

Solid State Physics from the Mathematicians' Point of View

G. Ali · R. Beneduci · G. Mascali · F.E. Schroeck Jr. · J. J. Sławianowski

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Abstract We propose, for a finite crystal, that the entire system be expressed in terms of the phase space, including momentum, configuration position and spin. This is to be done both classically and quantum mechanically. We illustrate this with a silicon crystal. Then, quantum mechanically measuring with a wire containing electrons, we obtain a theoretically good approximation for an electron in one semiconductor. As well, we outline what has to be done for any crystal.

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1 Introduction

The field of solid state physics is over a century old, but has not been advanced on the foundational level to any great extent during that time. We take the position that it is high time. For example, Bloch took the eigenfunctions of the energy for an infinite crystal to be of a particular form (see the next section) completely

G. Ali and R. Beneduci
Department of Physics,
University of Calabria, Italy and INFN-Gruppo c. Cosenza, 87036 Cosenza, Italy
E-mail: g.ali@mat.unical.it, rbeneduci@unical.it

G. Mascali
Department of Mathematics,
University of Calabria, Italy and INFN-Gruppo c. Cosenza, 87036 Cosenza, Italy
E-mail: g.mascali@unical.it

F.E. Schroeck
Department of Mathematics
University of Denver, Colorado, USA
and Florida Atlantic University
Boca Raton, Florida, U.S.A.
E-mail: fschroec@du.edu

J. J. Sławianowski
Institute of Fundamental Technological Research
Polish Academy of Sciences
Warsaw, Poland
E-mail: jslawian@ippt.gov.pl

overlooking the fact that there may be no eigenfunctions at all. There are also no periodic (eigen)functions as they would not be square integrable over the entire space \mathbb{R}^3 , and hence would not be interpretable in terms of any probability. On the other hand, Bloch and others defined a particular type of lattice and formulated the equations for the eigenfunctions on them. We could take that lattice and factor "the space" by it, working on the factor space for the quantum mechanical representations. But what kind of a "the space" will we be working on? The answer to this is "the phase space" for the crystal. This brings us to the theory of quantum mechanics on phase space. We have also the fact that the ions that carry the potentials with which the electrons interact are not stationary, but have momenta based on the temperature of the crystal. The theory must have these momenta in it; i.e., again the theory must have momenta and positions in it. We wish to make a theory based on that phase space and obtain the relations of the representations of the original symmetry group for electrons (spin 1/2) but on the phase space of a crystal. Again, that phase space must have the rotations (spins) in it.

In this paper, we will concentrate on finite perfect crystals, develop the theory in the standard classical framework, then the classical theory in the framework of Hilbert space, and then in the related framework of quantum mechanics on phase space. In particular, we wish to have massive particles with spin in the formalism. We shall treat the general construction of a phase space, and derive the special case of the periodic lattice in the setting of a finite crystal in phase space in the next section. We give examples by deriving or discussing the phase space from the Heisenberg group, the Heisenberg \times rotation group, the Galilei group, and the Poincaré group. We then go on to discuss the quantum mechanical as well as classical mechanical "quantizations" involved. In section 3, we will consider the "periodic" potential. In section 4, we will treat the Heisenberg group in the two standard representations as well as the phase space representation, and consider connections between them. We will obtain that the phase space representation is not the product of the other two. We will discuss the band gap in section 5. In section 6, we will compare the Wannier basis with the phase space basis. In section 7, we shall discuss how we place the conduction electrons in an environment with a wire containing other electrons which we then measure. Finally, in section 8, we summarize the advantages of treating the crystal in phase space.

2 Perfect Finite Crystals

2.1 Why Phase Space?

The first fact that we have to address is that there is no crystal of infinite extent in quantum mechanics, or in classical mechanics for that matter. A crystal is a structure that has a "periodic" potential as you travel across it - and then you come to a boundary! First, we shall review the current formalism and obtain the form of a crystal there. Then we shall take that formalism and, by a mathematical trick of factoring, derive the phase space formalism for that crystal.

By definition, a "Bravais lattice" is a term for a crystal that is infinite in extent in all directions. We shall abbreviate "a crystal that is infinite in extent in all directions" by the moniker "an infinite crystal." Infinite crystals have cer-

tain symmetries, namely those of certain translations, rotations, inversions, and inversion-rotations. We shall deal only with translations and rotations here.

Historically, one defines the Schroedinger equation with a periodic potential on this lattice, and obtains "eigenvectors" of Schroedinger's Hamiltonian, H. Bloch takes these "eigenvectors" to be of the form

$$\psi(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r}) \quad (1)$$

where

$$u_{n,\mathbf{k}}(\mathbf{r}) = u_{n,\mathbf{k}}(\mathbf{r} + \mathbf{R}) \quad (2)$$

for all \mathbf{R} in the Bravais lattice, $n \in \mathbb{Z}$, and "crystal momentum" $\mathbf{k} \in \mathbb{R}^3$. Thus

$$\psi(\mathbf{r} + \mathbf{R}) = e^{-i\mathbf{k}\cdot\mathbf{R}} \psi(\mathbf{r}). \quad (3)$$

The condition $\mathbf{k} \cdot \mathbf{R} = 2\pi n'$ for some $n' \in \mathbb{Z}$ gives rise to the "reciprocal lattice" of the Bravais lattice for the "crystal momenta" \mathbf{k} .

The formulation for a finite crystal is done by imposing the Born and von Karman boundary condition [2]

$$\psi(\mathbf{r} + N_i \mathbf{a}_i) = \psi(\mathbf{r}), \quad i = 1, 2, 3 \quad (4)$$

for

$$\{\mathbf{a}_i \mid i \in \{1, 2, 3\}\} \quad (5)$$

the primitive vectors in the lattice and N_i integers such that $N_1 N_2 N_3 = N$ with N total number of primitive cells in the crystal.

We give reasons why each and every statement above is not very clear in a strict interpretation; we modify those comments with what could be the way they were meant.

1) There are no boundary conditions for an infinite lattice because there is no boundary for an infinite lattice. But periodic boundary conditions are still called boundary conditions in a different sense of the word "boundary." There may be actual boundary conditions on a finite crystal, however. We will derive the mathematical description of a finite crystal under a group of symmetries. (Subsections 2.3, 2.4, and 2.5.) The periodic boundary conditions will then make sense.

2) Any such eigenvector ψ satisfying (2.1)–(2.3) or (2.4) is necessarily not quantum mechanical as it is not square integrable over \mathbb{R}^3 . But it must be, as $|\psi(\mathbf{q})|^2$, \mathbf{q} designating configuration position, must be interpretable as a probability density. The fact that ψ "works" for the description of physical systems means that it does have some meaning in the quantum mechanical sense. It is incumbent on us to derive such a quantum mechanical meaning.

3) By what stretch of the imagination is there any eigenvector of the Schroedinger equation, much less a basis of eigenvectors? Bloch's theorem states that any eigenvector of the Schroedinger equation must be of the form given in (2.1)–(2.2). It does not say there are any. We have information on the existence of eigenvalues only in particular situations. For example, we know [1] that if the potential $V(\mathbf{x})$ is of class $C^\infty(\mathbb{R}^n)$, has a unique non-degenerate global minimum at $\mathbf{x} = 0$, and there is an $\varepsilon > 0$ such that $V^{-1}([0, \varepsilon])$ is compact, then there is a number h_0 such that $\hbar < h_0$ implies that the spectrum of the operator $-\hbar^2 \nabla^2 + V(\mathbf{x})$ in a small interval $[0, \delta]$ consists of a finite number of eigenvalues. Furthermore, the

Schroedinger operator does have eigenvalues if it is quadratic though, and one might use these eigenvalues and eigenvectors as an approximation for the general Schroedinger operator in some appropriate mathematical sense. By comparison, in a finite crystal what is the status of eigenvectors of the general Schroedinger equation? In particular, what is the Schroedinger equation for a finite crystal?

4) There is a potential error in the interpretation of the crystal momentum (the vectors \mathbf{k}), namely, in the paraphrased words of Ashcroft and Mermin [2], " \mathbf{k} is not the momentum as it is not an eigenvalue of the momentum operator $\mathbf{p} = -i\hbar\nabla$ corresponding to eigenvector ψ ." But this operator is derived from the fact that it is the representation of the Lie algebra operator \mathbf{P} in the representation of the Heisenberg group as acting on \mathbb{R}^3 . We don't have \mathbb{R}^3 anywhere in the actual picture. In general, what is the status of the crystal momentum on a manifold?

5) There is no apparent consideration of the fact that if we put this in a system over a phase space (with all that that entails: a Poisson bracket, a set of pairs of canonical observables, a Hamiltonian, etc.) we will obtain a truer picture of the set of momenta and (configuration) position. What are the implications of putting this system in a phase space?

6) We have in mind placing phonons as well as electrons in the crystal, and this entails treating the problem relativistically, in the Galilei group, or in an extension of the Heisenberg group to include the rotation group which has the electron with one of its various representations. In any event, it is not just a theory of a "scalar" particle such as a phonon. This will have the added attraction of possibly defining the crystal partially by certain rotations which are also symmetries of the crystal.

2.2 The Phase Space Formalism:

These are six items that we may want to address in a restriction of a truer picture for a finite crystal, and then ask what are the models when we approximate with various of these six problems. But what is the "truer picture"? We will obtain the phase space from the symmetry group of the system by a very well defined procedure. Then we will formulate the problem in the phase space formalism, obtaining a theory of the crystal that circumvents all of these problems. We will proceed as follows:

A) First, we should obtain the group, G , of symmetries of the space in which the crystal is immersed. We will choose the Heisenberg group as a first approximation; this will cover the first five problems. Later, we will choose either an extension of the Heisenberg group, or the Galilei group, or the Poincaré group so as to include the spin of the electron. This entails treating the configuration position in the Cayley representation so that one may have half-odd integer representations of the rotation subgroup.

Call this symmetry group G , the continuous part of which we recognize as a Lie group (a differentiable group) that is locally compact. For what follows, see any book on "Lie Algebras" or see [3].

Let the Lie algebra of the group G , also known as the system of generators of G , be denoted \mathfrak{g}_e . Here e denotes the identity of the group. $X \in \mathfrak{g}_e$ means there is a curve, φ , in the group such that $\varphi(0) = e$, and, for any function $f \in C^\infty(G)$, $Xf = \frac{d}{dt}f(\varphi(t))|_{t=0}$. The elements of \mathfrak{g}_e form the tangent space, $\mathfrak{g}_e = TG_e$ of G at e . We assume that $\dim(TG_e) < \infty$. We may define the dual space $\mathfrak{g}_e^* = (TG_e)^*$ of TG_e ,

consisting of the linear functionals on TG_e . If $\{X_j\}$ is a basis of TG_e , then the dual basis $\{X_k^*\}$ of $(TG_e)^*$ is given by $X_k^*(X_j) = \delta_{j,k}$. We may obtain the commutation relations by taking the t and s derivatives of $f(\varphi(t)\psi(s)\varphi^{-1}(t)\psi^{-1}(s))$, for ψ another curve in G , and setting $t = s = 0$.

We may generalize all this by defining $L_g(h) = g \circ h$, $g, h \in G$, and for the action on $C^\infty(G)$, $[L_g f](h) = f(g \circ h)$ and defining the derivative analogously at any $g \in G$ by $XL_g f = \frac{d}{dt} f(g \circ \varphi(t))|_{t=0}$. Then we have the invariance condition $L_g X f = X L_g f$, i.e., $L_g X = X L_g$ on functions. For L_g as a function on X , we write $(L_g)_* X$. We obtain $(TG)_g = TG_g$, the tangent space of G at g . By the same invariance condition, we obtain the same abstract commutation relations for the $(L_g)_* X$ as for at $g = e$. Thus we take $X = \{L_g X \mid g \in G\}$ as a general element of the tangent spaces in $\mathfrak{g} = TG = \cup'_{g \in G} TG_g$. Here \cup' denotes the disjoint union. They are made disjoint by taking (g, TG_g) for TG_g (especially in case that some of the TG_g are parallel). The TG_g are the image of the TG_e under the left-action of the group, $g \in G$. We can therefore form the disjoint union of the set of the action on TG_e over the group. Similarly $\mathfrak{g}^* = TG^* = \cup'_{g \in G} TG_g^*$. We also define the n -forms as the set of objects in $(TG^*)^{\wedge n}$. For example, $(TG^*)^{\wedge 2} = TG^* \wedge TG^*$. For the purposes of Lie algebras, we take all the TG_g as linear spaces with constant coefficients that are real.

Similarly, we have the right action of G on G given by $R_g(h) = h \circ g$ and for the action on $C^\infty(G)$, $[R_g f](h) = f(h \circ g)$ for all $h \in G$. Then we have, as a right-action of G on TG , $(R_g)_* X$, and on TG^* , $(R_g)^* X^*$.

We note that, for the cases of the Heisenberg, Galilei, and Poincaré groups, $\{X_j\}$ may be composed of the coordinates of the momentum, position, and angular momentum, as well as the time in the former two cases. We also could use the common notation dX_j for X_j^* .

B) Define the "coboundary operator" δ on \mathfrak{g}^* as a graded operator with

$$\begin{aligned} \delta f &= \sum_j [X_j f] X_j^*, \quad f \in C^\infty(G); \\ \delta \sum_j f_j X_j^* &= \sum_{j,k} (X_k f_j) X_k^* \wedge X_j^*, \quad f_j \in C^\infty(G), \\ \delta(X^* \wedge Y^*) &= (\delta X^*) \wedge Y^* + (-1)^n X^* \wedge (\delta Y^*) \end{aligned} \quad (6)$$

for X^* an n -form and Y^* an m -form. Then automatically $\delta^2 = 0$. We define the set of 2-cocycles $Z^2(\mathfrak{g}) = \{\omega \in (TG^*)^{\wedge 2} \mid \delta\omega = 0\}$. Common alternate notations are $Z^2(G) = Z^2(\mathfrak{g}) = Z^2(\mathfrak{g}^*)$.

Pick any (left-invariant) cocycle ω in $Z^2(\mathfrak{g})$. [4] Form $\mathfrak{h}_\omega = \{X \in \mathfrak{g} \mid \omega(X, \cdot) = 0\}$. \mathfrak{h}_ω is a Lie subalgebra of \mathfrak{g} ; so, we may form the subgroup $H_\omega = \exp(\mathfrak{h}_\omega)$ of G by exponentiation. (Exponentiation is the opposite of forming the tangent space starting now from the Lie algebra.) We suppose that G is locally compact and H_ω is a closed subgroup of G so that G/H_ω is a Hausdorff manifold. Then we use the theorem [4] that every transitive phase space that has G as the group of symmetries is either equivalent to G/H_ω , or to a disjoint union over the G -orbit of spaces of the form G/H_ω . Acting on G/H_ω , this ω acts non-degenerately since $\omega(X, Y) = 0$ for all $Y \in \mathfrak{g}$ implies $X \in \mathfrak{h}_\omega$ implies X is equivalent to $\mathbf{0}$ in \mathfrak{h}_ω . In general, G/H_ω is the phase space of the system. We will have to factor further to obtain a correct form having the physical properties of the crystal and/or the phonon or electron in the crystal.

For ease of computation, we note that, if $\{X_j\}$ is a basis for \mathfrak{g} , then the commutation relations for the basis are of the form

$$[X_j, X_k] = \sum_l c_{j,k}^l X_l, \quad (7)$$

the $c_{j,k}^l \in \mathbb{R}$ being the structure constants. Then a simple computation from $\delta^2 = 0$ yields

$$\delta X_l^* = \frac{1}{2} \sum_{j,k} c_{j,k}^l X_j^* \wedge X_k^*. \quad (8)$$

Thus δX_l^* may be read off of the commutation relations in \mathfrak{g} .

C) Let μ be a G -left-invariant measure on G/H_ω , which exists because G/H_ω is a phase space. In fact we have, up to an isomorphism and a multiplicative constant,

$$\mu \approx \omega \wedge \omega \wedge \cdots \wedge \omega = \omega^{\wedge n} \quad (9)$$

where

$$\omega^{\wedge(n+1)} = 0, \omega^{\wedge n} \neq 0. \quad (10)$$

In the case in which we have an orbit of G/H_ω 's, we shall use the notation as if we have only one μ . (Only in the case that H_ω is normal in G will μ be a Haar measure; G/H_ω is just a general phase space as a manifold.)

D) It will be convenient to use the following actions of G on G/H_ω from the left and from the right (we are slightly changing the definition of the left action):

$$\begin{aligned} \text{From the left: } & (L_g) * (g_1 \circ H_\omega) \equiv (g^{-1} \circ g_1) \circ H_\omega; \\ \text{from the right: } & (R_g) * (g_1 \circ H_\omega) \equiv (g_1 \circ H_\omega) \circ g. \end{aligned} \quad (11)$$

We will drop the $*$ from the notation. Also, note that we have $L_g R_h = R_h L_g$ for all $g, h \in G$.

Now, the left action takes you from G/H_ω to G/H_ω ; so, the left action is clearly a representation of G . What about the right action?

Write

$$x = g_1 \circ H_\omega \in G/H_\omega.$$

Then

$$\begin{aligned} R_g * (g_1 \circ H_\omega) &= (g_1 \circ H_\omega) \circ g \\ &= (g_1 \circ g) \circ (g^{-1} \circ H_\omega \circ g); \end{aligned} \quad (12)$$

so, R_g takes you from G/H_ω to $G/(g^{-1} \circ H_\omega \circ g)$. Now

$$\begin{aligned} g^{-1} \circ H_\omega \circ g &= g^{-1} \circ \exp(\mathfrak{h}\omega) \circ g \\ &= \exp((R_g) * (L_g) * \mathfrak{h}\omega) \\ &= \exp(\mathfrak{h}_{R_g^* L_g^*} \omega) \\ &= \exp(\mathfrak{h}_{R_g^*} \omega) \\ &= H_{R_g^* \omega} \end{aligned}$$

by the left-invariance of ω . Consequently, we have that $R_g : G/H_\omega \rightarrow G/H_{R_g^* \omega}$. Similarly for $R_h : G/H_{R_g^* \omega} \rightarrow G/H_{R_h^* R_g^* \omega}$. Consequently we may consider the

action of $g \in G$ not on a single G/H_ω but on the disjoint union over the orbit of the G/H_ω . We will treat functions over $\cup'_{g \in G}(g, G/H_{R_g^* \omega}) \equiv \cup'_{g \in G} G/H_{R_g^* \omega}$, and then $\{R_g \mid g \in G\}$ is a right-representation of G on $\cup'_{g \in G} G/H_{R_g^* \omega}$.

Only if H_ω is normal in G may we consider the right action as an action on G/H_ω as then we have $H_\omega = g^{-1} \circ H_\omega \circ g$ for all $g \in G$.

We note that in [6,7] we have shown that, if $\pi(X)$ is the right action of X on G/H_ω , then a condition for $\pi(X)$ and $\pi(Y)$ to effectively commute on G/H_ω , is that

$$[\pi(X), \pi(Y)] \subseteq \pi(\mathfrak{h}_\omega) + \mathbb{R}\mathbf{1}. \quad (13)$$

We include that this is true if we have $[\pi(X), \pi(Y)] = \pi(Z)$ where $\pi(Z) \neq 0$, and we may perform a spectral resolution on $\pi(Z)$ so that it is diagonal in this representation. This is especially the case if the representations of $\pi(X)$ and $\pi(Y)$ are not diagonal in this representation although $\pi(Z)$ is. Then we may conclude that in this representation, we have $[\pi(X), \pi(Y)] = \lambda\mathbf{1}$, where λ is an (approximate) eigenvalue of $\pi(Z)$.

Now, we have to promote this to an action on the disjoint union, $\cup'_{g \in G} G/H_{R_g^* \omega}$, over the orbit of G/H_ω . But the condition (2.13) is equivalent to

$$[\pi((R_g)_* X), \pi((R_g)_* Y)] \subseteq \pi((R_g)_* \mathfrak{h}_\omega) + \mathbb{R}\mathbf{1}.$$

Hence, when representing G from the right, if we can obtain the vanishing of all the commutation relations for all the relevant X, Y , then we have achieved the goal of taking classical mechanics and reproducing it on $\cup'_{g \in G} G/H_{R_g^* \omega}$.

This will be very important when we wish to include the rotation group in our considerations.

E) Now take the action of G on functions over G/H_ω or over the orbit of G/H_ω . The action from the left:

$$\Psi \in L_\mu^2(G/H_\omega); [L_g \Psi](\mathbf{x}) = \Psi(L_g \mathbf{x}) = \Psi(g^{-1} \mathbf{x}), \mathbf{x} \in G/H_\omega. \quad (14)$$

The action from the right: Here, set $\mathbf{x} \in G/H_{R_g^* L_g^* \omega} = G/H_{R_g^* \omega}$, $\mathbf{x} = g_2 \circ H_{R_{g_1}^* \omega}$; then

$$\begin{aligned} \Psi &= \{\Psi_{g_1} \mid g_1 \in G, \Psi_{g_1} \in L_\mu^2(G/H_{R_{g_1}^* \omega}), \|\Psi_{g_1}\| = 1\}; \\ [R_g \Psi_{g_1}](\mathbf{x}) &= \Psi_{g_1}(R_g \mathbf{x}) = \Psi_{g_1}(R_g(g_2 \circ H_{R_{g_1}^* \omega})) \\ &= \Psi_{g_1}((g_2 \circ H_{R_{g_1}^* \omega}) \circ g) = \Psi_{g_1}((g_2 \circ g) \circ (g^{-1} \circ H_{R_{g_1}^* \omega} \circ g)) \\ &= \Psi_{g \circ g_1}((g_2 \circ g) \circ H_{R_{g_1}^* R_{g_1}^* \omega}) \\ &= \Psi_{g \circ g_1}((g_2 \circ g) \circ H_{R_{g \circ g_1}^* \omega}), \end{aligned} \quad (15)$$

for all $g, g_1, g_2 \in G$.

Now, we have, for

$$\begin{aligned} \Psi &= \{\Psi_{g_1} \mid g_1 \in G\} \in \cup'_{g_1 \in G}(g_1, L_\mu^2(G/H_{R_{g_1}^* \omega})) \\ &= \cup'_{g_1 \in G} L_\mu^2(G/H_{R_{g_1}^* \omega}), \\ \|\Psi\| &\equiv \|\Psi_{g_1}\| = 1, \text{ for any } g_1 \in G. \end{aligned} \quad (16)$$

The action from the left will correspond to the quantum mechanical representations, and those from the right will correspond to the classical representations

on the phase space. We do not claim that the right or left representations are exclusively classical and quantum, but just that they are the way that classical representations can be done [6, 7] and quantum representations are usually done. See eg. [8][9].

F) To proceed further, we need to define several things. We first let $\sigma : G/H_\omega \rightarrow G$ be a Borel cross section:

$$\begin{aligned}\sigma &: G/H_\omega \rightarrow G, \\ \sigma &: \mathbf{x} \mapsto \sigma(\mathbf{x}), \quad \mathbf{x} \in G/H_\omega.\end{aligned}\tag{17}$$

For $\mathbf{x} \in G/H_\omega$, and $g \in G$, it follows that $g \circ \sigma(\mathbf{x}) \circ H_\omega = g\mathbf{x} = \sigma(g\mathbf{x}) \circ H_\omega$. Thus there is a unique $h(g, \mathbf{x}) \in H_\omega$ such that

$$g \circ \sigma(\mathbf{x}) \circ h(g, \mathbf{x}) = \sigma(g\mathbf{x}).\tag{18}$$

Consequently, from the associative property of G , we have the generalized cocycle condition

$$h(g_1 \circ g_2, \mathbf{x}) = h(g_2, \mathbf{x})h(g_1, g_2\mathbf{x}).\tag{19}$$

Finally, let there be a unitary 1-dimensional representation of H_ω given by

$$\alpha : H_\omega \rightarrow S^1 \equiv \{c \in \mathbb{C} \mid |c| = 1\}.\tag{20}$$

Now induce a representation, V^α , for all of G , on functions on G/H_ω . Take $f : \sigma(G/H_\omega) \rightarrow \mathbb{C}$. Extend this f to $F : G \rightarrow \mathbb{C}$ by defining

$$F(\sigma(\mathbf{x}) \circ h) \equiv \alpha(h^{-1})f(\sigma(\mathbf{x})), \quad h \in H_\omega.\tag{21}$$

for the unitary representation α of H_ω . Next let

$$\begin{aligned}\mathcal{H} &= \{F : G \rightarrow \mathbb{C} \mid F(g \circ h) = \alpha(h^{-1})F(g) \\ &\text{for all } h \text{ in } H_\omega, g \text{ in } G\}.\end{aligned}\tag{22}$$

Define

$$\langle \cdot, \cdot \rangle_{\mathcal{H}} : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$$

by

$$\langle F, K \rangle_{\mathcal{H}} = \int_{G/H_\omega} d\mu(\mathbf{x}) F^*(\sigma(\mathbf{x})) K(\sigma(\mathbf{x}))\tag{23}$$

where we have defined $\mu(\sigma(\mathbf{x})) = \mu(\mathbf{x})$. Then $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ is independent of the choice of the $\sigma(\mathbf{x})$ by the unitarity of α ; so, it defines a pre-inner product on \mathcal{H} . [3, p. 322] Furthermore, \mathcal{H} is linear; so, close \mathcal{H} if necessary, to obtain a Hilbert space which we again will call \mathcal{H} . On \mathcal{H} , define the induced representation V^α by

$$[V^\alpha(g)F](g_1) = F(g^{-1} \circ g_1), \quad g, g_1 \in G.\tag{24}$$

V^α is automatically unitary, and is called the "induced left-regular representation." Note that actually we have defined the F 's on G/H_ω : $F(g) = f(gH_\omega)$.

Having the V^α will be important when we take G to have a spin group as a subgroup, for example.

One may also induce from a representation on S^1 to an induced right-regular representation, but we shall not do the details here.

Notice that there is no role played by \mathbb{C} other than that it is a Hilbert space in its own right. We may replace \mathbb{C} with the Hilbert space \mathcal{H}_0 in the above and obtain similar results. This is important when we proceed to induce representations of the Galilei group, the Poincaré group, and other groups. We will not do the details here as they may be found in [5].

Now, using (2.21) and supposing that H_ω is in the center of G , gives

$$\begin{aligned} [V^\alpha(h)F](g_1) &= F(h^{-1} \circ g_1) \\ &= F(g_1 \circ h^{-1}) \\ &= \alpha(h)F(g_1), \quad h \in H_\omega, g_1 \in G. \end{aligned} \quad (25)$$

If H_ω encodes the change from r to $r + R$ (see (2.51) - (2.58) for the Heisenberg group), we have generalized (2.1)-(2.4) from the case in which H_ω is in the center of G .

We may also obtain the action from the right on **the same** \mathcal{H} , see [6, 7].

Comment: The idea of using a symplectic space as the phase space is an old idea. See [10] for one example from 1967. There, the symplectic space is assumed as well as the expressions for the Hamiltonian, etc. What is different here is that we have derived the form of the symplectic spaces from the group, then have the Hamiltonian, etc. This gives us a great deal of freedom in that we may derive different symplectic spaces for the same group and then proceed.

2.3 Phase Spaces in the Heisenberg Group Case

We choose the Heisenberg group as the group of phase shifts, translations of \mathbb{R}^3 , and boosts of \mathbb{R}^3 . Specifically,

$$\mathcal{W} = \{(\lambda, \mathbf{q}, \mathbf{p}) \mid \mathbf{q}, \mathbf{p} \in \mathbb{R}^3, \lambda \in \mathbb{R}/2\pi\} \quad (26)$$

with the multiplication law

$$(\lambda', \mathbf{q}', \mathbf{p}') \circ (\lambda, \mathbf{q}, \mathbf{p}) = (\lambda' + \lambda + (\mathbf{q}' \cdot \mathbf{p} - \mathbf{q} \cdot \mathbf{p}')/2, \mathbf{q}' + \mathbf{q}, \mathbf{p}' + \mathbf{p}). \quad (27)$$

\mathcal{W} is locally compact. The center of \mathcal{W} is the set

$$Z(\mathcal{W}) = \{(\lambda, \mathbf{0}, \mathbf{0}) \mid \lambda \in \mathbb{R}/2\pi\}. \quad (28)$$

A basis of generators of \mathfrak{g} for \mathcal{W} are $\{\mathbf{1}, \mathbf{Q}_j, \mathbf{P}_k \mid j, k = 1, 2, 3\}$ satisfying

$$[\mathbf{Q}_j, \mathbf{P}_k] = -\delta_{j,k} \mathbf{1}, \quad (29)$$

the other commutators being zero.

Comment: The generators, X , in the Lie algebra are anti-adjoint; so, $\pm iX$ is self-adjoint in any complex representation of the group. Also, we have that the commutators of the X 's are real linear combinations of any basis of \mathfrak{g} . Furthermore, we have that an element of \mathcal{W} associated to $X \in \mathfrak{g}$ is in general of the form e^X which may also be written as e^{-iY} , with $Y = iX$ self-adjoint in any complex Hilbert space. Thus, we have a choice of writing everything as self-adjoint operators or in terms of X 's in \mathfrak{g} . Physicists usually use the self-adjoint option. We will use the other option.

Now, using

$$\mathbf{p} \cdot \mathbf{P} = \sum_j p_j \mathbf{P}_j, \quad p_j \in \mathbb{R}, \quad (30)$$

and

$$\mathbf{q} \cdot \mathbf{Q} = \sum_j q_j \mathbf{Q}_j, \quad q_j \in \mathbb{R}, \quad (31)$$

we obtain, for a general element X of \mathfrak{g}

$$X = (\lambda \mathbf{1} + \mathbf{q} \cdot \mathbf{Q} + \mathbf{p} \cdot \mathbf{P}) \quad (32)$$

for some $\lambda, q_j, p_j \in \mathbb{R}$.

Then,

$$[X, X'] = (\mathbf{q}' \cdot \mathbf{p} - \mathbf{q} \cdot \mathbf{p}') \mathbf{1}. \quad (33)$$

Also, we may denote elements of the group by

$$(\lambda, \mathbf{q}, \mathbf{p}) = \exp\{\lambda \mathbf{1} + \mathbf{q} \cdot \mathbf{Q} + \mathbf{p} \cdot \mathbf{P}\}. \quad (34)$$

(Notice again that we have used the convention that these generators $\mathbf{1}, \mathbf{Q}_j, \mathbf{P}_k$ are anti-adjoint in any complex representation. In particular, $\mathbf{1}$ is not the identity but is i times the identity.)

The dual basis for \mathfrak{g} is given by $\{\mathbf{1}^*, \mathbf{Q}_j^*, \mathbf{P}_k^* \mid j, k = 1, 2, 3\}$ such that

$$\begin{aligned} \mathbf{1}^*(\mathbf{1}) &= 1, \quad \mathbf{1}^*(\mathbf{Q}_k) = 0, \quad \mathbf{1}^*(\mathbf{P}_k) = 0, \\ \mathbf{Q}_j^*(\mathbf{1}) &= 0, \quad \mathbf{Q}_j^*(\mathbf{Q}_k) = \delta_{jk}, \quad \mathbf{Q}_j^*(\mathbf{P}_k) = 0, \\ \mathbf{P}_j^*(\mathbf{1}) &= 0, \quad \mathbf{P}_j^*(\mathbf{Q}_k) = 0, \quad \mathbf{P}_j^*(\mathbf{P}_k) = \delta_{jk}. \end{aligned} \quad (35)$$

From these equations and using (2.8), we obtain the coboundary operator, δ , (see [3, pp. 344-350] for this):

$$\delta(\mathbf{1}^*) = \sum_j \mathbf{Q}_j^* \wedge \mathbf{P}_j^*, \quad \delta(\mathbf{Q}_j^*) = 0, \quad \delta(\mathbf{P}_j^*) = 0, \quad (36)$$

and so for $j \neq k$,

$$\delta(\mathbf{Q}_j^* \wedge \mathbf{Q}_k^*) = \delta(\mathbf{P}_j^* \wedge \mathbf{Q}_k^*) = \delta(\mathbf{P}_j^* \wedge \mathbf{P}_k^*) = \delta(\mathbf{1}^* \wedge \mathbf{1}^*) = 0.$$

Thus the coboundary of a general two-form ω_2 is of the form

$$\begin{aligned} \delta\omega_2 &= \delta \left(\sum_j (\alpha_j \mathbf{1}^* \wedge \mathbf{Q}_j^* + \beta_j \mathbf{1}^* \wedge \mathbf{P}_j^*) \right) \\ &= \delta(\mathbf{1}^*) \wedge \sum_j (\alpha_j \mathbf{Q}_j^* + \beta_j \mathbf{P}_j^*) \end{aligned} \quad (37)$$

for $\alpha_j, \beta_j \in \mathbb{R}$; so, $Z^2(\mathfrak{g}) \equiv \text{Kernel}(\delta|_{2\text{-forms}}) = \{\omega_2 \text{ not involving } \mathbf{1}^* \wedge \sum (\alpha_j \mathbf{Q}_j^* + \beta_j \mathbf{P}_j^*)\}$, or

$$Z^2(\mathfrak{g}) = \left\{ \omega_2 = \sum_{j,k} (\alpha_{jk} \mathbf{P}_j^* \wedge \mathbf{P}_k^* + \beta_{jk} \mathbf{Q}_j^* \wedge \mathbf{P}_k^* + \gamma_{jk} \mathbf{Q}_j^* \wedge \mathbf{Q}_k^*) \right\}, \quad (38)$$

for $\alpha_{jk}, \beta_{jk}, \gamma_{jk} \in \mathbb{R}$.

We may choose (almost) any ω from $Z^2(\mathfrak{g})$, obtain \mathfrak{h}_ω and H_ω from it, and then form the phase space G/H_ω if H_ω is closed. To obtain the usual phase space, which we shall not use here except as an illustration, we take

$$\omega_0 = \delta(\mathbf{1}^*) = \sum_j \mathbf{Q}_j^* \wedge \mathbf{P}_j^*. \quad (39)$$

Then

$$\mathfrak{h}_{\omega_0} = \{\lambda \mathbf{1} \mid \lambda \in \mathbb{R}\}$$

from which we obtain

$$H_{\omega_0} = \{e^{\lambda \mathbf{1}} \mid \lambda \in \mathbb{R}\}.$$

But H_{ω_0} is closed as a subgroup of \mathcal{W} ; so, \mathcal{W}/H_{ω_0} is a phase space. H_{ω_0} is also a normal subgroup; so, \mathcal{W}/H_{ω_0} is even a group, and there is no significant difference in the action of \mathcal{W} on \mathcal{W}/H_{ω_0} from the left or right. \mathcal{W}/H_{ω_0} just is the usual phase space of \mathbf{q} 's and \mathbf{p} 's.

We now search for another phase space, one more suited to the problem of a crystal. For the crystal, let us define the basic lattice \mathcal{L}' of the physical system of the crystal as the set of linear combinations of the non-coplanar "primitive vectors" $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3\}$ with coefficients in \mathbb{Z} . Notice that such a set of primitive vectors defines a primitive or basic cell and the cell tiles \mathbb{R}^3 . Then a crystal lattice is defined as the set of linear combinations of the primitive vectors. (There are several ways to pick the primitive vectors; pick one.) This lattice is invariant under translation by the primitive vectors, and inversions in a finite class of planes (and by certain finite rotations which we will not consider until we include the rotations as a subgroup). We note that we may not choose these \mathbf{a} 's arbitrarily, but only those associated with some crystal. By including the rotation symmetries, there are only a finite number of crystal shapes available.

Set

$$\nu = 2\pi(\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3))^{-1} \quad (40)$$

and

$$\mathbf{b}_1 = \nu \mathbf{a}_2 \times \mathbf{a}_3, \quad \mathbf{b}_2 = \nu \mathbf{a}_3 \times \mathbf{a}_1, \quad \mathbf{b}_3 = \nu \mathbf{a}_1 \times \mathbf{a}_2. \quad (41)$$

The vectors that are linear combinations of the $\{\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3\}$ with coefficients in \mathbb{Z} form a lattice \mathcal{L}'' , called the Heisenberg lattice. Furthermore, we have

$$\mathbf{a}_j \cdot \mathbf{b}_k = 2\pi \delta_{jk}. \quad (42)$$

The lattice \mathcal{L}'' is also called "the reciprocal lattice" to \mathcal{L}' , and is recognized as the lattice of the momenta. See, for example, [2]. We will set

$$\mathcal{L} = \mathcal{L}' \times \mathcal{L}''. \quad (43)$$

We shall refer to \mathcal{L} as "the" crystal lattice.

We take as a basis for \mathfrak{g} the set

$$\{\mathbf{1}, \mathbf{a}_j \cdot \mathbf{Q}, \mathbf{b}_j \cdot \mathbf{P} \mid j \in \{1, 2, 3\}\}, \quad (44)$$

with commutation relations

$$[\mathbf{a}_j \cdot \mathbf{Q}, \mathbf{b}_k \cdot \mathbf{P}] = -2\pi \delta_{j,k} \mathbf{1}, \quad (45)$$

and the rest of the commutation relations equalling zero.

We now have the notation necessary to define a different phase space for the Heisenberg group, one which we shall use for the crystal. Define

$$\begin{aligned}\omega &= \delta(2\pi\mathbf{1}^*) \\ &= \sum_{j \in \{1,2,3\}} (\mathbf{a}_j \cdot \mathbf{Q}^* \wedge \mathbf{b}_j \cdot \mathbf{P}^*).\end{aligned}\quad (46)$$

But this is just the previous result with a new basis. Thus, we obtain again

$$\mathfrak{h}_\omega = \{\lambda\mathbf{1} \mid \lambda \in \mathbb{R}\} \quad (47)$$

and

$$H_\omega = \{e^{\lambda\mathbf{1}} \mid \lambda \in \mathbb{R}\}.\quad (48)$$

Hence \mathcal{W}/H_ω is just the usual phase space.

Next, we take the Heisenberg group for \mathcal{L} by which we mean

$$D = \left\{ \exp \left(\left[\sum_{\substack{n_j \in \mathbb{Z}, \\ j \in \{1,2,3\}}} n_j \mathbf{a}_j \cdot \mathbf{Q} + \sum_{\substack{m_j \in \mathbb{Z}, \\ j \in \{1,2,3\}}} m_j \mathbf{b}_j \cdot \mathbf{P} \right] \right) \right\}.\quad (49)$$

Furthermore, from the group relations, D is normal in \mathcal{W} , and hence in \mathcal{W}/H_ω :

$$\begin{aligned} & e^{(\lambda\mathbf{1} + \mathbf{q} \cdot \mathbf{Q} + \mathbf{p} \cdot \mathbf{P})} e^{(\mathbf{c} \cdot \mathbf{P} + \mathbf{d} \cdot \mathbf{Q})} e^{-(\lambda\mathbf{1} + \mathbf{q} \cdot \mathbf{Q} + \mathbf{p} \cdot \mathbf{P})} \\ &= e^{(\mathbf{c} \cdot \mathbf{P} + \mathbf{d} \cdot \mathbf{Q})}.\end{aligned}$$

Hence $(\mathcal{W}/H_\omega)/D$ is a group. D is also commutative, as one may easily check. These two properties have as consequences the fact that $(\mathcal{W}/H_\omega)/D$ is a very special phase space as we shall see, and one that is not necessary for the phase spaces of a general Lie group. It will be the phase space for \mathcal{L} , with the left-invariant volume measure on $(\mathcal{W}/H_\omega)/D$ coming directly from the volume measure on \mathcal{W}/H_ω . That $(\mathcal{W}/H_\omega)/D$ is a phase space, follows from the fact that D is closed in \mathcal{W}/H_ω ; so, $(\mathcal{W}/H_\omega)/D$ is Hausdorff, and that it is a manifold of dimension 6, and that any function on $(\mathcal{W}/H_\omega)/D$ comes from periodic functions on \mathcal{W}/H_ω with periods of length in $\{\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3\}$. We reiterate, $(\mathcal{W}/H_\omega)/D$ is the phase space for a crystal in the Heisenberg case.

The first step in obtaining an irreducible unitary representation of \mathcal{W} on \mathcal{W}/H_ω , is to obtain an irreducible unitary representation of H_ω . For that, we may either obtain a one-dimensional representation, α , of H_ω , or we may follow the procedure of Mackey [5]. Since H_ω is a commutative group, this is simply

$$\alpha(e^{\lambda\mathbf{1}}) = e^{i\lambda\epsilon}$$

for some $\epsilon \in \mathbb{R}$. We will take the choice $\epsilon = 0$. Consequently we obtain a representation of \mathcal{W}/H_ω from this. Then, we may obtain a representation, α' , of D (commutative) by

$$\begin{aligned}\alpha'(e^{(\mathbf{c} \cdot \mathbf{Q} + \mathbf{d} \cdot \mathbf{P})}) &= \alpha(e^{(\mathbf{c} \cdot \mathbf{Q} + \mathbf{d} \cdot \mathbf{P})}) \\ &= \exp\{i(\mathbf{c} \cdot \boldsymbol{\beta} + \mathbf{d} \cdot \boldsymbol{\gamma})\}\end{aligned}\quad (50)$$

where in $(\mathbf{c} \cdot \mathbf{Q} + \mathbf{d} \cdot \mathbf{P})$ we take $(\mathbf{c}, \mathbf{d}) \in \mathcal{L}$, for some choice of β , and $\gamma \in \mathbb{R}^3$. The α act unitarily on S^1 or on any complex vector space. The choices $\beta \in \mathcal{L}'$, $\gamma \in \mathcal{L}'$ are most convenient as they give $\alpha(e^{\lambda^1 D}) \equiv 1$.

Next we have to make a choice of $\sigma(\mathbf{x}) : (\mathcal{W}/H_\omega)/D \rightarrow \mathcal{W}$ that is Borel. This is easy:

$$\begin{aligned} \sigma(\mathbf{x}) &= \sigma(((\lambda, \mathbf{q}, \mathbf{p})/H_\omega)/D) \mapsto (0, \mathbf{q}/\mathcal{L}', \mathbf{p}/\mathcal{L}''), \\ \lambda &\in \mathbb{R}, \text{ and } \mathbf{q}, \mathbf{p} \in \mathbb{R}^3. \end{aligned} \quad (51)$$

We mean by this,

$$\begin{aligned} \mathbf{q}/\mathcal{L}' &= \{\mathbf{q}' \approx_{\mathcal{L}'} \mathbf{q} \mid 0 \leq q'_j < |\mathbf{a}_j|, j = 1, 2, 3\}, \\ \mathbf{p}/\mathcal{L}'' &= \{\mathbf{p}' \approx_{\mathcal{L}''} \mathbf{p} \mid 0 \leq p'_j < |\mathbf{b}_j|, j = 1, 2, 3\} \end{aligned} \quad (52)$$

where \mathbf{a} is the set of three primitive vectors of the crystal and \mathbf{b} is the set of three primitive vectors in the corresponding Heisenberg lattice given by (2.43). Since $\mathbf{x} \mapsto \sigma(\mathbf{x})$ is continuous except at the (boundary) points of \mathcal{L} , it is Borel.

Take $f : \sigma((\mathcal{W}/H_\omega)/D) \rightarrow \mathbb{C}$, extend it to \mathcal{W} . Then following (2.20)-(2.24), one obtains a representation

$$[V^\alpha(g)F](g_1) = F(g^{-1} \circ g_1), g, g_1 \in \mathcal{W}.$$

Hence, one obtains a unitary representation \mathcal{W} on a compact set! Here, we also have the direct interpretation of the $\mathbf{q}' \cdot \mathbf{Q}$ and $\mathbf{p}' \cdot \mathbf{P}$ being the translations and boosts. There is no question of \mathbf{p}' denoting a boost of \mathbf{p}' , unlike 4) in section 2.1.

Next we take the representations of \mathcal{W} on square integrable functions, Ψ , in $L^2((\mathcal{W}/H_\omega)/D)$, or the disjoint union of these over an orbit of ω . One may easily check that the $L(\mathcal{W})$ and $R(\mathcal{W})$ are representations of \mathcal{W} . In particular, there is no difficulty in showing that a given Ψ is square integrable or not, the integral being an integral over a compact set. This is much different from the mathematically questionable claim that in \mathbb{R}^3 , the periodic analogs of ψ and $\mathcal{F}\psi$, \mathcal{F} the Fourier transform, are square integrable over all of \mathbb{R}^3 . We have satisfied 1) and 2) of section 2.1.

Now we may see that, for $G = \mathcal{W}$, the Schroedinger equation is an equation on a compact set. It may have no eigenfunctions still! We will revisit this in a while.

We see that it has been very profitable to express the results in terms of the crystal lattice \times reciprocal lattice, as this has allowed us to express the restrictions on both the position and momentum vectors at the same time. We also remark that we could have made the factoring by any lattice that has begun with primitive vectors of the form $(n_1 \mathbf{a}_1, n_2 \mathbf{a}_2, n_3 \mathbf{a}_3)$, $n_j \in \mathbb{Z}_{>0}$. This would take care of the case of a finite crystal, and not just a single crystal cell.

2.4 Phase Spaces in the Heisenberg Group \times Rotation Group Case

In order to have the spin of the electron in our theory, we must add to our considerations a treatment of the rotation group. We will either take the group G defined as the Heisenberg group \times the rotation group or equivalently take G to be the continuous part of the symplectic group of $(\mathcal{W}/H_\omega, \mu)$. The group we obtain is isomorphic to the isochronous Galilei group, and is locally compact.

We have that the Lie algebra, \mathfrak{g} , is just the sum of the Lie algebras $\mathfrak{g}_{Heisenberg}$ and $\mathfrak{g}_{Rotation}$ with the basis $\{\mathbf{1}, \mathbf{Q}_j, \mathbf{P}_j, \mathbf{M}_j \mid j \in \{1, 2, 3\}\}$, the commutation relations of $\{\mathbf{1}, \mathbf{Q}_j, \mathbf{P}_j\}$ being given by (2.30), of the basis of the rotations $\{\mathbf{M}_j\}$ being given by

$$[\mathbf{M}_j, \mathbf{M}_k] = \sum_{l \in \{1, 2, 3\}} \epsilon_{jkl} \mathbf{M}_l, \quad (54)$$

and the remaining non-zero commutations of the basis being

$$[\mathbf{M}_j, \mathbf{P}_k] = \sum_l \epsilon_{jkl} \mathbf{P}_l, \text{ and } [\mathbf{M}_j, \mathbf{Q}_k] = \sum_l \epsilon_{jkl} \mathbf{Q}_l, \quad (55)$$

where

$$\begin{aligned} \epsilon_{jkl} &= 1 \text{ if } (j, k, l) \text{ is an even permutation of } (1, 2, 3), \\ \epsilon_{jkl} &= -1 \text{ if } (j, k, l) \text{ is an odd permutation of } (1, 2, 3), \\ \epsilon_{jkl} &= 0 \text{ otherwise.} \end{aligned} \quad (56)$$

From the Lie algebra, we may compute many expressions in $Z^2(\mathfrak{g}^*)$. In particular, we obtain in $\mathfrak{g}^* \wedge \mathfrak{g}^*$,

$$\begin{aligned} \delta(\mathbf{1}^*) &= \sum_{j=1}^3 \mathbf{Q}_j^* \wedge \mathbf{P}_j^*, \\ \delta(\mathbf{Q}_i^*) &= \mathbf{M}_j^* \wedge \mathbf{Q}_k^* - \mathbf{M}_k^* \wedge \mathbf{Q}_j^*, \\ \delta(\mathbf{P}_i^*) &= \mathbf{M}_j^* \wedge \mathbf{P}_k^* - \mathbf{M}_k^* \wedge \mathbf{P}_j^*, \\ \delta(\mathbf{M}_i^*) &= \mathbf{M}_j^* \wedge \mathbf{M}_k^*, \\ (j, k, l) &\in \text{cyclic}(1, 2, 3). \end{aligned} \quad (57)$$

The results are clearly in $Z^2(\mathfrak{g}^*)$ since $\delta^2 = 0$. This is also valid for any coordinate system; so, in fact we have the results for $\delta(\mathbf{u} \cdot \mathbf{Q}^*)$, $\delta(\mathbf{u} \cdot \mathbf{P}^*)$, $\delta(\mathbf{u} \cdot \mathbf{M}^*)$, as well where \mathbf{u} is a unit vector in \mathbb{R}^3 .

We use these results to form a particular $\omega \in Z^2(\mathfrak{g}^*)$, then \mathfrak{h}_ω , and then H_ω . But we would have to get G/H_ω to be 8-dimensional or 6-dimensional to be possibly a phase space, given that it has the \mathbf{Q} 's and \mathbf{P} 's in it. So, we could remove either one or all three of the \mathbf{M}_j 's. But taking away all three of the \mathbf{M}_j 's would give us the phase space of a particle of spin zero, which is what we would get in the treatment of the Heisenberg group. So we look for applications in which we eliminate just one of the \mathbf{M}_j 's. But this is easy! We only have to look at the classical photon which has the momentum perpendicular to the electric and magnetic forces or the Stern-Gerlach device which has the angular momentum around the magnetic field of the device as being irrelevant to what we get on the screen. Call this direction the 3-direction. Thus, we take \mathbf{M}_3 to be something that may be ignored; i.e., factored out of the space. This removes one dimension, and is true to the physics. In general we may factor out by placing $\delta(i\mathbf{u} \cdot \mathbf{M}^*)$ in ω . Hence, we will have

$$\begin{aligned} \omega &= m\delta(\mathbf{1}^*) + s\delta(\mathbf{u} \cdot \mathbf{M}^*) \\ &= m \sum_{j=1}^3 \mathbf{Q}_j^* \wedge \mathbf{P}_j^* + s\delta(\mathbf{u} \cdot \mathbf{M}^*), \end{aligned} \quad (58)$$

where m (mass) and s (spin) are real numbers. That they are positive we will leave out of our discussion. We could also choose $\delta(\mathbf{1}^*) + b\delta(\mathbf{u} \cdot \mathbf{Q}^*)$, or $\delta(\mathbf{1}^*) + c\delta(\mathbf{u} \cdot \mathbf{P}^*)$ in place of $\delta(\mathbf{1}^*)$. But what would that give in terms of the \mathfrak{h}_ω ? The answer is "the same thing." Thus, for

$$\begin{aligned} \omega &= m\delta(\mathbf{1}^*) + s[a\delta(\mathbf{u} \cdot \mathbf{M}^*) + b\delta(\mathbf{u} \cdot \mathbf{Q}^*) + c\delta(\mathbf{u} \cdot \mathbf{P}^*)], \\ a, b, c &\in \mathbb{R}, \quad a \neq 0, \end{aligned} \quad (59)$$

we obtain

$$\mathfrak{h}_\omega = \{\lambda \mathbf{1} + \kappa \mathbf{u} \cdot \mathbf{M} \mid \lambda, \kappa \in \mathbb{R}\}. \quad (60)$$

From here we obtain

$$H_\omega = \{\exp(\lambda \mathbf{1} + \kappa \mathbf{u} \cdot \mathbf{M}) \mid \lambda, \kappa \in \mathbb{R}\}. \quad (61)$$

This is clearly closed as a subgroup of G , and hence G/H_ω is a phase space. In this case, H_ω is not normal in G though. The measure on G/H_ω is in any case

$$d\mu = d^3q d^3p d\Omega([\mathbf{u} \cdot \mathbf{M}]^\perp) \quad (62)$$

where, for example,

$$d\Omega([\mathbf{M}_3]^\perp) = d(\theta_1, \theta_2)$$

where we have abbreviated $(\theta_1, \theta_2) \equiv \exp\{\theta_1 \mathbf{M}_1\} \exp\{\theta_2 \mathbf{M}_2\}$.

We should check that we obtain commutation relations that are zero on the right for all vectors in G/H_ω : Take the example where $\mathbf{u} = (0, 0, 1)$. Then

$$\begin{aligned} &\mathbf{x} \exp\{\theta_1 \mathbf{M}_1 + \theta_2 \mathbf{M}_2\} \\ &= \mathbf{x} \exp\{\theta_3 \mathbf{M}_3\} \exp\{\theta_1 \mathbf{M}_1\} \exp\{\theta_2 \mathbf{M}_2\} \\ &= \mathbf{x} \exp\{\theta_1 \mathbf{M}_1\} \exp\{\theta_2 \mathbf{M}_2\} \end{aligned} \quad (63)$$

for all $\mathbf{x} \in G/H_\omega$ and where we have used the fact that, for $\mathbf{x} \in G/H_\omega$, $\mathbf{x} \exp\{\theta_3 \mathbf{M}_3\} = \mathbf{x}$. Similarly for $\mathbf{x} \exp\{\theta_2 \mathbf{M}_2\} \exp\{\theta_1 \mathbf{M}_1\}$ to obtain

$$\mathbf{x} \exp\{\theta_1 \mathbf{M}_1\} \exp\{\theta_2 \mathbf{M}_2\} = \mathbf{x} \exp\{\theta_2 \mathbf{M}_2\} \exp\{\theta_1 \mathbf{M}_1\}.$$

Alternatively, we may work in a representation space in which M_3 is diagonal (see 2.2D), having eigenvalue $i2\pi n$ for $n \in \mathbb{Z}$. Hence $[\mathbf{M}_1, \mathbf{M}_2] = \mathbf{0}$ on G/H_ω from the right. Similarly for the commutator of the \mathbf{Q} 's and \mathbf{P} 's. Similarly for $[\mathbf{M}_1, \mathbf{P}_2]$ and $[\mathbf{M}_2, \mathbf{P}_1]$, and for $[\mathbf{M}_1, \mathbf{Q}_2]$ and $[\mathbf{M}_2, \mathbf{Q}_1]$, since we may choose a representation in which both \mathbf{P}_3 and \mathbf{Q}_3 are diagonal. In fact, it is hard not to choose a representation in which all of the \mathbf{Q} 's and \mathbf{P} 's are diagonal! Thus we obtain commutation relations that are effectively zero on G/H_ω when acting on the right.

We may transform this into the form for $\delta(\mathbf{u} \cdot \mathbf{Q}^*)$, $\delta(\mathbf{u} \cdot \mathbf{P}^*)$, $\delta(\mathbf{u} \cdot \mathbf{M}^*)$ instead of the corresponding terms in the three-direction, and obtain the corresponding relations. Thus, in G/H_ω , the $\delta(\mathbf{u} \cdot \mathbf{Q}^*)$, $\delta(\mathbf{u} \cdot \mathbf{P}^*)$, $\delta(\mathbf{u} \cdot \mathbf{M}^*)$ must have simultaneous diagonal representations.

Taking into account also the symmetry rotations of the crystal under consideration, in general, it is not possible to choose a basis for the Lie algebra of the

Heisenberg group \times rotation group adapted to the lattice, however in any case we can define

$$D = \left\{ \exp \left(\left[\sum_{\substack{l_j \in \mathbb{Z}, \\ j \in \{1,2,3\}}} m_j \mathbf{a}_j \cdot \mathbf{Q} + \sum_{\substack{l_j \in \mathbb{Z}, \\ j \in \{1,2,3\}}} m_j \mathbf{b}_j \cdot \mathbf{P} + \sum_{\substack{k_l \in \mathbb{Z}, \\ l \in \{1, \dots, l_R\}}} k_l \theta_l \mathbf{n}_l \cdot \mathbf{M} \right] \right) \right\}, \quad (64)$$

where l_R is the number of independent symmetry rotations of the crystal under consideration, (which can also be null, in the case of the triclinic lattice) \mathbf{n}_l , $l = 1, \dots, l_R$, are the directions of these rotations, and θ_l , $l = 1, \dots, l_R$, are the elementary rotation angles.

For example, for a cubic crystal, we can take $\mathbf{n}_1, \mathbf{n}_2$ and \mathbf{n}_3 along the edges of the cube. For any crystal shape, one is guaranteed that D is a group. Furthermore, one has that $(G/H_\omega)/D$ is another phase space since the primitive lattice tiles the space G/H_ω . We will discuss a specific example next.

For a tetragonal crystal ($\mathbf{a}_1 = \mathbf{a}_2 \neq \mathbf{a}_3$) with the center of the tetragon as the center of the rotations, then the axes of rotations are in the directions of \mathbf{a}_1 , \mathbf{a}_2 , \mathbf{a}_3 , $\mathbf{a}_1 + \mathbf{a}_2$, and $\mathbf{a}_1 - \mathbf{a}_2$. It is enough to know that the symmetry group of the crystal is a (finite) subgroup of G and in fact a subset of G/H_ω . We take that as given.

Alternatively, we could write the symmetry group of the crystal in terms of the Lie algebra of the original group. The moral of the story is that here again we obtain a lattice group, D , for the crystal that has the exponentials of the $\mathbf{a}_k \cdot \mathbf{Q}$'s, the $\mathbf{b}_k \cdot \mathbf{P}$'s, and the rotations $\mathbf{n}_l \cdot \mathbf{M}$'s in it and with the restrictions on the coefficients that they are in \mathbb{Z} times the primitive angles. It is similar for any crystal. We obtain the closure of the commutation relations for the crystal shape in the "right" basis.

We again take G/H_ω and factor it by D . $(G/H_\omega)/D$ is locally 3-dimensional in the \mathbf{Q} 's, 3-dimensional in the \mathbf{P} 's, and 2-dimensional in the \mathbf{M} 's. Hence, we have a phase space in which you have a crystal lattice for the space in which you have the elements with integer spin angular momentum. This will do for obtaining a representation of the phonons.

To obtain a theory for half-integer spin, we must convert the group to

$$G = G_{\text{Heisenberg}} \times (SO(3))^\sim \quad (65)$$

acting on the Cayley representation of \mathbb{R}^3 , where $(SO(3))^\sim$ is the double cover of $SO(3)$:

$$\mathbf{q} \in \mathbb{R}^3 \rightarrow \mathcal{C}(\mathbf{q}) = q_1 \sigma_1 + q_2 \sigma_2 + q_3 \sigma_3 = \mathcal{C}(\mathbf{q})^\dagger, \quad (66)$$

where $\{\sigma_1, \sigma_2, \sigma_3\}$ is the set of Pauli spin matrices:

$$\begin{aligned} \{\sigma_1, \sigma_2\}_+ &= 0, \\ (\sigma_j)^2 &= 1, \\ (\sigma_j)^\dagger &= \sigma_j, \\ \sigma_1 \sigma_2 &= -i \sigma_3 \end{aligned} \quad (67)$$

and cyclically, with $\{\}_+$ the anticommutator, and

$$\det(\mathcal{C}(\mathbf{q})) = - \|\mathbf{q}\|^2. \quad (68)$$

Then, for any complex 2×2 matrix $A \in [SO(3)]^\sim$, $C^{-1}(AC(\mathbf{q})A^\dagger)$ has determinant equal to $-\|\mathbf{q}\|^2$, and so is a rotation. From here, everything is similar to the case of integer angular momentum.

2.5 Phase Spaces in the Galilei Group Case

We now consider the non-relativistic spinning electron, which means we must obtain a representation of the Galilei group for it.

We have the Galilei group [11]

$$\mathcal{G}_{10} = \{(t, \mathbf{q}, \mathbf{p}, R) \mid t \in \mathbb{R}; \mathbf{q}, \mathbf{p} \in \mathbb{R}^3; R \in SO(3)\} \quad (69)$$

with group multiplication rule

$$(t', \mathbf{q}', \mathbf{p}', R') \circ (t, \mathbf{q}, \mathbf{p}, R) = (t' + t, \mathbf{q}' + R'\mathbf{q} + t\mathbf{p}', \mathbf{p}' + R'\mathbf{p}, R'R). \quad (70)$$

Here, t equals time shift, \mathbf{q} configuration translation, \mathbf{p} a boost, and R a rotation. The generators are $\tau, \mathbf{Q}, \mathbf{P}, \mathbf{M}$, respectively, and form a basis for \mathfrak{g}_{10} . (Note that there are ten of these; hence \mathcal{G}_{10} and \mathfrak{g}_{10} .) The Lie algebra is computed to be given by the following for $j, k, l \in \{1, 2, 3\}$:

$$\begin{aligned} [\mathbf{M}_j, \mathbf{M}_k] &= \sum_l \epsilon_{jkl} \mathbf{M}_l, \quad [\mathbf{M}_j, \mathbf{P}_k] = \sum_l \epsilon_{jkl} \mathbf{P}_l, \\ [\mathbf{M}_j, \mathbf{Q}_k] &= \sum_l \epsilon_{jkl} \mathbf{Q}_l, \quad [\mathbf{P}_j, \tau] = \mathbf{Q}_j, \end{aligned} \quad (71)$$

and the rest of the commutators of the basis of generators equalling zero. Then,

$$(t, \mathbf{q}, \mathbf{p}, R) = \exp\{t\tau + \mathbf{q} \cdot \mathbf{Q} + \mathbf{p} \cdot \mathbf{P} + \boldsymbol{\theta} \cdot \mathbf{M}\} \quad (72)$$

where $R = \exp\{\boldsymbol{\theta} \cdot \mathbf{M}\}$.

There are a one parameter set of central extensions of \mathcal{G}_{10} , for which we shall call the parameter the mass m . We extend the group to obtain

$$\mathcal{G} = \{(\zeta, t, \mathbf{q}, \mathbf{p}, R) \mid \zeta, t \in \mathbb{R}; \mathbf{q}, \mathbf{p} \in \mathbb{R}^3; R \in SO(3)\} \quad (73)$$

with the group now represented by

$$\begin{aligned} (\zeta, t, \mathbf{q}, \mathbf{p}, R) &= \exp\{\zeta \mathbf{1} + t\tau + \mathbf{q} \cdot \mathbf{Q} + \mathbf{p} \cdot \mathbf{P} + \boldsymbol{\theta} \cdot \mathbf{M}\}, \\ R &= \exp\{\boldsymbol{\theta} \cdot \mathbf{M}\}, \end{aligned}$$

and with group multiplication rule

$$\begin{aligned} &(\zeta', t', \mathbf{q}', \mathbf{p}', R') \circ (\zeta, t, \mathbf{q}, \mathbf{p}, R) \\ &= (\zeta' + \zeta + m(\frac{1}{2}t\mathbf{p}'^2 + \mathbf{p}' \cdot R'\mathbf{p}), t' + t, \mathbf{q}' + R'\mathbf{q} + t\mathbf{p}', \mathbf{p}' + R'\mathbf{p}, R'R). \end{aligned} \quad (74)$$

Here, ζ = the amount the phase shifts. Let \mathfrak{g} be the Lie algebra for \mathcal{G} . Since we have a central extension, the commutators of \mathfrak{g} are just the commutators for \mathfrak{g}_{10} augmented by the commutators of the generator for ζ with those of \mathfrak{g}_{10} , which are all zero. See [12] for a systematic treatment of the extensions. From here, we put

$t = 0$ and $m = 1$ and obtain the case considered in the previous subsection. This justifies the claim made there that that case was the orthochronous Galilei group.

For the representation on $(\mathcal{G}/H_\omega)/D$ with D as the group of the crystal, we see that we may use the same analysis as in the Heisenberg \times rotation group case and with the additional term $\delta(\tau)$ ($= 0!$) added to the formula for $\omega \in Z^2(\mathfrak{g})$, then talk about \mathcal{L}' and \mathcal{L}'' , etc. We may also perform the same trick with the Cayley transform of \mathbb{R}^3 to obtain the double cover of $SO(3)$ for the purposes of obtaining representations for half-integer spins. Thus we will include the electron in our Galilean considerations of the crystal.

2.6 The Phase Space in the Poincaré Case

We should do a similar thing starting with the Poincaré group. This is especially true for treating electrons, as we usually speak of the electron in terms of the Poincaré group and relativistic quantum mechanics. We should also obtain a representation for the phonons working in the same system. As this is all similar to what we have done in the non-relativistic cases, we will leave that for consideration in a sequel to this paper.

2.7 Some Operators on L^2 (phase space)

Suppose we have a Hamiltonian, H , as a function of the \mathbf{p} 's and \mathbf{q} 's on the classical phase space G/H_ω , which we shall abbreviate for a general G and H_ω by

$$\Gamma \equiv G/H_\omega. \quad (75)$$

We note that we have a measure μ on Γ which is G -left-invariant. μ comes from the form ω as in (2.9)-(2.10). From here, it is easy to form the Hilbert space $L^2_\mu(\Gamma)$ of μ -measurable and square integrable functions.

On $L^2_\mu(\Gamma)$ define a (quantum-like) representation, V_L , of G by

$$\begin{aligned} [V_L(g)\Psi](\mathbf{x}) &= \Psi(g^{-1}\mathbf{x}) = \Psi(L_g\mathbf{x}), \\ \Psi &\in L^2_\mu(\Gamma), g \in G, \mathbf{x} \in \Gamma = G/H_\omega. \end{aligned} \quad (76)$$

Also, define a projective representation, V_L^α , by

$$\begin{aligned} [V_L^\alpha(g)\Psi](\mathbf{x}) &= \alpha(h(g^{-1}, \mathbf{x})^{-1})\Psi(L_g\mathbf{x}), \\ \Psi &\in L^2_\mu(\Gamma), g \in G, \mathbf{x} \in \Gamma = G/H_\omega, \end{aligned} \quad (77)$$

with h defined by (2.18) and α as defined by (2.20). We have that V_L^α is easily shown to be unitary, and is a projective representation of G .

We may also define unitary representations V_R and V_R^α of G by

$$[V_R(g)\Psi](\mathbf{x}) = \Psi(R_g\mathbf{x}) \quad (78)$$

and

$$[V_R^\alpha(g)\Psi](\mathbf{x}) = \alpha(h(g^{-1}, \mathbf{x})^{-1})\Psi(R_g\mathbf{x}), \quad (79)$$

but now these Ψ take the form of (2.15), (2.16): For $\mathbf{x} \in G/H_{R_{g_1}^* \omega}$, $\mathbf{x} = g_2 H_{R_{g_1}^* \omega}$, define

$$\begin{aligned} \tilde{V}_R^\alpha(g) &: \cup'_{g_1 \in G} L^2(G/H_{R_{g_1}^* \omega}) \rightarrow \cup'_{g_1 \in G} L^2(G/H_{R_{g_1}^* \omega}), \\ \Psi &= \{\Psi_{g_1}\} \in \cup'_{g_1 \in G} L^2(G/H_{R_{g_1}^* \omega}), \end{aligned}$$

through

$$\begin{aligned} [V_R^\alpha(g)\Psi_{g_1}](\mathbf{x}) &= \alpha(h(g^{-1}, \mathbf{x})^{-1})\Psi_{g_1}(R_g g_2 \circ H_{R_{g_1}^* \omega}) \\ &= \alpha(h(g^{-1}, \mathbf{x})^{-1})\Psi_{g \circ g_1}((g_2 \circ g) \circ H_{R_{g \circ g_1}^* \omega}). \end{aligned} \quad (80)$$

The V_L^α give us a (projective) quantum mechanical like representation of G , and the V_R^α give us a (projective) classical mechanical like representation of G .

On $L_\mu^2(\Gamma)$, the Hamiltonian H will take the form of a multiplication operator, $A(H)$. In fact, for any function f of Γ (of the \mathbf{p} 's and \mathbf{q} 's), $A(f)$ is given by

$$[A(f)\Psi](\mathbf{x}) = f(\mathbf{x})\Psi(\mathbf{x}), \quad \Psi \in L_\mu^2(\Gamma), \mathbf{x} \in \Gamma. \quad (81)$$

Such f 's are called "classical observables" if they are real valued and μ -measurable. Notice that the $A(f)$'s form a commuting set, and thus cannot be an informationally complete set on $L_\mu^2(\Gamma)$. [13]

We look for eigenfunctions of $A(f)$ as follows: Take the function f and partition it by taking

$$\{\mathbf{x} \in \Gamma \mid f(\mathbf{x}) = r\} \quad (82)$$

for $r \in \mathbb{R}$. The elements of these sets for f a continuous function are called the level curves of f . (For example, the level curves for $f(\mathbf{p}, \mathbf{q}) = \mathbf{p}^2 + \mathbf{q}^2$ are the spheres $\mathbf{p}^2 + \mathbf{q}^2 = r$ for some $r \geq 0$.) Specializing to the Hamiltonian function, we obtain

$$A(H)\Psi = \varepsilon\Psi \quad (83)$$

along the curves $H(\mathbf{x}) = \varepsilon$ only. But there is no function Ψ such that this holds for all of Γ except for the case in which H is a constant. For f a piecewise defined Borel step function, then by taking $\Psi = 0$ except on one piece, you have a solution for that value. This is not the case for any H that has the form $H(\mathbf{p}, \mathbf{q}) = \mathbf{p}^2/2m + V(\mathbf{q})$, V the potential energy, no matter what form the potential V takes. The problem is with the fact that \mathbf{p}^2 is continuous. Similarly for a case in which you have a spin-orbit interaction or if you treat the case relativistically. We conclude that we have no eigenfunctions of a non-trivial Hamiltonian when treated in the phase space Γ . (There is a different conclusion for a representation of G on a quantum mechanical Hilbert space.)

2.8 Some Operators on a Quantum Mechanical Hilbert Space

Let us suppose we have a Hilbert space, \mathcal{H} , for particles of some mass and spin. Let Γ be the phase space for the same mass and spin. Let U be a representation of G on \mathcal{H} . (Here G may be either the Galilei or Poincaré group.) Let $\omega \in Z^2(\mathfrak{g})$ be such that it describes particles of that mass and spin. Then $\Gamma = G/H_\omega$. Let us choose some $\eta \in \mathcal{H}$. Then let

$$[W^\eta \phi](\mathbf{x}) = \langle U(\sigma(\mathbf{x}))\eta, \phi \rangle \quad (84)$$

for all $\phi \in \mathcal{H}$, and σ a Borel choice function from G/H_ω to G . With very mild restrictions on η , called the α -admissibility conditions, α as before, it can be shown that W^η is an isometry from \mathcal{H} to a closed subspace of $L_\mu^2(\Gamma)$. [3, pp. 321-322] Let

$$P^\eta : L_\mu^2(\Gamma) \rightarrow W^\eta \mathcal{H} \quad (85)$$

be the canonical projection. Then let

$$A^\eta(f) = [W^\eta]^{-1} P^\eta A(f) W^\eta. \quad (86)$$

This is the quantization of the classical operator f in our quantization.

Because the operators P^η and $A(f)$ do not commute, the corresponding $A^\eta(f)$ do not form a commuting set. In fact, the $A^\eta(f)$ form an informationally complete set in \mathcal{H} . [14][15] They correspond to the usual canonical operators with canonical commutation relations if the f 's are monomials in the basic classical variables.

We also have that W^η intertwines U and V_L^α under these α -admissibility conditions on η :

$$W^\eta U = V_L^\alpha W^\eta. \quad (87)$$

For completeness, we make the following

Definition 1 [3, pp. 319-320] Let H be a closed subgroup of a locally compact group G , and let U be a strongly continuous unitary representation of G on the Hilbert space \mathcal{H} . Let G/H have a Borel cross-section $\sigma : G/H \rightarrow G$ and a left-invariant measure μ on G/H . Then $\eta \in \mathcal{H}$ is admissible with respect to $\sigma(G/H)$ iff $\eta \neq 0$ and $\int_{G/H} | \langle U(\sigma(\mathbf{x})\eta, \eta \rangle |^2 d\mu(\mathbf{x}) < \infty$. If the representation U is also irreducible, then we say that U is square integrable over $\sigma(G/H)$. If η satisfies the admissibility condition as well as $\{ \text{there exists } \alpha : H \rightarrow \mathbb{C} \text{ such that } U(h)\eta = \alpha(h)\eta, \forall h \in H \}$, then η is α -admissible.

Thus, by the passage $H \rightarrow A^\eta(H)$, we may quantize any classical one-particle Hamiltonian. For an n -particle Hamiltonian, we may use an η of the form

$$\eta = \eta_1 \otimes \cdots \otimes \eta_n$$

in

$$\mathcal{H} = \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n,$$

use

$$U(g)\eta = U_1(g)\eta_1 \otimes \cdots \otimes U_n(g)\eta_n,$$

etc., and get similar results.

2.9 The Quantum Mechanical Theory of the Silicon Lattice

First we will treat the hydrogen atom. Hydrogen is treated quantum mechanically by having a charge 1 nucleus and a charge -1 electron around it; then writing a (Schroedinger) Hamiltonian for it and then solving $H\psi = E\psi$ for it, where E is the eigenvalue and ψ is the corresponding eigenvector. It is found that the ψ 's (the orbitals) are of the following types:

The lowest eigenvalue is for the 1S orbital where S stands for symmetric and 1 for the lowest eigenvalue. Plotting the level surface corresponding to the highest

value of the modulus of its eigenvector, $|\psi(\mathbf{x})|$, yields the surface of a sphere. $\psi(\mathbf{x})$ has a probability amplitude density $|\psi(\mathbf{x})|^2$ that is never equal to zero in any finite region and goes to zero at infinity as $\exp(-c \|\mathbf{x}\|^2)$.

The next lowest eigenvalue has again a S orbital, but a higher energy; so it is of type 2S. The next lowest eigenvalue has 2P orbitals of which there are three independent ones. Plotting the highest value of $|\psi(\mathbf{x})|$ for them yields a loop. (The loops may go in three orthogonal directions.) Again the probability density for each of these goes to zero exponentially with the square of the distance. Then one has the D orbitals, then the F orbitals, and so forth.

The spin variables for the electron (spin 1/2) give you two orbitals of each S type, 6 of each P type, etc.

One assumes that one may simply increase the charges to get similar results for higher weight atoms.

Free Si has 14 protons and some neutrons in its nucleus; its 14 electrons are in a $1S^2 2S^2 2P^6 3S^2 3P^2$ configuration where nX^m denotes that there are m electrons in the nX orbital, n referring to the particular energy level of the orbital and X the type. In a silicon lattice, the silicon is ionized once (there is one conduction electron); so, it has a "closed shell" of 10 electrons ($1S^2 2S^2 2P^6$) plus three electrons in orbitals that are linear combinations of the 3S and 3P orbitals. Thus there are three directions in which the plot of the maximum $|\psi(\mathbf{x})|$ may point. Thus, with covalent bonding and from energy considerations, they make up a crystal lattice, and the linear combinations of 3S and 3P orbitals are 120 degrees apart, the crystal being tetrahedral.

Similarly for any crystal of any ions or molecular ions. You obtain various shapes for the various crystals, as well.

3 The Potential in Γ

Now, if the theory is non-relativistic, $A^\eta(H)$ is the Schroedinger operator on \mathcal{H} . It is well known that this may be self-adjoint and may have eigenvalues. But it may not! It depends on the potential! If the potential is $V(\mathbf{p}, \mathbf{q}) \sim \mathbf{q}^2$, then it does have eigenvalues. This is all the subject for an industry in quantum theory. We are particularly interested in the case in which V is a periodic potential over an (in)finite lattice. If $A^\eta(H)$ has eigenfunctions at all, then they are of the form of (2.1)-(2.4). We may also obtain the bound electrons (which have wave functions that are eigenfunctions) and the conduction electrons (which don't). But in a lattice consisting of a finite number of single cells, we must use the formalism for a finite lattice.

We first obtain the classical Hamiltonian for the system. We will consider placing an "electron" in a perfect crystal which has a classical Hamiltonian H which is periodic in space:

$$H(\mathbf{p}, \mathbf{q} + \mathbf{R}) = H(\mathbf{p}, \mathbf{q}) \quad (88)$$

where \mathbf{R} is a lattice vector of the crystal:

$$\mathbf{R} = \sum_{i=1}^3 n_i \mathbf{a}_i, \quad (89)$$

the n_i and \mathbf{a}_i being as before. We note that this is not a Hamiltonian for an electron since there is no spin involved in it. Really, what we want is

$$H = \sum_{j=1}^7 V_j, \quad (90)$$

where

V_1 = free energy of the conduction electrons,

V_2 = free energy of the ions,

V_3 = Coulomb energy of the ions in interaction,

V_4 = Coulomb energy of the ions in interaction
with the conduction electrons,

V_5 = Coulomb energy of the conduction electrons
in interaction with each other,

V_6 = spin-orbit energy of the conduction electrons'
spin and the ions' spin,

V_7 = spin-spin energy between conduction electrons.

We have for initial consideration several forms of the Hamiltonian of the conduction electron only via the adiabatic approximations plus the one electron approximation: [21]

a) $H(\mathbf{p}, \mathbf{q}) = \mathbf{p}^2/2m + V(\mathbf{q})$ (due to Schroedinger),

b) $H(\mathbf{p}, \mathbf{q}) = \mathbf{p}^2/2m + V(\mathbf{q}) + (e^2/[4m^2c^2])\mathbf{p} \cdot (\boldsymbol{\sigma} \times \nabla V(\mathbf{q}))$ (due to Pauli),

c) $H(\mathbf{p}, \mathbf{q}) = \beta mc^2 + c\boldsymbol{\alpha} \cdot \mathbf{p} + V(\mathbf{q})$ (due to Dirac),

where $V(\mathbf{q})$ is the periodic potential of the crystal, the $\boldsymbol{\sigma}$ are the Pauli spin matrices represented as a vector, $\boldsymbol{\alpha}$ and β are the Dirac spinors, m is the mass of the electron, etc.

The form (a) has no spin at all in it. Thus we will obtain solutions that are independent of spin. This is no good for us. Form (b) has spin in it; so, it will have the required solutions depending on spin. Blount [21] shows that then there is a problem defining \mathbf{q} as an operator; it has a part that depends on $\boldsymbol{\sigma}$ in the usual representation space. It follows that \mathbf{p} also has a new form, and then you have to get the commutator to satisfy the canonical commutation relations. Then he derives a theory that has everything in it as a complicated power series. We suggest that it would be much simpler to have the \mathbf{p} 's and \mathbf{q} 's satisfy the canonical commutation relations, which are the Lie algebra relations, from the start. This suggests we work in $L_\mu^2(G/H_\omega)$ in this case. For (c), we also remind the reader that the Dirac form for the electron is very deficient, having problems with zitterbewegung [22], lack of positivity of the free energy [3, p. 562], lack of a single particle theory [3, p. 562], etc. For this reason, we shall not use a Hamiltonian of type (c) at all, but will use the form in $L_\mu^2(G/H_\omega)$ which suffers from none of these problems.

Continuing with these usual single electron cases, we note that the conduction electrons may feel the presence of the charges of the nuclei and their bound electrons in three ways: by either a screened charge, or by a function of the density in configuration space, $\rho_j(\mathbf{q})$, where j indicates which position $\mathbf{d}(j)$ one has for

the j th nucleus, or by the density as a function of the reciprocal lattice vector \mathbf{k} proportional to the Fourier transform of the electric charge distribution

$$f_j(\mathbf{k}) = -e^{-1} \int d^3(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} \rho_j(\mathbf{r}) \quad (91)$$

of the ion in position $\mathbf{d}(j)$ of the basis of the nuclei, where e is the electron charge. Thus, the conduction electrons feel the presence of a periodic potential.

For the screened charge, it may take the form of the Lennard-Jones potential

$$\phi(r) = -Ar^{-6} + Br^{-12}, A \geq 0, B \geq 0$$

or

$$\phi(r) = 4\varepsilon[(\sigma r^{-1})^{12} - (\sigma r^{-1})^6], \sigma = (B/A)^{1/6}, \varepsilon = A^2/(4B). \quad (92)$$

Alternatively, we may take the exact Coulomb potential and perform various approximations on that. In particular, we may use the Hartree-Fock approximation. There are many screenings that could be used.

But consider this. One has the wave function for the ion. This may be considered as the nucleus plus the closed shell plus symmetry adapted orbitals in the remaining electrons in the ion. The orbitals are distributions which extend everywhere. Treat these as each having the total charge of minus the charge of the electron and the conduction electrons as interacting with this distribution with a Coulomb interaction. Then no screening of the potential is necessary and no approximations have been used.

So far, we have treated the \mathbf{p} 's and \mathbf{q} 's as though they were vectors in \mathbb{R}^3 . In our formalism of $(G/H_\omega)/D$, they are not. In the Heisenberg group case,

$$(\mathcal{W}/H_\omega)/D = (\mathbb{R}^3/\mathcal{L}') \times (\mathbb{R}^3/\mathcal{L}'').$$

Thus one has both the momenta and positions bounded. It is similar in the Galilei and Poincaré cases.

Putting the entire discussion in this subsection in an overall review, we see that the explicit form of the Hamiltonian will have to be reformulated in the framework of the phase space, then converted to a theory on L^2 (phase space), and finally quantized to an irreducible representation space (the Hilbert space, \mathcal{H}). Instead of just using forms a), b), or c) for the Hamiltonian, we should use the assumptions that were used in deriving them but instead use the assumptions to derive them in phase space terms. Notice that we have not made any reference to the Hamiltonians having eigenvalues and eigenvectors, as they may not have them at all.

4 Momentum Space Versus Configuration Space Versus Phase Space

We wish to point out that a phase space distribution is much more than the product of the usual momentum space distribution and the usual configuration space distribution. We will show this by considering the Heisenberg group.

We have a very special situation in the Heisenberg group case that the momentum space representation and the configuration space representation are connected by the Fourier transform, \mathcal{F} . But what is the phase space representation? And how

is that representation connected with the two representations already mentioned. Also, what is the Hamiltonian function in these representations?

If we work in the configuration space representation, then we have

$$\begin{aligned} \mathbf{p} &\leftrightarrow -i\nabla_{\mathbf{q}}, \\ \mathbf{q} &\leftrightarrow \text{multiplication of } \psi(\mathbf{q}) \text{ by } \mathbf{q}, \\ \psi &\in L^2(\mathbb{R}_{\text{configuration}}^3). \end{aligned} \quad (93)$$

Now, if we have the Hamiltonian function given by $H(\mathbf{p}, \mathbf{q}) = \mathbf{p}^2/2m + V(\mathbf{q})$, one could argue that the direction of maximum increase in V is $\pm[\nabla_{\mathbf{q}}V](\mathbf{q})$. This is the method of steepest descent. As one ascends, then the momentum goes down and conversely. Thus one may argue that $\mathbf{p} = -\text{const.}\nabla_{\mathbf{q}}$.

Next, consider $[H(\mathbf{p}, \mathbf{q})\psi](\mathbf{q})$. It will transform to an expression $[\tilde{H}(\tilde{\mathbf{p}}, \tilde{\mathbf{q}})\tilde{\psi}](\mathbf{p}) = [\tilde{H}(\tilde{\mathbf{p}}, \tilde{\mathbf{q}})(\mathcal{F}\psi)](\mathbf{p})$ under the Fourier transform. But what is $\tilde{H}(\tilde{\mathbf{p}}, \tilde{\mathbf{q}})$? The answer is $\tilde{H}(\tilde{\mathbf{p}}, \tilde{\mathbf{q}}) = H(-\mathbf{q}, \mathbf{p})$ where we now represent

$$\begin{aligned} \tilde{\mathbf{q}} &\leftrightarrow -i\nabla_{\mathbf{p}}, \\ \tilde{\mathbf{p}} &\leftrightarrow \text{multiplication of } \varphi(\mathbf{p}) \text{ by } \mathbf{p}, \\ \varphi &\in L^2(\mathbb{R}_{\text{momentum}}^3). \end{aligned} \quad (94)$$

This is an instance of the "Born reciprocity principle." Thus $\tilde{H}(\tilde{\mathbf{p}}, \tilde{\mathbf{q}}) = -\nabla_{\tilde{\mathbf{p}}}^2/2m + V(\tilde{\mathbf{p}})$. This is all a realization of the fact that all irreducible representations of the Heisenberg group are connected by unitary mappings, and one such unitary map is the Fourier transform.

Assuming that the Hamiltonian has eigenvalues $\varepsilon_n(\mathbf{p})$, one may solve

$$[H(\mathbf{p}, \mathbf{q})\psi](\mathbf{q}) = \varepsilon_n(\mathbf{p})\psi(\mathbf{q}) \quad (95)$$

to obtain eigenvector ψ_n . Then for $\tilde{H}(\tilde{\mathbf{p}}, \tilde{\mathbf{q}})$ we would obtain the same eigenvalue but with eigenvector $\tilde{\psi}_n = \mathcal{F}\psi_n$. Hence, we could argue that in phase space the eigenvector would be $\tilde{\psi}_n(\mathbf{p})\psi_n(\mathbf{q})$ with eigenvalue $[\varepsilon_n(\mathbf{p})]^2$. This is wrong and not the way one may go from either of the representations to the phase space representation.

The proper way is the following. (See [3, pp. 405-413]. It is also the way the fast Fourier transform may be produced. [25]) Starting with $f \in L^2(\mathbb{R}_{\text{mom}}^3)$, define a linear map Θ by

$$[\Theta f](\boldsymbol{\xi}, \boldsymbol{\eta}) = \sum_{m_j=-\infty}^{\infty} f_m(\boldsymbol{\xi}) \exp(2\pi i \mathbf{m} \cdot \boldsymbol{\eta}), \quad (96)$$

η_j and ξ_j in $[0, 1)$, where $f_m(\boldsymbol{\xi}) = f(\mathbf{m} + \boldsymbol{\xi})$, $\mathbf{m} \in \mathbb{Z}^3$. Θ is an onto isometry:

$$\Theta : L^2(\mathbb{R}_{\text{mom}}^3) \rightarrow L^2(T^6), T = \mathbb{R}/\mathbb{Z}. \quad (97)$$

Next, define

$$\begin{aligned} L^2_{\mu}(\mathcal{W}/H) &\equiv \oplus_{m \in \mathbb{Z}} \mathcal{H}_m, \\ \mathcal{H}_m &\equiv \{f \in L^2_{\mu}(\mathcal{W}/H) \mid U^A(\alpha, \mathbf{0}, \mathbf{0})f = \exp(im\alpha)f\}. \end{aligned} \quad (98)$$

Follow this by a map

$$\mathcal{T} : L_\mu^2(T^6) \rightarrow L_\mu^2(\mathcal{W}/H) \quad (99)$$

given by the following:

$$\begin{aligned} \mathcal{T} &\equiv \bigoplus_{m \in \mathbb{Z}} \mathcal{T}_m \\ \mathcal{T}_m &: L_\mu^2(T^6) \rightarrow \mathcal{H}_m \\ (\mathcal{T}_m[f])(\alpha, \mathbf{x}, \mathbf{y}) &= \exp(im\alpha) f(\mathbf{x}, \mathbf{y}). \end{aligned} \quad (100)$$

Then \mathcal{T} is an onto isometry also. $\mathcal{T}\Theta$ is the desired unitary map from $L^2(\mathbb{R}_{mom}^3)$ to $L_\mu^2(\mathcal{W}/H)$. (One may then map from $L_\mu^2(\mathcal{W}/H)$ to $L_\mu^2(\mathcal{W}/H)$ by means of the Born reciprocity operator and obtain the fast Fourier transform by using $\mathcal{T}\Theta$ and $[\mathcal{T}\Theta]^{-1}$. See [3, pp. 408-413].)

On $L^2(\text{phase space}) = L_\mu^2(\mathcal{W}/H)$, one has

$$\hat{H} = \mathcal{T}\Theta H [\mathcal{T}\Theta]^{-1} \quad (101)$$

as the Hamiltonian. \hat{H} will have all eigenvalues that H does, if any.

There is another way we could obtain the Hamiltonian in $L^2(\text{phase space})$. We could start with the Hamiltonian, H , defined on the phase space, and then obtain $A(H)$ defined on $L_\mu^2(\Gamma)$ and $A^\eta(H)$ defined on \mathcal{H} for almost any vector $\eta \in \mathcal{H}$. Then the different forms of the Hamiltonian within unitarily equivalent irreducible representation spaces, $\mathcal{H}_1, \mathcal{H}_2$, are connected by the same transforms as the different η 's according to

$$\mathcal{H}_1 \mapsto \mathcal{H}_2 = V\mathcal{H}_1 \implies \mathcal{O} = VA^{\eta_1}(H)V^{-1}, \quad (102)$$

since $A^{\eta_1}(H)$ is the Hamiltonian operator in \mathcal{H}_1 and \mathcal{O} is an operator in \mathcal{H}_2 . Here V might be one of the various transforms we considered in this section for the Heisenberg group.

Note that we may generalize this to any Lie group using $\Gamma = G/H_\omega, L_\mu^2(G/H_\omega)$, and \mathcal{H} . In fact,

Theorem 1 *With the notation above, $VA^{\eta_1}(f)V^{-1} = A^{V\eta_1}(f) = A^{\eta_2}(f)$ for all f that are μ -measurable and real-valued.*

Proof First of all, ω is chosen so that \mathcal{H} encodes the mass and spin of the particle considered. Thus, any two irreducible Hilbert spaces, \mathcal{H}_1 and \mathcal{H}_2 , contained in $L_\mu^2(G/H_\omega)$ are unitarily equivalent. Assuming this is the case, then there exists a unitary V with $\mathcal{H}_2 = V\mathcal{H}_1$.

If $g \mapsto U(g)$ is a representation of G on \mathcal{H}_1 , and $\mathcal{H}_2 = V\mathcal{H}_1$, then $g \mapsto VU(g)V^{-1}$ is a representation of G on $\mathcal{H}_2 = V\mathcal{H}_1$. Thus [3, pg. 321]

$$\begin{aligned} [W^\eta \phi](x) &= \langle U(\sigma(x))\eta, \phi \rangle_{\mathcal{H}_1} \\ &= \langle (VU(\sigma(x))V^{-1})V\eta, V\phi \rangle_{V\mathcal{H}_1} \\ &= [W^{V\eta} V\phi](x); \end{aligned} \quad (103)$$

so, $W^\eta = W^{V\eta}V$. By [3, pg. 333] we also have

$$\begin{aligned} & [P^{V\eta}\Phi](y) \\ &= \|CV\eta\|_{\mathcal{H}_2}^{-2} \int_{G/H} d\mu(x) \langle (VU(\sigma(y))V^{-1})V\eta, (VU(\sigma(x))V^{-1})V\eta \rangle_{V\mathcal{H}_1} \Phi(x) \\ &= \|CV\eta\|_{\mathcal{H}_2}^{-2} \int_{G/H} d\mu(x) \langle U(\sigma(y))\eta, U(\sigma(x))\eta \rangle_{\mathcal{H}_1} \Phi(x) \\ &= (\|CV\eta\|_{\mathcal{H}_2} / \|C\eta\|_{\mathcal{H}_1})^{-2} P^\eta\Phi(y). \end{aligned}$$

Now, $\|CV\eta\|_{\mathcal{H}_2} = \|C\eta\|_{\mathcal{H}_1}$ since the normalization of $P^{V\eta}$ and P^η is the same. So,

$$P^{V\eta} = P^\eta. \quad (104)$$

Then, it follows that

$$\begin{aligned} A^{V\eta}(f) &= [W^{V\eta}]^{-1} P^{V\eta} A(f) W^{V\eta} \\ &= V[W^\eta]^{-1} P^\eta A(f) W^\eta V^{-1} \\ &= VA^\eta(f) V^{-1} \end{aligned} \quad (105)$$

for any f that is μ -measurable and real-valued. ■

In particular, we would have that $A^\eta(H)$ is the Hamiltonian in whatever representation we choose.

This shows that (5.9) - (5.10) is not restricted to the Heisenberg group.

Therefore, on $L_\mu^2(\Gamma)$, we may obtain wave functions of just \mathbf{p} or just \mathbf{q} by taking marginals, but still we do not obtain the wave function of both \mathbf{p} and \mathbf{q} as the product of these two marginals. This is just like taking a finite set, S , that is the cross product of two other sets S_1 and S_2 , taking a probability function P on S , and then taking the marginal probability densities P_1 and P_2 . Then you do not have $P(s_1, s_2) = P_1(s_1)P_2(s_2)$, except in the one case that $P = P_1 \times P_2$.

This also suggests that there is something wrong in making the identification of the momentum with \mathbf{p} and position by \mathbf{q} in (5.1) or in (5.2)! This heresy is verified for momentum in [26] and in [3, pp. 442-443 and 509], and for position in [27]. A correct identification is made in the phase space formalism, however.

5 The Band Gap in Γ

In the space $L^2(\mathbb{R}^3)$ with $\mathbb{R}^3 =$ configuration space representation of the Heisenberg group, one has the Schroedinger equation of the form

$$[i \frac{\partial}{\partial t} \psi](\mathbf{r}, t) = [-\frac{1}{2m} \nabla_{\mathbf{r}}^2 + V(\mathbf{r})] \psi(\mathbf{r}, t) = [H\psi](\mathbf{r}, t). \quad (106)$$

Then one assumes one has (an orthonormal basis of) eigenfunctions of the form

$$H\psi_{n,\mathbf{k}} = \varepsilon_{n,\mathbf{k}} \psi_{n,\mathbf{k}}. \quad (107)$$

We know that there is no guarantee that there are eigenvalues of the Hamiltonian, though. Hence, let us make a slight generalization. One says that one has an energy

band gap located around γ if the energies $\varepsilon_{n,\mathbf{k}}$ are such that there exists a partition $\{N_1, N_2\}$ of \mathbb{N} and an $\epsilon > 0$ such that

$$\begin{aligned} \sup_{\mathbf{k} \in \mathbb{R}^3} \varepsilon_{n,\mathbf{k}} &\leq \gamma - \epsilon \text{ for } n \in N_1, \\ \inf_{\mathbf{k} \in \mathbb{R}^3} \varepsilon_{n,\mathbf{k}} &\geq \gamma + \epsilon \text{ for } n \in N_2. \end{aligned} \quad (108)$$

There is even a problem with this if there are almost no eigenfunctions of the Schroedinger equation, but then you may have some solutions "lying below" $\gamma - \epsilon$ and other times "above" $\gamma + \epsilon$ in some sense, perhaps statistical. What is important for us to recognize is that this is a condition in the phase space of the $(\mathbf{k}, \mathbf{r})!$

In the representation on $L_\mu^2(\Gamma)$, we may put

$$[i \frac{\partial}{\partial t} \Psi](\mathbf{k}, \mathbf{r}, t) = [A^\eta(\mathbf{H})\Psi](\mathbf{k}, \mathbf{r}, t). \quad (109)$$

Then, if $A^\eta(\mathbf{H})$ has a purely discrete spectrum, we define

$$A^\eta(\mathbf{H})\Psi_n = \lambda_n \Psi_n \quad (110)$$

for $\{\Psi_n\}$ some orthonormal basis for $\mathcal{H} \hookrightarrow L_\mu^2(\Gamma)$. Hence we may use the same theory of the band gap as before. If $A^\eta(\mathbf{H})$ does not have a purely discrete spectrum but the assumption in (6.2) holds in some sense, then you have

$$A^\eta(\mathbf{H})\chi_{\Delta\mathbf{p}}\Psi_n = \overline{\varepsilon_{n,\Delta\mathbf{p}}}\Psi_n \quad (111)$$

for all $\Delta\mathbf{p} \in \text{Borel}(\mathbb{R}_{\text{mom}}^3/\mathcal{L}'')$, and for some orthonormal basis $\{\Psi_n\}$ of \mathcal{H} . Here we have taken

$$\begin{aligned} \overline{\varepsilon_{n,\Delta\mathbf{p}}} &= \left[\int \chi_{\Delta\mathbf{p}} d\mathbf{p} \right]^{-1} \int \varepsilon_{n,\mathbf{p}} d\mathbf{p}, \\ \inf_{\mathbf{p} \in \Delta\mathbf{p}} \varepsilon_{n,\mathbf{p}} &\leq \overline{\varepsilon_{n,\Delta\mathbf{p}}} \leq \sup_{\mathbf{p} \in \Delta\mathbf{p}} \varepsilon_{n,\mathbf{p}}. \end{aligned} \quad (112)$$

Then for $\{N_1, N_2\}$ a partition of \mathbb{N} ,

$$\begin{aligned} \text{Tr} (P_{\Psi_{n_1}} [\chi_{\Delta\mathbf{p}} \{A^\eta(\mathbf{H}) - \gamma + \epsilon\}]) &> 0 \quad \forall n_1 \in N_1, \\ \text{Tr} (P_{\Psi_{n_2}} [\chi_{\Delta\mathbf{p}} \{\gamma + \epsilon - A^\eta(\mathbf{H})\}]) &> 0, \quad \forall n_2 \in N_2 \end{aligned} \quad (113)$$

means that one has a band gap around γ .

In either case, when you have a band gap present and you measure the electrons with an electron state vector $\eta \in \mathcal{H}$ with a sufficiently fine variance, you expect to have the band gap persist, at least with high probability due to the non-local nature of $A^\eta(\mathbf{H})$.

6 The Wannier Basis and the Phase Space Basis

We first do a bit of history. First, Bloch wave functions are defined as the "functions $b(\mathbf{k}, \mathbf{x})$ of energy $W(\mathbf{k})$." Then "the 'required' functions are

$$a(\mathbf{x} - \mathbf{n}) = \frac{1}{N^{1/2}} \sum_{\nu} \exp[-i\mathbf{k}_{\nu}\mathbf{n}]b(\mathbf{k}_{\nu}, \mathbf{x}),$$

where N is the number of cells in the crystal and the \mathbf{k} 's are as usual determined by some boundary condition."

Wannier [28] then made "the *ad hoc* assumption (valid for free electrons) that b is of the form

$$b(\mathbf{k}_{\nu}, \mathbf{x}) = \exp[-i\mathbf{k}_{\nu}\mathbf{x}]b(\mathbf{x}),$$

where $b(\mathbf{x})$ " is periodic in an 'ideal crystal'. Then, Wannier goes on to prove that the $a(\mathbf{x} - \mathbf{n})$ are orthogonal by using the fact that

$$\sum_{\nu} \exp[-i\mathbf{k}_{\nu}(\mathbf{n} - \mathbf{x})] = (\text{const}) \prod_{j=1}^3 \sin \pi(x_j - n_j)/\pi(x_j - n_j).$$

This was all assuming that the crystal axes are orthogonal, but "this could easily be removed." He doesn't say how. Then he continues with a discussion of the Hamiltonian (which does not contain any spin terms) and converts \sum_{ν} to an integral.

He does not consider a finite crystal and nowhere in his paper is there any recognition of the fact that the electrons have spin! At least he considers the fact that the wave functions are functions over a phase space, albeit without spin. However he does not make any use of the fact that this "phase space" is a symplectic space and therefore the Hamiltonian has certain properties on it. He also takes the phase space as non-relativistic.

On the other hand, we may now take the actual phase space in either the case of the Heisenberg \times rotation group or the Galilei group, work on $(G/H_{\omega})/D$ or $L^2((G/H_{\omega})/D)$ with the right and left actions of the group. We will obtain representations that are truly functions on the phase space (including spin if you work within the Cayley representation). When we work in $(G/H_{\omega})/D$, we may assume that the wave functions for the conduction electrons are of the form

$$\psi(\mathbf{x}, \mathbf{p}, \mathbf{s}) = \sum c_{j,k,l} a_j(\mathbf{x}) b_k(\mathbf{p}) s_l(\mathbf{s})$$

with the $\{a_j\}$, $\{b_k\}$, $\{s_l\}$ being bases for the various spaces. Or we may take the bases (minus the $\{s_l\}$) being as Bloch did. But it would be much better to work with it all and obtain bases that were adapted to the phase space and the actual Hamiltonian. Then we take an actual Hamiltonian for this system and ask whether it has any eigenfunctions, or failing that, if it has any representations that are diagonal in the \mathbf{p} 's, or equivalently the \mathbf{k} 's. If it does, then we have the orthogonality automatically. We may continue by describing the band gap, etc. And we do not have to make any *ad hoc* assumptions this way.

7 Measuring the Conduction Electron

One places a wire in the silicon lattice and measures the electrons in the wire. But these electrons are themselves quantum mechanical. This set up is ideally suited for our form of measurement in phase space physics! We may consider single electrons in the wire as one having the wave function η , and another $U(\sigma(\mathbf{x}))\eta$, for \mathbf{x} a translation or boost or rotation (spin). Let ψ denote the wave function for the conduction electron. Then compute the transition probability

$$|\langle\psi, U(\sigma(\mathbf{x}))\eta\rangle|^2.$$

Next take the various $U(\sigma(\mathbf{x}))\eta$ in the wire to have probability density $f(\mathbf{x})$ of occurring. Then compute

$$\int_{\mathbf{x} \in \text{wire}} f(\mathbf{x}) |\langle\psi, U(\sigma(\mathbf{x}))\eta\rangle|^2 d\mu(\mathbf{x}).$$

This is the total transition from ψ to the wire. But we have proven in [3] that

$$\langle\psi, A^n(f)\psi\rangle = \int_{\mathbf{x} \in \text{wire}} f(\mathbf{x}) |\langle\psi, U(\sigma(\mathbf{x}))\eta\rangle|^2 d\mu(\mathbf{x}).$$

Taking η to be Gaussian in momentum with a certain average value of the momentum will do the job.

Notice that with this formula, for the conduction electron, the direction of the momentum, the spin of the electron, and the starting point in configuration space all are measured. There is no problem with the uncertainty principle, as we never ask the question of what the probability is of being at \mathbf{q} or moving at \mathbf{p} ; we only ask what the transition probability is between ψ and $U(\sigma(\mathbf{x}))\eta$. None-the-less, we have a complete measurement of ψ with the overcomplete set $\{U(\sigma(\mathbf{x}))\eta \mid \mathbf{x} \in G/H_\omega \text{ or } (G/H_\omega)/D\}$.

8 Summary of the Advantages

We have made the problems of an infinite lattice disappear by placing this theory in terms of the lattice in phase space and factoring. This procedure will work for any kinematical group and not just for the Heisenberg group. Thus we may have the conduction electron as a true spin 1/2 particle.

In the Heisenberg case, the theory is on a compact space, and one may use the Fourier transform.

Because of the vibrations of the crystal, the proper treatment of the conduction electrons is necessarily in phase space. Thus phonons are not necessary (but may be used).

The vibrations of the crystal may be related to the temperature through the principle of equipartition of the energy and dormant degrees of freedom, as well as using the crystal symmetry group to partition the energy into channels.

There is no reason to require that the Hamiltonian has eigenvalues and eigenvectors. There are no "secular determinant" and no "internal frequencies," but you may still have band gaps in a fuzzy sense.

When we measure the conduction electrons, we use the actual form of the probe with which we may measure. In this way we recover the method of measurement used in general in phase space.

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