Comments on the Weyl-Wigner calculus for lattice models

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Abstract

Here, we clarify the physical aspects between the discrete Weyl-Wigner (W-W) formalism, well-developed in condensed matter physics, and the so-called ‘precise Weyl-Wigner calculus for lattice models’ recently appearing in the literature. We point out that the use of compact continuous momentum space for a discrete lattice model is unphysically founded. It has an incommensurate phase space, highly unphysical, lacks the finite fields aspects, as exemplified by the Born-von Karman boundary condition of compactified Bravais lattice of solid-state physics, and leads to several ambiguities. This new W-W formalism simply lacks bijective Fourier transformation, which is well-known to support the uncertainty principle of canonical conjugate dynamical variables of quantum physics. Moreover, this new W-W formalism for lattice models failed to handle the quantum physics of qubits, representing two discrete lattice sites.

1 Introduction

There has been a surging interest in discrete Weyl-Wigner formulation of quantum physics in recent years [1–3]. Several recent W-W formulations for discrete lattice models have appeared in the literature. Here we give some clarifying comments on the physical merits of these various formulations. Specifically, our comments is essentially focused on the so-called precise W-W calculus for lattice models that has most recently appeared in the literature [1].

The discrete Weyl-Wigner (W-W) quantum physics has been well-developed in condensed matter physics with its various successful applications, including the IQHE [4–13]. It seems that it just needs to be properly applied or adapted to quantum field theory with ultraviolet cut-off. Below, I present a counter example that exposes the weakness, unnecessary complications, and corresponding physical and mathematical ambiguities of the new “precise” W-W formulation of discrete lattice models that has recently appeared, as well as other discrete W-W formulations, in the literature.

2 Wannier functions and Bloch functions physics

First of all, there are already long-standing existing quantum models in physics that has firmly and physically guided the discrete phase-space physics of the W-W formulation in condensed matter physics namely, (a) Localized Wannier function and extended Bloch function for discrete lattice in solid state physics, obeying the Born-von Karman boundary condition (or strictly speaking, modular arithmetic based on finite fields, akin to a group theory of integers), (b) Dirac delta function and plane waves in the continuum limit, i.e., physically and more importantly, only for continuous coordinate space can one have continuous momentum space (this quantum mechanical principle is violated in a recent unphysically-formulated W-W formalism, the so-called ‘precise’ Weyl-Wigner calculus for lattice models, where discrete lattice coordinates is unphysically and incommensurately matched with compact continuous momentum space)
In both (a) and (b), we have the eigenvector for positions (or discrete lattice position), \( |q\rangle \), and eigenvector for momentum (or discrete crystal momentum), \( |p\rangle \). Of course, all respective eigenspaces only go to continuum spaces in the limit of lattice constant goes to zero as in (b).

These respective eigenvectors, \( |q\rangle\) and \( |p\rangle \), in (a) and (b) are related bijectively by Fourier transformation, \( |q\rangle \to |p\rangle \) via \( \langle p | q \rangle \), and often produces results akin to quantum uncertainty principle in their probabilistic coordinate components. Thus, to construct a physically-based discrete phase space or discrete W-W quantum physics one must be guided by the following observations.

### 3 Construction of W-W formalism: Discrete phase-space based on finite fields

The physically-based construction of W-W formalism in condensed-matter physics is guided by the following well-known aspects of solid-state physics [4]. (i) The invariance of this physical scheme of complete and orthogonal set of \( \{|q\rangle\} \) and complete and orthogonal set of \( \{|p\rangle\} \), in going from discrete to continuum physics, provides a strong guide for formulating discrete quantum phase space W-W formalism in condensed matter physics, (ii) Another crucial guidance comes from the observation that the the number of discrete lattice points (and hence the number of discrete momentum points) must be an odd prime number for obvious inversion symmetry reason. Moreover, all arithmetic operations on this group of numbers must be closed, i.e., all arithmetic operation must be a modular arithmetic with prime number modulus \( (\text{akin to a group operation on prime number of integers}) \). In short, all arithmetic operation on these numbers is a modular arithmetic based on finite fields, since only for finite fields with prime number modulus does every nonzero element have well-defined multiplicative inverse, and hence modular division operation also provide closure.

### 4 Generalization to other discrete quantum and classical systems

**First Generalization:** Guidance (i) and (ii) allow us to generalize discrete phase space based on finite fields to be particularly useful when the quantum numbers involved, specifying the quantum states, are discrete configurations other than the particle position and momentum quantum numbers [11]. A simplest example is that of quantum bit or qubit, which will be discussed below. **Second Generalization:** The crucial importance and power of using finite fields is that one can easily generalized the discrete Wigner distribution construction based on the algebraic concept of finite fields, which are extension of prime fields, where \( q \) and \( p \) are field elements \( (\text{mod irreducible polynomial}) \), useful in quantum computing, visualization, and communication/information sciences. Here we have \( p^n \) elements for some prime \( p \) and some integer \( n > 1 \) useful for constructing the Wigner distribution function for \( \text{spin}=\frac{1}{2} \) systems [11,12].

I will detail below to show that the new 'precise' W-W formulation of lattice models is not consistent with the above-mentioned physically based models. It is essentially the misguided use of discrete lattice positions coupled with the compact continuous momentum space that complicate the new 'precise' W-W formulation and renders several ambiguities by incurring a non-bijective canonical conjugate dynamical variables, momentum \( p \) and coordinate \( q \). This, and together with the lack of modular arithmetic on finite fields, which is not invoked at all in this new W-W formulation is adding to several more ambiguities. These ambiguities stemmed from the use of the unphysical compact continuous momentum space corresponding to a discrete lattice space models.

### 5 The W-W formulation in condensed-matter physics

Let me first summarize the Bravais lattice vectors and their corresponding reciprocal lattice vectors, since this points to some generalities of the discrete W-W formulation in condensed matter physics. In 2-D lattice, we have the reciprocal lattice vectors, \( \vec{b}_1 \) and \( \vec{b}_2 \) given by the matrix,

\[
\left( \begin{array}{c} \vec{b}_1 \\ \vec{b}_2 \end{array} \right) = \frac{1}{\hat{n} \cdot (\hat{a}_1 \times \hat{a}_2)} \left( \begin{array}{c} \hat{a}_2 \times \hat{n} \\ \hat{n} \times \hat{a}_1 \end{array} \right)
\]  

(1)
which geometrically means that $\vec{b}_1$ is perpendicular to $\vec{a}_2$ and $\vec{b}_2$ perpendicular to $\vec{a}_1$. The $\hat{n}$ is the unit vector normal to the 2-D lattice plane.

In 3-D lattice, the reciprocal lattice vectors, $\vec{b}_1$, $\vec{b}_2$, and $\vec{b}_3$ are contained in the matrix

$$
\begin{pmatrix}
\vec{b}_1 & \vec{b}_2 & \vec{b}_3
\end{pmatrix}
= 
\begin{pmatrix}
\vec{a}_2 \times \vec{a}_3 & \vec{a}_3 \times \vec{a}_1 & \vec{a}_1 \times \vec{a}_2
\end{pmatrix}
$$

(2)

This is the form usually given in solid-state physics textbooks. It is worth mentioning that the above formulas are independent of any chosen coordinate system. Note that the matrix multiplication given by

$$(M)(M)^{-1} = I \tag{3}$$

becomes

$$
\begin{pmatrix}
\vec{a}_1 & \vec{a}_2 & \vec{a}_3
\end{pmatrix}
\begin{pmatrix}
\vec{b}_1 & \vec{b}_2 & \vec{b}_3
\end{pmatrix}^T = I
$$

$$
\begin{pmatrix}
\vec{a}_1 & \vec{a}_2 & \vec{a}_3
\end{pmatrix} \text{vectors in column}
\begin{pmatrix}
\vec{b}_1 \\
\vec{b}_2 \\
\vec{b}_3
\end{pmatrix} \text{vectors in rows (adjoint)}
= I_{3 \times 3} \tag{4}
$$

### 5.1 Translation symmetry

The overarching concept in solid state physics is the concept of translation symmetry along any symmetry directions of the lattice. Inversion symmetry of the lattice structure is also one of the symmetry properties. Thus, the Buot discrete phase space W-W formalism in condensed matter physics is compatible with any of the lattice structures defined by Eq. (1) – (2), i.e., not limited to cubic lattice structures only.

#### 5.1.1 Discrete momentum space

Each energy band corresponds to the splitting of the energy levels of one atomic site into $N$ levels where $N$ is the number of lattice sites in a compactified Bravais lattice obeying the Born-von Karman boundary condition in a given symmetry direction. This is the basis of energy band quantum dynamics. Therefore, the number of crystal momentum states in each band (in Brillouin zone) is exactly equal to the number of lattice sites. This is an important physical observation which is violated by the new ‘precise’ W-W calculus of lattice models. Hence, there has to be a bijective mapping between number of discrete lattice sites and the number of discrete crystal momentum states. This is the essence of the powerful theoretical concept of localized function around each lattice site, the so-called Wannier function $|q\rangle$, and the extended function over all lattice points, the so-called Bloch function $|p\rangle$, related through the bijective discrete Fourier transformation. The bijectivity aspect is crucial here to avoid ambiguities.

#### 5.1.2 Bijective Fourier transformation

In short, the crystal momentum space is essentially discrete to yield a bijective mapping to the discrete lattice sites in a discrete Fourier transformation, it should definitely not be a compact continuous momentum space, which is the highly unphysical basic assumption of the ‘precise’ W-W formulation. This would give an ambiguous or ill-defined correspondence between lattice sites and continuous momentum space in a Fourier transformation, a bijective deficiency. Moreover, without the provision of closure property based on modular arithmetic of the mathematics of finite fields, the use of continuous momentum space will lead to other ambiguities in taking the Weyl transform. To cure this deficiency would only lead to obscure and complex mathematics far from the simple basic physics, which is the characteristic of the new ‘precise’ W-W formalism, and other recent discrete W-W formalisms in the literature.

The Bloch function is an eigenfunction of crystal momentum and the Wannier function is the eigenfunction of lattice site position. Observe that these eigenfunctions of phase space operators are well established for gapped structures with translational symmetry, or energy band far removed from the other energy bands. Generalized Wannier function can also be defined for coupled energy bands, using decoupling scheme like the Foldy-Wouthuysen transformation for relativistic Dirac electrons. Indeed, it has been shown that counterparts of Wanner function and Bloch function exist for the decoupled positive energy states of relativistic
electrons, with the 'Dirac-Wannier function’ localization about the size of Compton wavelength. Electric Wannier function and magnetic Wannier function also exist, as well as their respective Bloch functions, for uniform external electromagnetic fields. This physical idea has been extended by Buot to formally construct the discrete phase space quantum mechanics based on finite fields for cases where $q$ and $p$ are not position and momentum variables, useful for quantum computing.

Now for the finite number of lattice points to have closure property under modular arithmetic operations of addition (includes inversion), multiplication, and division, the number of lattice points must be a prime number obeying the Born-von Karman boundary condition, i.e., of prime modulus obeying modular arithmetic of finite fields.

In general, the Buot formalism for discrete phase space in condensed matter physics is based on the mathematics of finite fields [14] and holds for any prime number of lattice points obeying the Born-von Karman boundary condition. It even holds for the most elementary prime number 2 of lattice points, to yield the $2 \times 2$ Pauli spin matrices and the well-known Hadamard transformation between “Wannier function” and “Bloch function”, i.e., discrete Fourier transformation of two points in “phase space” leading to transformation of qubits. Here the “Wannier function” and “Bloch function” simply become a guiding theoretical concept, i.e, has acquired the status of a simple theoretical device for discrete quantum physics. Indeed, the Buot formalism also gives the generalized Pauli spin operators for any given prime number of lattice points. It has also yielded all the entangled basis states for two and three qubits, crucial to the physics of quantum teleportation [11].

5.1.3 Phase-space point projectors in Hilbert space

In Buot W-W formalism, any quantum mechanical operator is meaningfully expanded in terms of phase-space point projectors in Hilbert space. The coefficient of expansion is precisely the phase-space distribution function (lattice Weyl transform), or the Wigner distribution function if the density operator is the one expanded in terms of phase-space point projectors [11]. The same phase-space point projector was obtained by Gibbons et al [14] constructed from the eigenstate of the equation of lines in discrete $(p, q)$-phase space based on finite fields.

6 Violations and weakness of the new 'precise’ W-W formulation

So, we see that the use of the theoretical and physically-based model pioneered by the concept of Wannier function and Bloch function in solid-state physics is essential to a formal discretization in phase space quantum physics based on the mathematics of finite fields. In contrast, the basic assumption of the new ‘precise’ W-W calculus for lattice models [1] has the following unphysical ingredients, some listed as follows.

1. It misses the use of Hilbert space of discrete lattice position eigenvectors and discrete crystal momentum eigenvectors, a powerful theoretical device for energy-band gapped structures,

2. It has a complete lack of the operational concept of modular arithmetic on finite fields, modulus prime number essential for modular-arithmetic closure property of a finite prime number of lattice points, to avoid ambiguous arithmetic manipulations [continuum limit only when lattice constant goes to zero],

3. It has incurred an unnecessary complications by considering two discrete lattices, physical and ancillary unphysical lattice, and the momentum space is erroneously (unphysically) assumed as a compact continuous space, this coupled with being devorced from the modular arithmetic of finite fields makes a direct Weyl transformation on momentum space totally ambiguous and not bijective.

Although every finite field, with $p^n$ elements for some prime $p$ and some integer $n \geq 1$, often deals with irreducible polynomials over ring $\mathbb{Z}$ of integers, or over field $\mathbb{Q}$ of rational numbers, or over field $\mathbb{R}$ of real numbers, or over field $\mathbb{C}$ of complex numbers, the role of irreducible polynomials can be played by prime numbers themselves for $n = 1$: prime numbers (together with the corresponding negative numbers of equal modulus) are the irreducible integers. They exhibit many of the general properties of the concept 'irreducibility' that equally apply to irreducible polynomials, such as the essentially unique factorization into prime or irreducible factors: Every polynomial $p(x)$ in ring of polynomials with coefficients in $F$, denoted by $F[x]$, can be factorized into polynomials that are irreducible over $F$. This factorization is unique up to permutation of the factors and the multiplication of constants from $F$ to the factors.

The simplest case of interest in Buot discrete W-W formulation is when $n = 1$. In this case the finite field $GF(p)$ is the ring $\mathbb{Z}/p\mathbb{Z}$. This is a finite field with $p$ elements, usually labelled $0, 1, 2, ..., p - 1$, where arithmetic is performed modulo $p$, where nonzero elements have multiplicative inverses.
(4) It has violated the bijective mapping in a Fourier transformation of discrete lattice position to discrete momentum phase space, rendering this ambiguous, i.e., not bijective since the momentum space is assumed compact continuous, incommensurate with the number of discrete lattice sites, and

(5) It needs a correct physically-based assumption, namely, that both spaces, lattice sites and momentum states, are discrete and exactly equal in number of points, i.e., appropriately a prime number obeying modular arithmetic of finite fields.

6.1 Counter example

A counter example can easily be given in which the use of discrete ‘lattice points’ paired with compact continuous momentum points \([1]\) will fail and does not make any sense at all. Take the simplest prime number 2 of lattice points \([0, 1]\), a qubit. If we follow the new ‘precise’ W-W formulation, the momentum space is a compact continuous space in the interval \([0, \pi]\) assuming lattice constant of unity. Clearly the resulting Fourier transformation between the two spaces is highly ambiguous and is not bijective at the very least. On the other hand, if we follow Buot W-W formulation in condensed matter physics based on the mathematics of finite fields of the prime modulus number 2, and the use of theoretical device in terms of Wannier function and Bloch function, a lot of interesting physics is revealed \([11]\). Indeed, the \(2 \times 2\) Pauli spin matrices emerge, as well as the well-known Hadamard transformation, which has become the standard transformation of a quantum bit or qubit in quantum computing.

The Hadamard matrix is the transformation from the ”Wannier function”, \(|q\rangle\), to the corresponding ”Bloch function”, \(|p\rangle\), for the two-state system. Consider the identity

\[
|p\rangle = \sum_q \langle q | p \rangle |q\rangle,
\]

where the \(\langle q | p \rangle\) is the transformation function. For discrete quantum mechanics, this is given by the discrete Fourier transform function,

\[
\langle q | p \rangle = \frac{1}{\sqrt{N}} \exp \left( -\frac{i}{\hbar} p \cdot q \right).
\]

Upon substituting the possible values of \(q\) and \(p\), namely, \([0, 1]\) and \([\frac{2\pi \hbar 0}{2}, \frac{2\pi \hbar 1}{2}]\), respectively, for our two-state system, we obtained the matrix for \(\langle q | p \rangle\)

\[
\langle q | p \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix}
1 & 1 \\
1 & -1
\end{pmatrix} \equiv H,
\]

which is the Hadamard matrix, \(H\), which is really a ”two-state discrete Fourier transform matrix”.

7 Concluding Remarks

In summary, the method of new ‘precise’ W-W calculus for lattice models \([1]\) seems unnecessarily complicated, is not physically founded, and is beset with ambiguities cited above. More importantly, it fails to handle the physics of the simplest prime number 2 of discrete lattice sites. At the very least the cited ambiguities and bijective deficiency of the so-called new precise Weyl-Wigner calculus for lattice models renders this instead as an ‘imprecise’ W-W formulation for lattice models. It is worth mentioning that the Buot W-W discrete phase space formalism has also been the basis of numerical Monte Carlo approach to quantum transport \([15][16]\).

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