifests as vertical strips.

4.1.2. Particle with spin

We return to the description of a particle with spin 1/2. Our purpose is to analyze the dynamics for such a system and compare it with the spinless case. To do so, we need to introduce some spin-dependent potential, or the different components in the WM will evolve in exactly the same way, and the results of the previous subsection apply. To make this comparison as close as possible, we will consider the time evolution under the effect of a



Hamiltonian of the form

$$H = J\left(T_{+} + T_{-}\right) + \sigma_z V,\tag{43}$$

where *V* is, as before, a site-dependent scalar potential. It is possible to obtain an evolution equation, similar to (28), when the particle is subject to the above Hamiltonian in the lattice. This derivation is made in the appendix, the main difference with the spinless case being that the diagonal and off-diagonal components of the WM evolve differently. In what follows, we concentrate on the particular example of a discretized linear potential, $V_n = \lambda an$, with λ being a real constant. Then, equation (A.6) particularizes to

$$\frac{\partial}{\partial t}W_{\alpha\alpha}(m,k,t) = 2J\sin k \Big[W_{\alpha\alpha}(m+1,k,t) - W_{\alpha\alpha}(m-1,k,t) \Big] + (-1)^{\alpha}\lambda a \frac{\partial}{\partial k} W_{\alpha\alpha}(m,k,t), \quad (44)$$

and

$$\frac{\partial}{\partial t}W_{\alpha\beta}(m,k,t) = 2J\sin k \Big[W_{\alpha\beta}(m+1,k,t) - W_{\alpha\beta}(m-1,k,t) \Big] - \mathrm{i}(-1)^{\alpha}\lambda am W_{\alpha\beta}(m,k,t)$$
(45)

(valid for $\alpha \neq \beta$).

The first equation can be easily solved by comparison to (31). We only have to perform the replacement, $\lambda \longrightarrow (-1)^{\alpha} \lambda$. Therefore, we can write the solution using the same procedure as in the case with no spin, to obtain

$$W_{\alpha\alpha}(m, k, t) = \sum_{l} J_{m-l} \left[-8 \frac{J}{\lambda a} \sin\left(k + (-1)^{\alpha} \frac{\lambda a t}{2}\right) \sin\frac{\lambda a t}{2} \right] W_{\alpha\alpha} \left(l, k + (-1)^{\alpha} \lambda a t, 0\right).$$
(46)

The same comments made in the previous section hold here: $W_{a\alpha}(m, k, t)$ is periodic in time, with the frequency given by $\omega_B = |\lambda| a$. Equation (45) can be solved by introducing a Fourier transform, as made with (31). We arrive, after some algebra, at

$$W_{\alpha\beta}(m, k, t) = e^{(-1)^{\alpha} \operatorname{im} \frac{\lambda a t}{2}} \sum_{l} e^{(-1)^{\alpha} \operatorname{il} \frac{\lambda a t}{2}} J_{m-l} \left[-8 \frac{J}{\lambda a} \sin k \sin \frac{\lambda a t}{2} \right] W_{\alpha\beta}(l, k, 0)$$
(47)

(valid when $\alpha \neq \beta$).

To illustrate the evolution of the WM elements under the effect of the Hamiltonian (43) with a linear potential, we followed this evolution for an initial separable state of the form (13), with ρ_s defined by the pure state, $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, and $W_L(m, k)$ corresponding to a Gaussian state, given by (cf equation (21))

$$W_L(m, k) = \frac{1}{2\pi N^2} e^{-\frac{a^2 + (m-a)^2}{2\sigma^2}} e^{ikm} \theta_3 \left(k + \frac{im}{2\sigma^2}, e^{-\frac{1}{\sigma^2}}\right)$$
(48)

and $\mathcal{N} = \sqrt{\theta_3(0, e^{-\frac{1}{\sigma^2}})}$ being the normalization constant. The results are presented in figure 3, which shows different snapshots of the diagonal components, $W_{00}(m, k, t)$ and $W_{11}(m, k, t)$ of the WM. We observe that both components present similar features to the case without spin, as plotted in figure 2. However, they evolve differently on the *m* axis: Initially, the $W_{00}(m, k, t)$ component moves to the left, while the $W_{11}(m, k, t)$





component moves to the right, as a consequence of the different time dependence, $(-1)^{\alpha} \lambda at$, in (46), a phenomenon that is reminiscent of the splitting into two beams in the Stern-Gerlach experiment, where the basic piece of the interaction is analogous to (43).

4.1.3. Decoherence

Another dynamical scenario of great relevance to the study of quantum systems is the presence of decoherence, which can be caused by interaction with the environment. In the following, we show how the WF formalism we are discussing also accommodates this situation. In particular, we explore some typical cases, in which the spin structure of the WM allows a simple visualization of the decoherence effects.

We consider the case where the interaction with the environment can be described by a Lindblad-type equation [45]

$$\frac{\partial}{\partial t}\rho = -\mathbf{i}[H,\rho] + \sum_{k} \gamma_k \left(A_k \rho A_k^{\dagger} - \frac{1}{2} A_k^{\dagger} A_k \rho - \frac{1}{2} \rho A_k^{\dagger} A_k \right),\tag{49}$$

where A_k are the Lindblad operators and γ_k represent the corresponding coupling constants.

If these operators act only on the spin space, the Lindblad (noise) term equation (49) immediate translates into an analogous equation for the WM. In other words, under this hypothesis, we can write for the WM

$$\frac{\partial}{\partial t}W(m, k, t) = \frac{\partial}{\partial t}W(m, k, t)|_{H} + \sum_{k}\gamma_{k}\left(A_{k}W(m, k, t)A_{k}^{\dagger} - \frac{1}{2}A_{k}^{\dagger}A_{k}W(m, k, t) - \frac{1}{2}W(m, k, t)A_{k}^{\dagger}A_{k}\right).$$
(50)

In the latter equation, $\frac{\partial}{\partial t}W(m, k, t)|_{H}$ denotes the contribution of the Hamiltonian to the dynamics (without decoherence), and we used a matrix notation so that spin indices were omitted.

As a simple example, let us consider the case where we only have a Lindblad operator, $A_1 = \sigma_z$ with $\gamma_1 \equiv \gamma$. We then have

$$\frac{\partial}{\partial t}W(m,k,t) = \frac{\partial}{\partial t}W(m,k,t)|_{H} + \begin{pmatrix} 0 & -2\gamma W_{01}(m,k,t) \\ -2\gamma W_{10}(m,k,t) & 0 \end{pmatrix},$$
(51)

whose solution can be readily obtained and expressed as

$$W(m, k, t) = \begin{pmatrix} W_{00}(m, k, t)|_{H} & e^{-2\gamma t} W_{01}(m, k, t)|_{H} \\ e^{-2\gamma t} W_{10}(m, k, t)|_{H} & W_{11}(m, k, t)|_{H} \end{pmatrix}.$$
(52)

In other words, in this example, decoherence leaves the diagonal terms unaltered, while the off-diagonal terms are exponentially damped with time.

Our second example is provided by the Lindblad operator, $A_1 = \sigma_x$ with $\gamma_1 \equiv \gamma$. In this case, equation (50) becomes

$$\frac{\partial}{\partial t}W(m,k,t) = \frac{\partial}{\partial t}W(m,k,t)|_{H} + \gamma \begin{pmatrix} W_{11}(m,k,t) - W_{00}(m,k,t) & W_{10}(m,k,t) - W_{01}(m,k,t) \\ W_{01}(m,k,t) - W_{10}(m,k,t) & W_{00}(m,k,t) - W_{11}(m,k,t) \end{pmatrix}.$$
(53)

This set of equations can be solved by elementary operations. We concentrate on the diagonal terms, for which the final solution reads

$$W_{00}(m, k, t) = \frac{1}{2} \left(1 + e^{-2\gamma t} \right) W_{00}(m, k, t) |_{H} + \frac{1}{2} \left(1 - e^{-2\gamma t} \right) W_{11}(m, k, t) |_{H},$$
(54)

$$W_{11}(m, k, t) = \frac{1}{2} \left(1 - e^{-2\gamma t} \right) W_{00}(m, k, t) |_{H} + \frac{1}{2} \left(1 + e^{-2\gamma t} \right) W_{11}(m, k, t) |_{H}.$$
 (55)

Similar equations can be obtained involving $W_{01}(m, k, t)$ and $W_{10}(m, k, t)$. As a result, in the limit $t \to \infty$, both $W_{00}(m, k, t)$ and $W_{11}(m, k, t)$ become an equally weighted mixture; the same happens with the off-diagonal terms.

4.2. Discrete time

4.2.1. Quantum walk

The examples studied in the previous section arise as a consequence of the continuous interaction of a particle with an external potential acting on the lattice. However, we can envision some situations in which we act on the particle with subsequent short pulses, or via some actions that appear suddenly but regularly in time. A paradigmatic example of this kind is provided by the quantum walk (QW) [39, 46], which has generated a lot of interest in recent years. In the discrete quantum walk, a quantum particle moves on a 1D lattice subject to the periodic influence of a displacement operator, which propagates the particle to the right or to the left, according to the state of a two-level system (the *coin*). The total Hilbert space has precisely the structure $\mathcal{H} = \mathcal{H}_l \bigotimes \mathcal{H}_s$, defined in section 2; in fact, we can associate the states of the coin to the spin of the particle without loss of generality. It is customary to use the basis states $|L\rangle$ and $|R\rangle$ in \mathcal{H}_s (instead of $|0\rangle$ and $|1\rangle$) and associate them to the left and right propagation, respectively. We consider the successive application of the unitary transformation

$$U(\theta) = \left\{ T_{-} \bigotimes |L\rangle \langle L| + T_{+} \bigotimes |R\rangle \langle R| \right\} \bigotimes C(\theta),$$
(56)

where $C(\theta) = I \bigotimes \sigma_z e^{-i\theta\sigma_y}$, $\theta \in [0, \pi/2]$ is a parameter defining the bias of the coin toss, *I* is the identity operator in \mathcal{H}_l , and σ_y and σ_z are Pauli matrices acting on \mathcal{H}_s . The QW dynamics can be described entirely in terms of the WM [47], via a recursion formula that relates W(m, k, t + 1) to other components of this function at time *t*. Using equation (56), one obtains, after some algebra:

$$W(m, k, t+1) = M_R W(m-2, k, t) M_R^{\dagger} + e^{-2ik} M_R W(m, k, t) M_L^{\dagger} + e^{2ik} M_L W(m, k, t) M_R^{\dagger} + M_L W(m+2, k, t) M_L^{\dagger},$$
(57)

where $M_L = (|L\rangle \langle L|) C(\theta)$ and $M_L = (|R\rangle \langle R|) C(\theta)$. A complete analysis of the time evolution in phase space with the help of the WF can be found in [47]. Note that a different definition of the WF was used in [48] for the reduced density matrix of the walker (after tracing the coin) to study the evolution and the effects of decoherence for the quantum walk.

4.2.2. Decoherence in discrete time

The WF formalism can easily accommodate the description of the general transformation of the quantum state via a completely positive map. In particular, we consider here trace-preserving maps. These maps could, for instance, represent a decoherent QW process, with Kraus operators modeling the interaction of the system with the environment. The discrete evolution is represented by

$$\rho(t+1) = \sum_{i} E_{i}\rho(t)E_{i}^{\dagger}, \qquad (58)$$

where E_i are Kraus operators with the property $\sum_i E_i^{\dagger} E_i = I$. As an example, we analyze two simple models of decoherence, which are applied as projective measurements in the different degrees of freedom of the system. The first model is defined as projectors in spin space, while the second model is defined by projecting in the lattice sites. We use the notation Π_i to designate the different projectors, which satisfy $\Pi_i^{\dagger} = \Pi_i$ and $\Pi_i \Pi_j = \delta_{ij} \Pi_i$. With probability *p*, the system is projected onto the spin (or space) basis, so that equation (58) will be rewritten as

$$\rho(t+1) = (1-p)\rho(t) + p \sum_{i} \Pi_{i} \rho(t) \Pi_{i}.$$
(59)

By iteration of the above equation and making use of the properties of projectors, one can derive the following formula relating the final and initial density operators of the system,

$$\rho(t) = (1-p)^{t} \rho(0) + \left[1 - (1-p)^{t}\right] \sum_{i} \Pi_{i} \rho(t) \Pi_{i}.$$
(60)

We start from a state consisting of the superposition of two deltas with orthogonal spin components: equation (15) with $\alpha = 1$. For the first projective model, we apply the spin projectors $\Pi_i = |i\rangle\langle i|, i = 0, 1$, while for the site projection they are given by $\Pi_n = |n\rangle\langle n|, n \in \mathbb{Z}$. The iterated density operator, $\rho(t)$, that is obtained from equation (60) is the same in both cases because of the spin and position entanglement structure in equation (15). The result is

$$\rho(t) = \frac{1}{2} \begin{pmatrix} |n_1\rangle\langle n_1| & (1-p)^t |n_1\rangle\langle n_2| \\ (1-p)^t |n_2\rangle\langle n_1| & |n_2\rangle\langle n_2| \end{pmatrix}.$$
(61)

The corresponding WM becomes

$$W(m, k, t) = \frac{1}{4\pi} \begin{pmatrix} \delta_{m,2n_1} & (1-p)^t \delta_{m,n_1+n_2} e^{-ik(n_1-n_2)} \\ (1-p)^t \delta_{m,n_1+n_2} e^{ik(n_1-n_2)} & \delta_{m,2n_2} \end{pmatrix}.$$
 (62)

Thus, as a consequence of the projective measurements, the nondiagonal components in the WM (62) tend to zero with time. This was expected from the intuitive idea that these components appear from interference between the two spin states in equation (15) or, correspondingly, between the two occupied positions. Once decoherence acts, this kind of interference is reduced and the responsible terms are consequently diminished. Qualitatively similar results are found if one starts from the superposition of two Gaussian states (19) and introduces projective measurements on the lattice states. Interestingly, these interference terms are nonpositive and tend to disappear as decoherence is acting. In the next section, we will discuss the consequences of this idea in more detail.

5. Negativity

In the context of continuous variables, it is well known that the WF may present some zones in phase space where it is negative. This is interpreted as an indication of quantumness, in the sense that the state would not have a classical analogue. To quantify this quantum feature, the negative volume of the WF has been defined as a measure on nonclassicality [6] and has been applied to distinguish quantum states from classical ones [8]. The only pure states with non-negative WFs are Gaussian states [49], but the classification is not complete for mixed states.

For the continuous phase space, the negativity of a state, ρ , becomes

$$\eta(\rho) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left[|W_{\varepsilon}(x,p)| - W_{\varepsilon}(x,p) \right] dp dx = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} |W_{\varepsilon}(x,p)| dp dx - 1.$$
(63)

The positive character of the WF has also been studied for discrete systems. In the finite-dimensional case and for odd dimensions, Gross showed [50] that the only pure states with positive WFs are stabilizer states. The presence of negative values in the WF has been, in this case, connected to a quantum resource related to a possible quantum speedup [28, 51] or the nonsimulability of certain quantum computations involving states with nonpositive WFs [7, 31].

In the case of spin $\frac{1}{2}$, the WF defined by Wooters [21] has been used to establish a separability criterion for a system of two particles [52]. A connection between entanglement and negative WFs was also established in [8] for two particles in a continuous space when the state is a hyperradial s-wave.

Even without the additional degree of freedom, the discreteness of the Hilbert space causes the appearance of spurious negative terms in the Wf, which do not correspond directly to nonclassical features of the state, but rather are due to the structure of the discrete phase space itself. Nevertheless, for the case of a spinless particle, we showed in [32] that it is possible to introduce a modified negativity measure that excludes such negative contributions and contains information about the quantumness of the states, consistent with the continuum limit.

Not being a true quantum observable, the meaning of such a negativity measure will depend strongly on the definition used for the Wf and on the characteristics of the particular system, as the discussion above illustrates. It is then reasonable to ask what natural extension corresponds to the system we are discussing, and what information it maintains about the characteristics of the states.

It is possible to think of several extensions of the WF. If we start with our definition (2) and trace out the spin, we are left with a scalar WF representing the state of the spatial degree of freedom, which in general will be mixed. To this function, we can immediately apply the definition of negativity discussed in [32]. It might be more interesting to think of a negativity definition, $\eta(\rho)$, that preserves some spin information.

One possibility is to define a negativity for the WM as in [47],

$$\eta(\rho) \equiv \sum_{m} \int_{-\pi}^{\pi} \left[||W(m,k)||_{1} - Tr(W(m,k)) \right] dk = \sum_{m} \int_{-\pi}^{\pi} ||W(m,k)||_{1} dk - 1,$$
(64)

where $||A||_1 \equiv Tr \sqrt{A^{\dagger}A}$ is the trace norm of matrix A and the second equality follows from normalization. We can easily check that this quantity fulfills the following desirable properties:

- 1. It reduces to equation (63) for product states in the continuum limit, with $W_c(x, p)$ obtained from $W_L(m, k)$ (see equation (13));
- 2. It is invariant under rotations in spin space.

The first property is also satisfied by the negativity computed after tracing out the spin. The second property, on the other hand, can be illustrated with the following example. We consider an electron, subject to an external magnetic field. To simplify, the electron is confined to a site on the lattice, so that its state is factorizable. The effect of the magnetic field manifests on the precession of the spin, which continuously changes the spin state of the electron. This property ensures that the value of the negativity is not influenced by the precession. In other words, simply changing the spin direction will not alter the negativity properties of the WM. Note that for some alternative definitions of the WF for a particle with spin [21], the function can contain negative values in the phase space for some states, while being completely positive for other states.

We can further explore the significance of definition (64) by considering different examples. We may then

investigate, as in [52], whether this quantity holds information about the entanglement in the state. We start by analyzing the cat state, $|\psi\rangle = \frac{1}{\sqrt{1+|\beta|^2}}(|a\rangle|\sigma_1\rangle + \beta |b\rangle|\sigma_2\rangle)$, where $a, b \in \mathcal{Z}$ label two different sites on the lattice, $\beta \in \mathbb{C}$ is a constant, and $\{|\sigma_1\rangle, |\sigma_2\rangle\}$ are two arbitrary, orthogonal spin states. The negativity of this state takes the form $\eta = \frac{2|\beta|}{1+|\beta|^2}$. It is easy to check that in this case, the entanglement and the negativity have the same behavior.

However, this is not the generic behavior, as illustrated by Werner states [53], $\rho = \frac{1-z}{4}I + z |\psi\rangle\langle\psi|$, where $|\psi\rangle = \frac{1}{\sqrt{2}}(|a\rangle|0\rangle + |b\rangle|1\rangle)$ and $a, b \in \mathbb{Z}$ label two different sites on the lattice. This state is entangled whenever $z \ge \frac{1}{3}$. The WM for this state takes the form

$$W(m,k) = \begin{pmatrix} \frac{1+z}{4} W_{aa}(m,k) + \frac{1-z}{4} W_{bb}(m,k) & \frac{z}{2} W_{ab}(m,k) \\ \frac{z}{2} W_{ab}(m,k) & \frac{1-z}{4} W_{aa}(m,k) + \frac{1+z}{4} W_{bb}(m,k) \end{pmatrix},$$
(65)

with the definition $W_{ln}(m, k) = \frac{1}{2\pi} \delta_{m,l+n} e^{-ik(l-n)}$ and $l, n \in \{a, b\}$. The corresponding negativity is simply $\eta(\rho) = z$. This result implies that for these states, entanglement and negativity are not correlated.

Another scenario where the emergence of classical behavior is often discussed is that of decoherent dynamics. It is thus reasonable to study how this quantity, η , changes under decoherence. To do so, we consider a very simple situation, in which the initial state subject to decoherence is the double delta considered in section 3. To simplify, we restrict ourselves to the discrete time dynamics already studied in section 4, with decoherence arising from projections on spin or lattice sites. Similar qualitative conclusions can be drawn if we allow for continuous time dynamics or if we consider a double Gaussian state (19), although the calculations are more involved. A simple application of (64) to equation (62) leads to the result

$$\eta(t) = (1 - p)^t$$
(66)

for the negativity as a function of time. This simple result can be interpreted as the damping of the out-ofdiagonal terms in (62). As time goes on, these interference terms tend to fade away, and one is left with an incoherent state with a positive WF. This transition from a coherent superposition to an incoherent one is, of course, a well-known phenomenon in the theory of open quantum systems, which shows a change in the nature of the Wigner function that is monitored by our definition of the corresponding negativity.

Although it is obvious from this discussion that in the presence of spin the negativity does not have the clear unique physical meaning it had in the purely spatial case (either continuous or discrete), the quantity, η , introduced here may be useful to characterize some features of the quantum state or the dynamics when the study is restricted to particular families of states. The topic is nevertheless far from being closed, and could be the subject of further debate.

6. Conclusions

In this paper, we have elaborated on the previously introduced Wigner formalism for a particle in an infinite 1D lattice to account for dynamics and for the presence of an additional, finite-dimensional degree of freedom. Our goal was to describe the dynamics on the phase space associated with this problem. Although we have concentrated, for simplicity, on the case where such an additional degree of freedom corresponds to a spin 1/2, one can envision more general situations where higher spins or different properties, such as the polarization of a photon, are considered. As we have shown, the matrix formalism is especially well suited to describe the interaction of the particle with a spin-dependent Hamiltonian on a fixed basis, and it keeps a close resemblance to the relativistic WF formalism [9, 11], a fact that might be useful in the investigation of the nonrelativistic limit of a given problem. We have illustrated the construction of the WF by first analyzing some simple static examples, like the 'Schrodinger cat' double delta or two-Gaussian states. For these states, the position and spin variables are entangled, and this entanglement manifests in a particular structure of the WM.

We have studied the time evolution of the WM for some simple cases. We have explicitly shown the equation governing the evolution of the WF for a general space-dependent potential. This equation, however, can only be exactly solved for some special cases, as we have done for the case of a linear potential, where one recovers the well-known phenomenon of Bloch oscillations. A similar statement is valid for a Hamiltonian that can be factored as a scalar part and a spin operator. We have obtained the equation of motion for a general scalar term, and solved it in the linear case, which allows us to compare it with the dynamics in the spinless case. The presence of a 'spin-dependent force' introduces new features on the dynamics that manifest in phase space. To complete the above description, we have incorporated the role of decoherence which, for some simple examples, can be implemented for the WM in a closed form.

In some physical situations, the interaction appears as short pulses acting on the particle, a paradigmatic example being the quantum walk. It is also possible to analyze the role of decoherence in this case, and we have analyzed a simple example for the double delta state, when decoherence appears as projections either on the spatial or in the original spin basis. We have showed that both mechanisms produce the same effect, which translates into a damping of the off-diagonal matrix components.

Finally, we have explored a possible extension of the concept of negativity, as defined for the scalar WF, to the spin 1/2 case. While it is not evident what the physical meaning of such negativity might be once the spin is incorporated into the particle, we have proposed the minimum requirements that, in our opinion, this magnitude should obey, and we have suggested a definition of negativity that fulfills these requirements. Following this proposal, we analyzed how decoherence translates into a decreasing of negativity in the above decoherence model. We also showed that our definition of negativity does has not have trivial correspondence with entanglement, as clearly indicated by an analysis of the Werner state. We think, however, that it is worth further study of the relationship of the Wigner description to the quantum properties of general states in a lattice.

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Appendix. Dynamics of the Wigner function on a lattice for a particle subject to a potential

We will derive the differential equation that is obeyed by the WM in two cases: I) a particle interacting with a position-dependent potential V(x), and II) a spin 1/2 particle under the effect of a spin-position Hamiltonian of the form (43).

I) We start with the Hamiltonian defined in (23). The interaction in this case only affects the phase space variables (m, k); therefore, spin indices can be omitted for the moment, but can be recovered in the final expression by replacing $W(m, k, t) \longrightarrow W_{\alpha\beta}(m, k, t)$. Of course, for a spinless particle no replacement is necessary.

The evolution equation is obtained from the von Neumann equation for the density operator (26). Using the properties of the T_{\pm} operators, one obtains

a

$$\frac{\partial}{\partial t}W(m, k, t) = 2J \sin k [W(m+1, k, t) - W(m-1, k, t)] + D,$$
(A.1)

where

$$D \equiv -\frac{\mathrm{i}}{2\pi} \sum_{l} \mathrm{e}^{-\mathrm{i}(2l-m)k} \Big(V_l - V_{m-l} \Big) \langle l|\rho(t)|m-l \rangle.$$
(A.2)

We assume that V(x) is continuous and infinitely derivable at any point. Remembering that $V_l = V(la)$, we Taylor expand both V_l and V_{m-l} around the point $\frac{m}{2}a$, so that

$$D = -\frac{i}{2\pi} \sum_{l} e^{-i(2l-m)k} \sum_{p=0}^{\infty} \frac{a^{p}}{p!} \frac{d^{p}V(x)}{dx^{p}} \Big|_{x=ma/2} \frac{(2l-m)^{p}}{2^{p}} \Big[1 - (-1)^{p} \Big] \langle l|\rho(t)|m-l\rangle.$$
(A.3)

With the help of the WF definition, equation (2), one arrives at

$$D = -i\sum_{p=0}^{\infty} \frac{a^p}{p!} \frac{d^p V(x)}{dx^p} \bigg|_{x=ma/2} \frac{1}{(-2i)^p} \bigg[1 - (-1)^p \bigg] \frac{\partial^p W(m, k, t)}{\partial k^p}.$$
 (A.4)

Note that even values of *p* do not contribute in the above sum, so we restrict ourselves to odd values, p = 2s + 1 with $s \in \mathbb{N}$. After simplifying, we finally obtain

$$\frac{\partial}{\partial t}W(m, k, t) = 2J \sin k \left[W(m+1, k, t) - W(m-1, k, t) \right] + \sum_{s=0}^{\infty} \frac{(-1)^s a^{2s+1}}{2^{2s}(2s+1)!} \frac{d^{2s+1}V(x)}{dx^{2s+1}} \bigg|_{x=ma/2} \frac{\partial^{2s+1}W(m, k, t)}{\partial k^{2s+1}}.$$
 (A.5)

II) We now develop an equation of motion for a spin 1/2 particle, which is subject to a spin positiondependent interaction given by equation (43). Following similar steps to the previous case and making use of $\sigma_z |\alpha\rangle = (-1)^{\alpha} |\alpha\rangle, \alpha = 0, 1$, one gets

$$\frac{\partial}{\partial t}W_{\alpha\beta}(m,k,t) = 2J\sin k \Big[W_{\alpha\beta}(m+1,k,t) - W_{\alpha\beta}(m-1,k,t) \Big] + D_{\alpha\beta}, \tag{A.6}$$

with

$$D_{\alpha\beta} \equiv -\frac{i}{2\pi} \sum_{l} e^{-i(2l-m)k} \Big[(-1)^{\alpha} V_{l} - (-1)^{\beta} V_{m-l} \Big] \langle n, \alpha | \rho | m - n, \beta \rangle.$$
(A.7)

After expanding V_l and V_{m-l} around the point $\frac{m}{2}a$ as before, we arrive at

$$D_{\alpha\beta} = -\frac{i}{2\pi} \sum_{l} e^{-i(2l-m)k} \sum_{p=0}^{\infty} \frac{a^p}{p!} \frac{d^p V(x)}{dx^p} \bigg|_{x=ma/2} \frac{(2l-m)^p}{2^p} (-1)^{\alpha} \Big[1 - (-1)^p (-1)^{\alpha+\beta} \Big] \langle l|\rho(t)|m-l\rangle.$$
(A.8)

In terms of the WM,

$$D_{\alpha\beta} = -i\sum_{p=0}^{\infty} \frac{a^p}{p!} \frac{d^p V(x)}{dx^p} \bigg|_{x=ma/2} \frac{1}{(!-2i)^p} (-1)^{\alpha} \Big[1 - (-1)^p (-1)^{\alpha+\beta} \Big] \frac{\partial^p W_{\alpha\beta}(m, k, t)}{\partial k^p}.$$
 (A.9)

In order to determine the values of p that contribute to the above sum, one has to consider two different cases.

If $\alpha = \beta$, only odd values p = 2s + 1 with $s \in \mathbb{N}$ have to be considered, and one is lead to

$$D_{\alpha\alpha} = (-1)^{\alpha} \sum_{s=0}^{\infty} \frac{(-1)^{s} a^{2s+1}}{(2s+1)!} \frac{1}{2^{2s}} \frac{d^{2s+1}V(x)}{dx^{2s+1}} \bigg|_{x=ma/2} \frac{\partial^{2s+1} W_{\alpha\alpha}(m, k, t)}{\partial k^{2s+1}},$$
(A.10)

whereas for the off-diagonal elements $\alpha \neq \beta$, we now have only the contribution from even values of p = 2s, and we can easily obtain

$$D_{\alpha\beta} = -2\mathrm{i}(-1)^{\alpha} \sum_{s=0}^{\infty} \frac{(-1)^{s} a^{2s}}{(2s)!} \frac{1}{2^{2s}} \frac{\mathrm{d}^{2s} V(x)}{\mathrm{d}x^{2s}} \bigg|_{x=ma/2} \frac{\partial^{2s} W_{\alpha\beta}(m, k, t)}{\partial k^{2s}}.$$
 (A.11)

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