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LETTER TO THE EDITOR

Wilson-like functions on von Neumann lattices

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Abstract

An orthonormal set of functions is defined on a von Neumann lattice in phase space. There is one function assigned to each unit cell of area h. The functions are of the Wilson type in that in the x-direction they are obtained from one another by uniform translations, while in the p-direction they are double-peaked, and cannot be obtained by translations. A similar construction is also carried out with the x- and p-axes interchanged. The results apply to any dimension. An explicit example is worked out for the ground state of a harmonic oscillator, and a relation to coherent states is pointed out.

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The conventionally used Wannier functions in condensed matter physics are orthonormal functions localized around sites of a crystalline lattice in configuration space [1]. For an isolated energy band these functions have an exponential fall off. The situation is different when a magnetic field is present. The localization and orthogonality of the magnetic functions depend on whether or not the magnetic energy band carries a non-zero quantum Hall coefficient [2]. There is a connection between magnetic functions and the localization problem in phase space on a von Neumann lattice [3], the latter being a lattice in phase plane with area h (Planck constant) of the unit cell [4]. This connection enters via the magnetic translation group which is the symmetry group of a Bloch electron in a magnetic field [5, 6]. The localization of wavefunctions on a von Neumann lattice is controlled by the Balian–Low theorem [7] according to which the fall-off of these functions and their orthogonality are mutually exclusive, a feature that is well known in quantum mechanics [8]. This theorem has been explicitly demonstrated for the magnetic field problem in [9, 10]. Much attention has been given to expansions in sets of function on lattices in phase plane by the signal processing community [11]. In the original construction of von Neumann sets the states are constructed from a single function on a lattice with unit cell area h. One of the ideas to bypass the Balian–Low theorem is to use the concept of frames [12]. This leads to lattices in phase plane with a unit cell area smaller than h and, respectively, to highly overcomplete and non-orthogonal sets of states. Another idea of bypassing the Balian–Low theorem was raised by Wilson [13], who suggested to use a lattice with a unit cell of area $\frac{h}{2}$ in an ingenious numerical iteration procedure for constructing a complete and orthogonal set of

states. Following this development, Daubechies *et al* [14] have given an analytic construction of such a set of states and called it the Wilson orthonormal basis. What is characteristic about these functions is the asymmetry between the x- and p-axes: on the x-axis they behave like the usual von Neumann set (they can be obtained from one another by translations by a lattice constant a), but on the p-axis, they are doubly peaked, and cannot be obtained from one another by translations. As such, these functions do not violate the Balian–Low theorem, which applies to functions that are obtained from a single function by translation in both x- and p-directions. The construction of these functions appears like a brilliant guess (the authors of [14] call it a trick), which leaves, however, a number of questions unanswered. Like, why is there an asymmetry between the x- and p-axes? Or how does one generalize them to more than one dimension? This is an important issue for three-dimensional electronic structure calculations [13]. Also, can one construct additional Wilson-like orthonormal bases?

In this letter we construct a great variety of Wilson-like orthonormal bases by building for them a general framework. The latter puts the x- and p-axes on an equal footing, and enables direct generalization to any dimension of the space. The construction relies to a great extent on the kq-representation, in general, and on its symmetry transformation properties, in particular.

We start with a few remarks about the transformation properties under inversion of a wavefunction $C(k,q)$ in the kq-representation [15]. Let $(I|2\alpha)$ be the inversion around the point α on the x-axis

$$(I|2\alpha)x = -x + 2\alpha. \tag{1}$$

Under this transformation $C(k,q)$ becomes

$$(I|2\alpha|C(k,q) = C(-k,-q+2\alpha) \tag{2}$$

which follows from the connection between $C(k,q)$ and the wavefunction $\psi(x)$ in the x-representation [15]

$$C(k,q) = \left(\frac{a}{2\pi}\right)^{\frac{1}{2}} \sum_{\ell} \exp(\mathrm{i}ka\ell)\psi(q-\ell a) \tag{3}$$

where a is an arbitrary constant. From equation (3) it also follows that if $\psi(x)$ is real then

$$C^*(k,q) = C(-k,q) \tag{4}$$

where $C^*(k,q)$ is the complex conjugate of $C(k,q)$. Let us now define an even, $C^{(e)}(k,q)$, and odd, $C^{(o)}(k,q)$, function under the operation $(I|2\alpha)$

$$(I|2\alpha)C^{(e)}(k,q) = C^{(e)}(k,q) \qquad (I|2\alpha)C^{(o)}(k,q) = -C^{(o)}(k,q). \tag{5}$$

We also assume that $C^{(e)}(k,q)$ and $C^{(o)}(k,q)$ satisfy equation (4).

With these preliminary remarks in mind one can prove a very far-reaching result, namely, that the functions

$$C_{\ell m}(k,q) = \frac{1}{\sqrt{2}}\exp(-\mathrm{i}kam)\left\{\exp\left[\mathrm{i}\frac{2\pi}{a}(q-\alpha)\ell\right]C^{(e)}(k,q) + \exp\left[-\mathrm{i}\frac{2\pi}{a}(q-\alpha)\ell\right]C^{(o)}(k,q)\right\} \tag{6}$$

with ℓ and m integers which assume values from $-\infty$ to $+\infty$, form an orthonormal basis, under the condition that

$$\pi\left[\left|C^{(e)}(k,q)\right|^2 + \left|C^{(o)}(k,q)\right|^2\right] = 1. \tag{7}$$

As will be seen below, equation (7) is easy to satisfy. The proof is entirely elementary. We start with the proof of orthonormality,

$$\begin{aligned}
&\iint C^*_{\ell m}(k,q)C_{\ell' m'}(k,q)\,\mathrm{d}k\,\mathrm{d}q \\
&\quad= \frac{1}{2}\iint \exp[\mathrm{i}ka(m-m')]\left\{\exp\left[\mathrm{i}\frac{2\pi}{a}(q-\alpha)(\ell'-\ell)\right]\left|C^{(e)}(k,q)\right|^2\right. \\
&\quad\quad+\exp\left[-\mathrm{i}\frac{2\pi}{a}(q-\alpha)(\ell'-\ell)\right]\left|C^{(o)}(k,q)\right|^2 \\
&\quad\quad+\exp\left[-\mathrm{i}\frac{2\pi}{a}(q-\alpha)(\ell+\ell')\right]C^{(e)*}(k,q)C^{(o)}(k,q) \\
&\quad\quad\left.+\exp\left[\mathrm{i}\frac{2\pi}{a}(q-\alpha)(\ell+\ell')\right]C^{(e)}(k,q)C^{(o)*}(k,q)\right\}\mathrm{d}k\,\mathrm{d}q \\
&\quad= \frac{1}{2}\iint \exp\left[\mathrm{i}ka(m-m')+\mathrm{i}\frac{2\pi}{a}(q-\alpha)(\ell'-\ell)\right]\left[\left|C^{(e)}(k,q)\right|^2\right. \\
&\quad\quad\left.+\left|C^{(o)}(k,q)\right|^2\right]\mathrm{d}k\,\mathrm{d}q=\delta_{\ell\ell'}\delta_{mm'}. \qquad (8)
\end{aligned}$$

In obtaining the result in equation (8) we used the following:
(1) The sum of the third and fourth terms gives zero which can be seen by applying to these two terms, first the inversion operation $(I|2\alpha)$ and then changing k into $-k$.[1] By doing this and using equations (2), (4) and (5), the sum of the third and fourth terms goes into minus itself, meaning that this sum is zero. We would like to remind the reader that equation (4) uses explicitly the reality of the wavefunction $\psi(x)$ in the x-representation. (2) By applying $(I|2\alpha)$ to the first term in equation (8) and then changing k into $-k$, the product of the exponentials in the first term will become identical with that in the second term. One can then sum the first and second terms and use equation (7) in order to arrive at the result of equation (8) (since we are left with exponentials only in the integrand), which means orthonormality of the set of functions in equation (6).

In a similar way one can prove completeness of the set in equation (6). We have

$$\begin{aligned}
&\sum_{\ell m} C^*_{\ell m}(k,q)C_{\ell m}(k',q') \\
&\quad= \frac{1}{2}\sum_{\ell,m}\exp[\mathrm{i}(k-k')ma]\left\{\exp\left[-\mathrm{i}\frac{2\pi}{a}(q-q')\ell\right]C^{(e)*}(k,q)C^{(e)}(k',q')\right. \\
&\quad\quad+\exp\left[\mathrm{i}\frac{2\pi}{a}(q-q')\ell\right]C^{(o)*}(k,q)C^{(o)}(k',q') \\
&\quad\quad+\exp\left[-\mathrm{i}\frac{2\pi}{a}(q+q'-2\alpha)\ell\right]C^{(e)*}(k,q)C^{(o)}(k',q') \\
&\quad\quad\left.+\exp\left[\mathrm{i}\frac{2\pi}{a}(q+q'-2\alpha)\ell\right]C^{(o)*}(k,q)C^{(e)}(k',q')\right\}. \qquad (9)
\end{aligned}$$

Now, we use the Poisson summation formula for distributions for the variable y and constant c

$$\sum_m \exp(\mathrm{i}ymc)=\frac{2\pi}{c}\sum_m \delta\left(y-\frac{2\pi}{c}m\right) \qquad (10)$$

[1] The application of the latter two operations, $(I|2\alpha)$ and $k\to -k$, to a kq-function is equivalent to operating by $(I|2\alpha)$ on the q-coordinate only, which is a special transformation property under an inversion operation in the kq-representation [15].

and the boundary conditions on the kq-function [15]

$$C\left(k+\frac{2\pi}{a},q\right)=C(k,q)=\exp(-\mathrm{i}ka)C(k,q+a). \tag{11}$$

Equation (9) turns into

$$\sum_{\ell,m}C^{*}_{\ell m}(k,q)C^{*}_{\ell m}(k',q')=\pi\left[\left|C^{(e)}(k,q)\right|^{2}+\left|C^{(o)}(k,q)\right|^{2}\right]\langle kq|k'q'\rangle=\langle kq|k'q'\rangle \tag{12}$$

where equation (7) was used and also the following notation

$$\sum_{m}\delta\left(k-k'-\frac{2\pi}{a}m\right)\sum_{n}\exp(\mathrm{i}kan)\delta(q-q'-na)=\langle kq|k'q'\rangle. \tag{13}$$

In arriving at equation (12) one has to show that the third and fourth terms in equation (9) cancel, which follows directly from equations (4) and (5). Having proven orthogonality and completeness, this completes the proof that the set in equation (6) forms an orthonormal basis, under the condition that equation (7) is satisfied.

In order to appreciate the wide variety of orthonormal bases that are contained in equation (6), we remark that for $C^{(e)}(k,q)$ and $C^{(o)}(k,q)$ in equation (6) we can choose completely arbitrary even and odd functions with the only condition that they satisfy equation (7). For example, $C^{(e)}(k,q)$ can be the ground state of the harmonic oscillator and $C^{(o)}(k,q)$—the first excited state. This is a case for $\alpha=0$ in equation (6). For making them satisfy the condition given by equation (7), one can define new even and odd functions,

$$\varphi^{(e,o)}(k,q)=\frac{C^{(e,o)}(k,q)}{\left\{\pi\left[\left|C^{(e)}(k,q)\right|^{2}+\left|C^{(o)}(k,q)\right|^{2}\right]\right\}^{\frac{1}{2}}}. \tag{14}$$

These new functions $\varphi^{(e,o)}(k,q)$ clearly satisfy equation (7). The assumption is that the denominator in equation (14) does not vanish.

Next, let us point out that given any function $C(k,q)$ (whose $\psi(x)$ is real) we can always decompose it into an even and odd part with respect to a general point $\alpha\neq 0$ on the x-axis ($\alpha=0$ are the common even and odd functions)

$$\begin{aligned}C(k,q)&=\tfrac{1}{2}[C(k,q)+(I|2\alpha)C(k,q)]+\tfrac{1}{2}[C(k,q)-(I|2\alpha)C(k,q)]\\&=\tfrac{1}{\sqrt{2}}\left[C^{(e)}(k,q)+C^{(o)}(k,q)\right]\end{aligned} \tag{15}$$

where the factor $\frac{1}{\sqrt{2}}$ is needed for normalization of $C^{(e)}(k,q)$ and $C^{(o)}(k,q)$ to 1, if $C(k,q)$ is normalized to 1. $C^{(e)}(k,q)$ and $C^{(o)}(k,q)$ in equation (15) can be used for constructing the functions in equation (6). Certainly, one has to make sure that they satisfy equation (7), for which one can use equation (14). With the definition of equation (15), the basis functions of equation (6) become (ℓ, m run from $-\infty$ to ∞)

$$\begin{aligned}C_{\ell m}(k,q)=\exp(-\mathrm{i}kam)&\left\{\cos\left[\frac{2\pi}{a}\left(q-\frac{a}{4}\right)\ell\right]C(k,q)\right.\\&\left.+\mathrm{i}\sin\left[\frac{2\pi}{a}\left(q-\frac{a}{4}\right)\ell\right]C\left(k,q-\frac{a}{2}\right)\right\}.\end{aligned} \tag{16}$$

These functions were written for $\alpha=\frac{a}{4}$ in order to show their connection to the Daubechies *et al* [14] set of functions $\psi_{\ell m}(x)$, which we present here for comparison. Also for comparison with [14] it was assumed that $C(k,q)$ in equation (16) is even. The $\psi_{\ell m}(x)$ are built from a single function $\phi(x)$ as follows (with $\ell\geqslant 0$ and m running from $-\infty$ to ∞):

$$\left.\begin{aligned}&\psi_{om}(x)=\phi(x-ma)\\&\psi_{\ell m}(x)=\sqrt{2}\cos\left(\tfrac{2\pi}{a}x\ell\right)\phi\left(x-m\tfrac{a}{2}\right)\qquad\text{if}\quad\ell>0\quad\ell+m\equiv\text{even}\\&\psi_{\ell m}(x)=\sqrt{2}\sin\left(\tfrac{2\pi}{a}x\ell\right)\phi\left(x-m\tfrac{a}{2}\right)\qquad\text{if}\quad\ell>0\quad\ell+m\equiv\text{odd}\end{aligned}\right\} \tag{17}$$

where a is the same lattice constant as above. In order to see the relation between the functions in equations (16) and (17), let us first point out that for $\ell = 0$, they are identical. This is because the second term in equation (16) vanishes for $\ell = 0$, and the first term is nothing else but the kq-transform of $\phi(x - ma)$ in equation (16) (see the definition of $C(k, q)$ in equation (3), and the boundary conditions on the kq-function in equation (11)). For $\ell > 0$, it is easy to see that the functions in equation (16) are linear combinations of those in equation (17). We would also like to point out that one can check directly for orthonormality and completeness of the functions in equation (16) for ℓ, m running from $-\infty$ to ∞.

One immediate advantage of the set of functions in equation (6) (also equation (16)) is in their unique form for all ℓ and m running from $-\infty$ to ∞. In addition, because of their elementary structure, one can extend the functions in equation (6) in two ways.

First, in a way similar to the construction of the set in equation (6), one can build functions which are double-peaked in the x-direction, and are obtained from one another by translations in the p-direction by $\frac{2\pi}{a}\hbar$. These functions are

$$A_{\ell m}(k, q) = \frac{1}{\sqrt{2}} \exp\left(\mathrm{i}q\frac{2\pi}{a}\ell\right)\left\{\exp(-\mathrm{i}kam)C^{(e)}(k, q) + \exp(\mathrm{i}kam)C^{(o)}(k, q)\right\} \tag{18}$$

where $C^{(e)}(k, q)$ and $C^{(o)}(k, q)$ are even and odd functions like in equation (5) but with $\alpha = 0$.[2] Also, unlike for the functions in equation (6) we require that the Fourier transforms $F(p)$ are real. It then follows that the $C(k, q)$-function satisfies the relation

$$C^*(k, q) = C(k, -q) \tag{19}$$

instead of equation (4) when $\psi(x)$ is real. Let us remind the reader of the connection between the Fourier transform $F(p)$ and the kq-function [15],

$$C(k, q) = \left(\frac{\hbar}{a}\right)^{\frac{1}{2}} \exp(\mathrm{i}kq) \sum_n \left(\mathrm{i}\frac{2\pi}{a}qn\right) F\left(\hbar k + \frac{2\pi}{a}n\right). \tag{20}$$

Under these conditions, it is easy to check that the functions in equation (18) form an orthonormal basis. As we have already pointed out, these functions are double-peaked on the x-axis and have identical shapes on a lattice of spacing $\frac{2\pi}{a}\hbar$ in the p-direction.

Second, it is simple to generalize the functions in equation (6) (or equally in equation (18)) to higher dimension. In three dimensions the functions of equation (6) become

$$\begin{aligned} C_{\vec{K}_\ell \vec{R}_m}(\vec{k}, \vec{q}) = \frac{1}{\sqrt{2^3}} \exp(-\mathrm{i}\vec{k} \cdot \vec{R}_m)\{&\exp[\mathrm{i}(\vec{q} - \vec{\alpha}) \cdot \vec{K}_\ell]C^{(e)}(\vec{k}, \vec{q}) \\ &+ \exp[-\mathrm{i}(\vec{q} - \vec{\alpha}) \cdot \vec{K}_\ell]C^{(o)}(\vec{k}, \vec{q})\} \end{aligned} \tag{21}$$

where $\vec{R}_m$ and $\vec{K}_\ell$ are, respectively, the Bravais and reciprocal lattice vectors, and $\vec{\alpha}$ is a constant vector in configuration space. The even and odd functions, $C^{(e)}(\vec{k}, \vec{q})$ and $C^{(o)}(\vec{k}, \vec{q})$ have to satisfy equation (7), with π replaced by π^3. Equally, the definition for the functions $\varphi^{(e,o)}(\vec{k}, \vec{q})$ holds also in three dimensions, again with π replaced by π^3. In a similar manner one can extend the function in equation (18) to three dimensions. For all the orthonormal sets we have constructed, both in one and three dimensions, there is one state assigned to a unit cell. The area of this cell is h in one dimension and h^3 in three dimensions.

We now consider an example when $C(k, q)$ in equation (16) is the ground state of a harmonic oscillator

$$\psi_o(x) = \left(\frac{1}{\lambda^2\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{x^2}{2\lambda^2}\right) \tag{22}$$

[2] Only under inversion around the origin of the coordinate system is there a full symmetry between x and p, $x \to -x$, $p \to -p$. This is the reason for choosing $\alpha = 0$ for the functions in equation (18).

where λ is the width of the Gaussian. In the kq-representation we have (see equation (3))

$$C_0(k,q) = \left[\frac{a}{2\lambda\pi^{\frac{3}{2}}}\right]^{\frac{1}{2}} \sum_n \exp\left[\mathrm{i}kan - \frac{(q-na)^2}{2\lambda^2}\right]. \tag{23}$$

One can show that the denominator of equation (14) becomes (see equation (15))

$$\begin{aligned}\pi\left[\left|C^{(e)}(k,q)\right|^2 + \left|C^{(o)}(k,q)\right|^2\right] &= \pi\left[|C_0(k,q)|^2 + \left|C_0\left(k, q-\frac{a}{2}\right)\right|^2\right] \\ &= \theta_3\left(\frac{ka}{2}\middle|\,\mathrm{i}\frac{a^2}{4\pi\lambda^2}\right)\theta_3\left(\frac{2\pi q}{a}\middle|\,\mathrm{i}\frac{4\pi\lambda^2}{a^2}\right)\end{aligned} \tag{24}$$

where $\theta_3(z|\tau)$ is the Jacobi theta function [16]

$$\theta_3(z|\tau) = \sum_{-\infty}^{\infty} \exp(2\mathrm{i}zn + \mathrm{i}\pi\tau n^2). \tag{25}$$

With this in mind we get an exact closed form for the orthonormal set of states in equation (16) in the case when $C(k,q)$ is the ground state of the harmonic oscillator

$$C_{\ell m}(k,q) = \frac{\exp(-\mathrm{i}kam)\left\{\cos\left[\frac{2\pi}{a}\left(q-\frac{a}{4}\right)\ell\right]C_o(k,q) + \mathrm{i}\sin\left[\frac{2\pi}{a}\left(q-\frac{a}{4}\right)\ell\right]C_o\left(k,q-\frac{a}{2}\right)\right\}}{\left[\theta_3\left(\frac{ka}{2}\middle|\,\mathrm{i}\frac{a^2}{4\pi\lambda^2}\right)\theta_3\left(\frac{2\pi q}{a}\middle|\,\mathrm{i}\frac{4\pi\lambda^2}{a^2}\right)\right]^{\frac{1}{2}}}. \tag{26}$$

From the properties of θ_3-functions, it is well known [16] that the denominator in equation (26) vanishes at no real kq-point. The reason that we have a single denominator in equation (26) is because it is periodic in q with period $\frac{a}{2}$. There is a very simple approximation for the denominator in equation (26) for the case when $\frac{a^2}{4\pi\lambda^2} = 1$. We then have, to a very good approximation,

$$\theta_3\left(\frac{ka}{2}\middle|\,\mathrm{i}\right)\theta_3\left(\frac{2\pi q}{a}\middle|\,\mathrm{i}\right) \approx 1 + 2\,\mathrm{e}^{-\pi}\left[\cos(ka) + \cos\left(\frac{4\pi q}{a}\right)\right] + \cdots \tag{27}$$

where we neglect terms of the order of $\mathrm{e}^{-4\pi}$. By using this approximation one can find a connection between the functions in equation (26) and the coherent states[3].

In conclusion, let us mention a number of possible uses of the Wilson-like functions on a von Neumann lattice. Originally, these functions were designated for large-scale electronic structure calculations [13]. Having now defined them in three dimensions, one can reconsider this designation. In this connection it is of interest to point out the following. The Wilson-like functions in equation (6) can be written in a product from (this holds also for the three-dimensional case in equation (21))

$$C_{\ell m}(k,q) = \exp(\mathrm{i}kam)C_\ell(k,q) \tag{28}$$

$$C_\ell(k,q) = \frac{1}{\sqrt{2}}\left\{\exp\left[\mathrm{i}\frac{2\pi}{a}(q-\alpha)\ell\right]C^{(e)}(k,q) + \exp\left[-\mathrm{i}\frac{2\pi}{a}(q-\alpha)\ell\right]C^{(o)}(k,q)\right\}. \tag{29}$$

From what was previously shown (see equation (8)), $C_\ell(k,q)$ in equation (28) satisfies the relation

$$\int |C_\ell(k,q)|^2\,\mathrm{d}q = \frac{a}{2\pi} \tag{30}$$

[3] This will be done in a separate publication.

and the functions in equation (28) can be considered to be Wannier functions of a hypothetical solid [15]. The corresponding Bloch functions in the kq-representation are

$$C_{\ell k_B}(k,q) = \left(\frac{a}{2\pi}\right)^{\frac{1}{2}} \sum_n \exp(\mathrm{i}k_B na) C_\ell(k, q-na) = \left(\frac{2\pi}{a}\right)^{\frac{1}{2}} C_\ell(k,q) \sum_n \delta(k - k_B - na). \tag{31}$$

Because of the special structure of the Wannier functions in equation (28), one can check that applying the p^2 operator to them leads for large ℓ's to the equation

$$p^2 C_{\ell m}(k,q) = \hbar^2 \left(\frac{2\pi}{a}\right) \ell^2 C_{\ell m}(k,q). \tag{32}$$

This shows that for large ℓ's the functions in equation (28) represent Wannier functions for an infinite square well potential.

Finally, forming an orthonormal basis, the Wilson-like functions (equations (6), (18) and (21)) can readily be used in expansions of other functions. This might, in particular, be useful for the magnetic field problem [9, 10]. In the latter, the degree of freedom of the orbit centre (which does not appear in the Hamiltonian) forms a phase plane on which the Wilson-like functions can be constructed. In general, the orthonormal bases of this letter can practically be built for any function (see equation (15)) and they replace the original von Neumann set with one function per unit cell of area h.

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