Eur. Phys. J. D **8**, 165–168 (2000)

THE EUROPEAN PHYSICAL JOURNAL D

EDP Sciences

A one-dimensional lattice model for a quantum mechanical free particle

A.C. de la Torre[a] and A. Daleo

Departamento de Física, Universidad Nacional de Mar del Plata, Funes 3350, 7600 Mar del Plata, Argentina

Received 25 March 1999 and Received in final form 20 August 1999

Abstract. Two types of particles, A and B with their corresponding antiparticles, are defined in a one-dimensional cyclic lattice with an odd number of sites. In each step of time evolution, each particle acts as a source for the polarization field of the other type of particle with nonlocal action but with an effect decreasing with the distance: $A \to \cdots \bar{B}B\bar{B}B\bar{B}\cdots$; $B \to \cdots A\bar{A}A\bar{A}A\cdots$. It is shown that the combined distribution of these particles obeys the time evolution of a free particle as given by quantum mechanics.

PACS. 03.65.Bz Foundations, theory of measurement, miscellaneous theories (including Aharonov-Bohm effect, Bell inequalities, Berry's phase) – 03.65.Ca Formalism

The modeling of physical reality by means of fictitious particles that move and react in a substrate of different geometrical structures has been a fruitful strategy that has extended our analysis capabilities beyond the domain associated with differential equations [1]. The particles involved in these models are classical in the sense that they are given precise location and velocity. This is clearly inadequate for the modeling of quantum systems that require, not only the indeterminacies imposed by Heisenberg's principle, but also nonlocal correlations between *commuting* observables, suggested by the Einstein Podosky Rosen argument [2] and empirically established in the violation of Bell inequalities [3,4]. However this does not forbid the modeling of quantum systems if we *do not* identify the particles of the model with the quantum particles. It is possible, as will be seen in this work, to associate the real quantum particle to a combined distribution of two types of fictitious particles with nonlocal interaction. This simple example model can be trivially extended to higher dimensions of space and to a higher number of non-interacting quantum particles and it provides a new point of view to study the peculiarities of quantum mechanics.

Let us assume a one-dimensional lattice with N sites on a circle and lattice constant a. We assume N to be an *odd* integer. The reason for this restriction will become clear later. The inclusion of *even* values for N would introduce unwanted complications in the model. Each site can be occupied by any number of particles of type A, B or by their corresponding antiparticles $\bar{A}$, $\bar{B}$. Particles and antiparticles of the same type annihilate in each site of the lattice leaving only the remaining excess of particles or antiparticles of both types A and B. At each time step, $t \to t+1$, corresponding to a time evolution by a small amount τ, the particles of type A create antiparticles $\bar{B}$ in the same site, particles B in the first neighboring sites, $\bar{B}$ in the second neighboring sites and so on. In a similar way, particles B create particles A and $\bar{A}$

$$\begin{aligned} A &\longrightarrow \cdots \bar{B}\,B\,\bar{B}\,B\,\bar{B}\cdots \\ B &\longrightarrow \cdots A\,\bar{A}\,A\,\bar{A}\,A\cdots \end{aligned} \tag{1}$$

The same reactions occur exchanging particles and antiparticles. This creation process extends to the right and left of each site up to the two opposing sites in the circle. Since N is odd, in these two sites particles of the same sign (either particles or antiparticles) are created. The *number* of particles or antiparticles created decreases with the distance d roughly like $1/d^2$ for a distribution of particles confined in a small region within a large lattice as will be precisely stated later. Before we write the master equation for the time evolution, we can notice some qualitative features of the process. It is easy to see that the process has diffusion. If we start, for instance, with some number of A particles in one site, after *two* time steps, some $\bar{A}$ antiparticles have been created at the same site reducing the number of A particles, but also some A particles appear in the first neighboring sites. The net effect is diffusion. It is less obvious that, even though the process has left-right symmetry, we may also have drift to the right or to the left. In order to see how this is possible we notice that A particles *reject* B particles from the site because $\bar{B}$ are created there, whereas B particles *attract* neighboring A particles to his site. Therefore if we have an asymmetric configuration like AB, the center of the combined distribution will move towards B. The drift direction and velocity is then *encoded* in the shape and relative distribution of both types of particles. We will see that, although the distribution of particles are widely

[a] e-mail: dltorre@mdp.edu.ar

distorted after few time steps, the drift direction and velocity remain invariant.

A convenient way to label the sites of the circular lattice is by an index s running from $-L$ to L. Since the number of sites $N = 2L+1$ is odd, the index s will be integer. It is of course irrelevant which site has the label $s = 0$. Let $a_s(t)$ and $b_s(t)$ be the number of particles of type A and B respectively at the site s at time t, normalized in a way that will be specified later (anyway the master equation is independent of the normalization). When $a_s(t)$ or $b_s(t)$ take negative values they denote the number of *antiparticles*. At a particular site of the lattice, the number of particles change as particles or antiparticles are created in it by the particles in other sites. The time evolution of the process is then defined by the equations

$$\begin{aligned} a_s(t+1) &= a_s(t) + \tau g^2 \sum_{d=-L}^{L} b_{[s+d]}(t) F(d) \\ b_s(t+1) &= b_s(t) - \tau g^2 \sum_{d=-L}^{L} a_{[s+d]}(t) F(d), \end{aligned} \tag{2}$$

where the square brackets in the index, $[s+d]$, denotes "modulo N", that is, with a value in the closed interval $[-L, L]$; g is related to the lattice constant a by $g = (2\pi)/(Na)$ (it corresponds to the reciprocal lattice constant); τ is a time scale small enough to make $\tau g^2 N^2 \ll 1$, and the function of the distance $F(d)$ is defined as

$$\begin{aligned} F(d) &= \frac{1}{N} \sum_{k=-L}^{L} k^2 \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}kd} \\ &= \begin{cases} (-1)^d \dfrac{\cos(\pi d/N)}{2\sin^2(\pi d/N)} & \text{if } d = \pm 1, \pm 2, ..., \pm L \\ \dfrac{1}{12}(N^2-1) & \text{if } d = 0 \end{cases}. \end{aligned} \tag{3}$$

For later use we define a similar function $G(d)$ as:

$$\begin{aligned} G(d) &= \frac{\mathrm{i}}{N} \sum_{k=-L}^{L} k \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}kd} \\ &= \begin{cases} \dfrac{(-1)^d}{2\sin(\pi d/N)} & \text{if } d = \pm 1, \pm 2, ..., \pm 2L \\ 0 & \text{if } d = 0 \end{cases}. \end{aligned} \tag{4}$$

The alternating sign in the definition of $F(d)$ corresponds to the fact that particles and antiparticles are created at alternating sites, and the different sign in equation (2) is due to the difference in the role of particle and antiparticle in relation (1). If the particles are confined in a small region within a large lattice, the main contribution in the sums of equation (2) comes from terms with distance $|d| \ll N$. In this limit we have $|F(d)| \approx 1/d^2$ as mentioned before.

The number of A or B particles are not conserved in the time evolution. Neither is the sum of particles conserved. A quantity that is approximately conserved in the time evolution of the process is the sum of the square of the number of A particles (or antiparticles) plus the sum of the square of the number of B particles (or antiparticles). This approximately conserved quantity can be used for normalization and can be given a physical meaning like energy density or probability density. It is therefore relevant to define a *combined distribution* $a_s^2(t) + b_s^2(t)$, associated to this approximately conserved quantity. We will see that the drift velocity of this combined distribution, given by

$$\langle V \rangle = 4g \sum_{s,r} a_s(t) b_r(t) G(s-r), \tag{5}$$

is also approximately conserved in the time evolution. Given a distribution $\{a_s(t), b_s(t)\}$, we can change the drift velocity by an amount v, *without* changing the shape of the combined distribution by means of the local transformation

$$\begin{aligned} a'_s(t) &= a_s(t)\cos(vas/2) - b_s(t)\sin(vas/2) \\ b'_s(t) &= a_s(t)\sin(vas/2) + b_s(t)\cos(vas/2). \end{aligned} \tag{6}$$

Both quantities mentioned are "approximately" and not strictly conserved due to the discrete nature of the model. We will see that taking smaller time steps τ leads to better conservation. These features have been checked in a computer simulation of the process. A circular lattice with $N = 801$ sites ($L = 400$) and with lattice constant $a = 1$ was chosen. Several shapes of initial distributions were tried: Gaussian, uniform and random, with several widths and drift velocities. The time dependence of $M(t) = \sum_s (a_s^2(t) + b_s^2(t))$ and of the drift velocity given in equation (5) was studied. Taking a time step $\tau = 10^{-3}$, we found that these quantities remain constant after $t = 1000$ time steps, with a relative variation less than 10^{-5} for the Gaussian case, 4×10^{-4} for the uniform distribution, and 0.04 for the random distribution. For larger time steps, $\tau = 0.005$, these quantities remain constant (less than 1% relative variation) for the Gaussian and uniform case at $t = 1000$ but the random case begins to show significant departure from constancy. At $\tau = 0.010$ only in the Gaussian case these quantities remain constant (less than 0.1%). The time evolution of the shape of the combined distribution is strongly reminiscent of the time evolution of quantum mechanical wave packets. For instance, a Gaussian distribution for A and B particles, modified by equation (6) in order to have drift, will evolve increasing the width and drifting but maintaining the Gaussian shape. A uniform distribution will develop side lobes in the evolution. A remarkable feature is that the process smooths out the random fluctuations of an initial distribution.

The resemblance of the process with quantum mechanics is striking. We will indeed show that the process here defined corresponds to a quantum mechanical free particle in a lattice. An extensive numerical simulation of the process is therefore not necessary because quantum mechanics provides a faithful representation for it. Let us define then an N-dimensional Hilbert space spanned by a basis

$\{\varphi_s\}$ $s = -L, -L+1, \cdots, L$ corresponding to the eigenvectors of the position operator X. Then, $X\varphi_s = as\varphi_s$. In this finite dimensional Hilbert space, we can not define the momentum operator P by means of the usual commutation relation. The alternative way to define P is to choose first an *unbiased basis* [5–7] $\{\phi_k\}$,

$$\phi_k = \frac{1}{\sqrt{N}} \sum_{s=-L}^{L} \mathrm{e}^{\mathrm{i}\frac{2\pi}{N}ks}\varphi_s, \tag{7}$$

and with it, we define the momentum by the spectral decomposition

$$\begin{aligned} P &= \sum_{k=-L}^{L} gk\phi_k\langle\phi_k, \cdot\rangle \\ &= \frac{1}{N}\sum_{k,s,r} gk\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}k(s-r)}\varphi_s\langle\varphi_r, \cdot\rangle. \end{aligned} \tag{8}$$

The momentum eigenvalues and the relative phases to build the basis $\{\phi_k\}$ have been chosen such that P is the generator of translations. That is, with this choice, the operator $U_a = \exp(-\mathrm{i}aP)$ is such that $U_a\varphi_s = \varphi_{s+1}$. The translation is cyclic at the border, $U_a\varphi_L = \varphi_{-L}$. If we had taken N even, the right hand side of this equation should have a minus sign. This would complicate the model of relation (1) introducing a change of sign at some appropriated places. In order to have a simple lattice model for the quantum free particle we prefer to restrict ourselves to odd values of N.

The state of a free quantum particle, given by

$$\Psi(t) = \sum_{s=-L}^{L} c_s(t)\varphi_s, \tag{9}$$

will change according to the time evolution operator (we set $\hbar = 2m = 1$)

$$U_t = \exp(-\mathrm{i}P^2 t). \tag{10}$$

Let us consider the evolution of the coefficients of the expansion given in equation (9), in one step of discretized time: $t_0 = \tau t$ and $t_1 = \tau(t+1)$ with a small time scale τ and t positive integer. We have

$$c_s(t+1) = \sum_{r=-L}^{L} c_r(t)\langle\varphi_s, U_\tau\varphi_r\rangle. \tag{11}$$

For τ small enough such that $\tau\|P^2\| \ll 1$, that is $\tau \ll (a/\pi)^2$, the time evolution operator can be linearized and we obtain

$$c_s(t+1) = c_s(t) - \mathrm{i}\tau\sum_{r=-L}^{L} c_r(t)\langle\varphi_s, P^2\varphi_r\rangle. \tag{12}$$

Using equation (8) we calculate the matrix element

$$\langle\varphi_s, P^2\varphi_r\rangle = g^2\frac{1}{N}\sum_{k=-L}^{L} k^2\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}k(s-r)}. \tag{13}$$

We have then

$$c_s(t+1) = c_s(t) - \mathrm{i}\tau g^2\sum_{r=-L}^{L} c_r(t)F(s-r). \tag{14}$$

Reordering the terms in the sum and using the "modulo N" notation, we get

$$c_s(t+1) = c_s(t) - \mathrm{i}\tau g^2\sum_{d=-L}^{L} c_{[s+d]}(t)F(d). \tag{15}$$

Finally if we explicitly write the coefficients with real and imaginary part, $c_s(t) = a_s(t) + \mathrm{i}b_s(t)$, we get equation (2) above.

We can here check that $M(t) = \sum_s |c_s(t)|^2$ is approximately conserved

$$\begin{aligned} M(t+1) &= M(t) \\ &\quad + \tau^2 g^4\sum_{r,u} c_r(t)c_u^*(t)\sum_s F(r-s)F(s-u). \end{aligned} \tag{16}$$

The term linear in τ vanishes because the symmetric function F appears multiplied by an anti-symmetric factor. We see here that the "derivative" $(M(t+1) - M(t))/\tau$ vanishes like τ in agreement with the numerical simulation of the process. We can write the functions F in their summation representations and, performing the sum over s, we get

$$\sum_s F(r-s)F(s-u) = \frac{1}{N}\sum_{k=-L}^{L} k^4\mathrm{e}^{\mathrm{i}\frac{2\pi}{N}k(r-u)}. \tag{17}$$

This sum can be evaluated as was done in equations (3, 4) but we don't need it. In the limit $N \gg d = r-u$, that is, when the particles are confined in a small region of a large lattice, we get

$$M(t+1) = M(t) + \tau^2\frac{\pi^4}{5}\left(2\sum_{r\neq u} c_r(t)c_u^*(t)\frac{(-1)^{(r-u)}}{(r-u)^2} + M(t)\right). \tag{18}$$

A similar result is obtained for the drift velocity, proportional to the expectation value of P

$$\langle P\rangle_t = -\mathrm{i}g\sum_{s,r} c_s^*(t)c_r(t)G(s-r). \tag{19}$$

In terms of $a_s(t)$ and $b_s(t)$ this equation becomes the equation (5) above. Here again, considering the time evolution $\langle P\rangle_{t+1}$, the term linear in τ vanishes because it contains $\sum_s[F(u-s)G(s-r) - G(u-s)F(s-r)]$ which is zero as can be calculated with the summation representation of the functions F and G. We obtain then

$$\begin{aligned} \langle P\rangle_{t+1} &= \langle P\rangle_t - \mathrm{i}\tau^2 g^5 \\ &\quad \times \sum_{u,v} c_u^*(t)c_v(t)\sum_{s,r} F(u-s)G(s-r)F(r-v). \end{aligned} \tag{20}$$

showing that the drift velocity is constant to order τ, that is, the "derivative" vanishes with τ in agreement with the numerical simulation of the process. Finally, applying a boost transformation $\exp(\mathrm{i}Xv/2)$ to the state of equation (9), we prove equation (6).

The one-dimensional lattice model here presented provides a simple representation for the position and momentum of a free quantum mechanical particle. In this model we require that N should be odd. Let us see what happens in the case where N is even. In this case, the model evolves according to equation (2) with the summations running from $-N/2$ to $N/2$ and with the same function $F(d)$ defined in equation (3). Notice that this function vanishes at the extreme values of d, that is $F(\pm N/2) = 0$. This model can be interesting in itself but it is no longer equivalent to the quantum mechanical system. The connection is lost in the step from equation (14) to equation (15). For the cases when the argument $s - r$ of the function F in equation (14) take values exceeding $N/2$, we should introduce a minus sign if we want to change the argument to d as in equation (15) (in the case N odd, no sign change is needed). The reason for this change can be traced to the change in sign produced by the translation operator when the site labeled by $\pm L$ is crossed as mentioned after equation (8). It would be possible to include even values for N but at the cost of complicating the model. For this we would have to change the rules of relation (1) exchanging particles and antiparticles when we cross the site with label $\pm L$. These complications are unwanted and we prefer to accept the fact that position and momentum of a quantum mechanical particle can be easily modeled only with a cyclic lattice with an odd number of sites. In the case of a quantum particle confined in a very small region (say, 10 sites) of a very large lattice (say, close to one million sites) it doesn't matter whether N is even or odd for all times until, due to drift or diffusion, the distribution reaches the sites with label close to $\pm N/2$. However for small lattices and for extended distributions it does matter, and only in the odd N case the model of relation (1) describes a quantum mechanical particle. This is a further indication of the essential nonlocal character of quantum mechanics. There is another case in quantum mechanics where an even or odd number of states has important qualitative consequences. This is in finite dimensional realizations of angular momentum. Whereas *intrinsic* angular momentum, the spin, of a particle can have an even or odd number of states, the *orbital* angular momentum, arising from position and momentum, can only have a realization with an odd number of states.

The model presented can be extended from the free particle to the case of a position dependent potential. The general structure of the process shown in relation (1) remains unchanged but the function F of equation (2) will not be given by equation (3) but will have to be calculated from an appropriate time evolution operator. The process can also be extended to two or three space dimensions but with larger computer requirements for the numerical simulations.

Since the advent of quantum mechanics, there have been numerous attempts to develop a classical image for quantum behavior. For the reasons already mentioned at the beginning, the attempts in terms of *particles* are doomed. The model here presented, besides being a "divertissement" in theoretical physics, also suggests the possibility of a classical image for quantum mechanics in terms of two *fields* $A(x,t)$ and $B(x,t)$ where each field acts as a source for the polarization of the other. Indeed, in the continuous limit, the particles and antiparticles of this work become creation and destruction quanta of two fields that turn out to be the real and imaginary part of the wave function; $\Psi(x,t) = A(x,t) + \mathrm{i}B(x,t)$. The continuous extension of equations (2, 3) provide the equations of motion for the fields that are equivalent to Schrödinger equation. This continuous study has been done somewhere else [8] and suggests an interpretation of quantum mechanics as a classical field theory, not more weird than classical electrodynamics. These considerations may provide a new point of view for studying the peculiarities of quantum mechanics.

We would like to thank H. Mártin for discussions and comments. This work has been done with partial support from "Consejo Nacional de Investigaciones Científicas y Técnicas" (CONICET), Argentina (PIP grant No. 4342/96). One of us (A.D.) would like to thank the "Comisión de Investigaciones Científicas" (CIC) for financial support.

References

1. E.V. Albano, Heter. Chem. Rev. **3**, 389 (1996); A.L. Barabási, H.E. Stanley, *Fractal Concepts in Surface Growth* (Cambridge University Press, 1995).
2. A. Einstein, B. Podolsky, N. Rosen, Phys. Rev. **47**, 777 (1935).
3. J.S. Bell, Physics **1**, 195 (1964).
4. S.J. Freedman, J.F. Clauser, Phys Rev. Lett. **28**, 938 (1972).
5. W.K. Wooters, Ann. Phys. **176**, 1 (1987).
6. A. Peres, *Quantum Theory: Concepts and Methods* (Kluwer Acad. Pub., 1993).
7. A.C. de la Torre, J.L. Iguain, Am. J. Phys. **66**, 1115 (1998).
8. A.C. de la Torre, A. Daleo, Mar del Plata preprint, LANL code `quant-ph/9905032`.