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Jauch–Piron System of Imprimitivities for Phonons. II. The Wigner Function Formalism

Zbigniew Banach[1] and Sławomir Piekarski[2]

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In 1932 Wigner defined and described a quantum mechanical phase space distribution function for a system composed of many identical particles of positive mass. This function has the property that it can be used to calculate a class of quantum mechanical averages in the same manner as the classical phase space distribution function is used to calculate classical averages. Considering the harmonic vibrations of a system of n atoms bound to one another by elastic forces and treating them as a gas of indistinguishable Bose particles, phonons, the primary objective of this paper is to show under which circumstances the Wigner formalism for classical particles can be extended to cover also the phonon case. Since the phonons are either strongly or weakly localizable particles (as described in a companion paper), the program of the present approach consists in applying the Jauch–Piron quantum description of localization in (discrete) space to the phonon system and then in deducing from such a treatment the explicit expression for the phonon analogue of the Wigner distribution function. The characteristic new features of the "phase-space" picture for phonons (as compared with the situation in ordinary theory) are pointed out. The generalization of the method to the case of relativistic particles is straightforward.

1. INTRODUCTION

In 1932 Wigner defined and described a quantum mechanical phase space distribution function $f(\lambda, \mathbf{x}, t)$ for a system composed of n identical particles of positive mass (Wigner, 1932). As is by now well known, the $f(\lambda, \mathbf{x}, t)$ cannot be regarded as being a μ-space density, because the

[1]Institute of Fundamental Technological Research, Department of Fluid Mechanics, Polish Academy of Sciences, Swietokrzyska 21, 00-049 Warsaw, Poland.
[2]Institute of Fundamental Technological Research, Department of Theory of Continuous Media, Polish Academy of Sciences, Swietokrzyska 21, 00-049 Warsaw, Poland.

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uncertainty principle makes it impossible to simultaneously specify the position $\mathbf{x}$ and momentum λ of a particle at a given time t. Nevertheless, this function has many properties analogous to those of the classical distribution function. For example, it turns out that $f(\lambda, \mathbf{x}, t)$ can be used to calculate a class of quantum mechanical averages in the same manner as the classical phase space distribution function is used to calculate classical averages. One merely multiplies the Wigner distribution function $f(\lambda, \mathbf{x}, t)$ and any classical one-particle additive phase space function $A(\lambda, \mathbf{x})$ whose average is desired, and then integrates the resulting product over the entire phase space. Also, when the function $f(\lambda, \mathbf{x}, t)$ is integrated over all momenta, it gives us the average density of particles at the space-time point $\mathbf{x}, t$. Further, if one integrates $f(\lambda, \mathbf{x}, t)$ with respect to $\mathbf{x}$, one obtains the average density of particles with momentum λ at time t, a result that was to be expected for the momentum space distribution function.

It should be emphasized that the Wigner distribution function $f(\lambda, \mathbf{x}, t)$ is not in general positive. Moreover, as demonstrated in a recent analysis by Davidović and Lalović (1992), it is too much to require that every $f(\lambda, \mathbf{x}, t)$ smoothed out over phase space regions of dimensions larger than those of minimum uncertainty be always positive. In spite of these properties of $f(\lambda, \mathbf{x}, t)$, Wigner was right in stressing that his function, which can be chosen as being real, is in a certain sense the simplest and most natural quantum analogue of the classical phase space distribution function.

The important assumption in Wigner's (1932) paper is that the states of the physical system considered can be identified with the density matrices,[3] i.e., with the self-adjoint, positive, linear operators $\hat{\rho}$ of unit trace acting on some suitably constructed Hilbert space $\mathscr{H}$. In order to study the time evolution of $f(\lambda, \mathbf{x}, t)$, Klimontovich (1975) introduced a phase space operator $\hat{f}(\lambda, \mathbf{x}, t)$, actually a quantum field in phase space, which has the property that its expectation value on a state $\hat{\rho}$ is equal to $f(\lambda, \mathbf{x}, t)$. The main justification for the detailed analysis of the properties of a phase space operator $\hat{f}(\lambda, \mathbf{x}, t)$ lies in the hope that this analysis may provide a means of describing transport phenomena in a self-contained way, starting from a systematic derivation of an equation of motion for $\hat{f}(\lambda, \mathbf{x}, t)$.

In a companion paper (Banach and Piekarski, 1993), we outlined the proof for the existence of a notion of localizability for phonons, i.e., quasiparticles arising from the harmonic vibrations of a system of n atoms bound to one another by elastic forces. The essential ingredient in the discussion was the postulate, first formulated by Mackey (1953, 1958) and Wightman

[3]As remarked already by Emch (1972), the universal validity of this assumption is by no means obvious.

(1962), that the adequate mathematical tools for the investigation of localizability are the projection operators $\hat{E}(\Delta)$ acting on the Hilbert space $\mathscr{H}^{(1)}$ of one-phonon states, where Δ is an arbitrary subset of the set D that consists of n vectors $\mathbf{x}$ specifying the equilibrium positions of n atoms. The expectation value of an observable $\hat{E}(\Delta)$ on a normalized state $|\mathfrak{Z}\rangle \in \mathscr{H}^{(1)}$ gives us the probability that the phonon belongs to the atoms whose equilibrium positions are characterized by the members of Δ. We presented (Banach and Piekarski, 1993) the elementary formalism pertinent to the explicit construction of projection operators $\hat{E}(\Delta)$ and subsequently recognized that if in the system of n atoms there exist normal modes of zero frequency, then the phonon is only weakly localizable. [The general properties of weakly localizable particles are discussed in Jauch and Piron (1967) and Amrein (1969).]

Using the results established in Banach and Piekarski (1993), the purpose of this paper is to define the number-of-phonons operator[4] $\hat{N}_t(\Delta)$ corresponding to Δ at time t, to introduce the phonon analogue of the Klimontovich phase space operator $\hat{f}(\boldsymbol{\lambda}, \mathbf{x}, t)$, to derive various relations satisfied by it, to obtain the closed equation of motion for it,[5] and finally to demonstrate that its expectation value has many similarities to the original Wigner distribution function $f(\boldsymbol{\lambda}, \mathbf{x}, t)$.

However, closer inspection shows that these similarities are rather formal and that the differences between classical particles and phonons are more fundamental. First, it should not be forgotten that, since a phonon is characterized by a label j (Banach and Piekarski, 1993), we must replace $\boldsymbol{\lambda}$ by j.[6] Second, for phonons the space is discrete [a finite or countably infinite set of degrees of freedom (Jensen, 1964; Jensen and Nielsen, 1969)], while it is continuous for particles in ordinary space (Wightman, 1962; Jauch and Piron, 1967; Amrein, 1969). Consequently, in the present case $\mathbf{x}$ can take on only discrete values. Finally, the phonon analogue of $\hat{f}(\boldsymbol{\lambda}, \mathbf{x}, t)$, denoted by $\hat{f}_\Delta(j, \mathbf{x}, t)$, depends in general on Δ. The quantum pseudofield $\hat{f}_\Delta(j, \mathbf{x}, t)$

[4]The restriction of $\hat{N}_t(\Delta)$ to the Hilbert space $\mathscr{H}^{(1)}$ of one-phonon states is equal to the projection operator $\hat{E}_t(\Delta)$ at time t.

[5]In obtaining this equation, we restrict attention to the harmonic model in which the interactions between phonons are not considered.

[6]In the important case of a perfect crystal subject to the Born–von Karman cyclic boundary conditions (Born and von Karman, 1913), we can identify j with a pair $(\mathbf{k}, s)$, where $\mathbf{k}$ is a discrete wave vector varying within the first Brillouin zone and s is an integer which runs from 1 to r (r denotes the number of atoms per unit cell). The (infinitesimal) space-rotational symmetry is broken by the appearance of the Born–von Karman conditions, although the effective cyclic Hamiltonian is still invariant under a continuous translation. (Obviously, the ground state of the system does not manifest this symmetry.) Thus, as $\mathbf{k} \Rightarrow \mathbf{0}$, three of the branches $\Omega_s(\mathbf{k})$ must have frequencies that approach zero. These are known as the acoustic branches.

is defined in such a way that[7]

$$\sum_{j=d+1}^{3n} \sum_{\mathbf{x}\in\Delta} \hat{f}_\Delta(j, \mathbf{x}, t)$$

represents the operator $\hat{N}_t(\Delta)$ corresponding to the number of phonons "localized in" Δ at time t. In addition, if we consider the phonons of a particular kind j and wish to know how the average number of them changes with time, we should calculate the expectation value of $\sum_{\mathbf{x}\in D} \hat{f}_D(j, \mathbf{x}, t)$ for every t.

Certainly, the most significant new feature that arises in our approach is the fact that only for phonons which are localizable in the ordinary sense [$d=0$ (Banach and Piekarski, 1993)] do the operators $\hat{f}_\Delta(j, \mathbf{x}, t)$ not depend on Δ. It is probably this new complication which has been most directly responsible for the delay in the explicit construction of a phonon analogue of the Wigner distribution function. Fortunately, if in the system composed of vibrating atoms there exist no normal modes of zero frequency, these additional complications may be avoided altogether, provided one considers the Hamiltonian which is *not* invariant under the (infinitesimal) translations and/or rotations. If needed, this may be enforced by altering the Hamiltonian or considering a situation in which there is interaction between particles and an external system. From the conceptual point of view, however, the above-mentioned complications are quite important, because, as first observed by Jauch and Piron (1967) and Amrein (1969), they characterize the typical properties of weakly localizable particles.

By way of digression, we mention that our elementary formalism can easily be modified to cover the crystal case as well (see footnote 6), with naturally the obvious exception that in solid-state physics it is the custom to introduce the complex eigenvectors of the dynamical matrix. In addition, we are able to generalize the method of this paper to the case of classical and relativistic particles.

Here we proceed as follows. To prepare for the analysis, in Section 2 we look more closely at the problem of defining the number-of-phonons operator. Section 3 first introduces the phonon analogue of the Klimontovich phase space operator and then derives the closed equation of motion satisfied by it. We conclude the paper with final remarks in Section 4.

[7]The notation in this paper is taken from our previous considerations (Banach and Piekarski, 1993); thus d denotes the number of normal modes of zero frequency, n signifies the total number of vibrating atoms, and Δ is an arbitrary subset of the set D that consists of n vectors $\mathbf{x}$ specifying the equilibrium or average positions of n atoms.

2. DEFINITION OF THE NUMBER-OF-PHONONS OPERATOR

2.1. The Case of Strongly Localizable Phonons

As demonstrated in a companion paper (Banach and Piekarski, 1993), the analysis of a notion of localizability for phonons is a matter of introducing the projection operators $\hat{E}_t(\Delta)$ acting on the Hilbert space $\mathscr{H}^{(1)}$ of one-phonon states $|\mathfrak{Z}\rangle$. Restricting attention to the system composed of strongly localizable phonons ($d=0$), these projection operators take the form

$$\hat{E}_0(\Delta) := \sum_{\alpha,\mathbf{x}} \chi_\Delta(\mathbf{x}) \mathfrak{Z}_\alpha(\mathbf{x}) \hat{Y}_\alpha^+(\mathbf{x})|\xi\rangle \tag{2.1}$$

at time $t=0$, where $\chi_\Delta(\mathbf{x})=1$ if $\mathbf{x}\in\Delta$, and 0 if $\mathbf{x}\in D\backslash\Delta$. Without further comment we shall use those symbols that either are reasonably standard or appear for the first time in Banach and Piekarski (1993). Here let us only recall that $\mathfrak{Z}_\alpha(\mathbf{x})$, $\alpha=1, 2, 3$, is the position-space Schrödinger function and that $\hat{Y}_\alpha(\mathbf{x})$ is the detection operator expressed in terms of the annihilation operators $\hat{a}_j$ and the eigenvectors $e_\alpha(\mathbf{x}\,|\,j)$ of the dynamical matrix $[\mathbf{K}]$:

$$\hat{Y}_\alpha(\mathbf{x}) := \sum_{j=d+1}^{3n} e_\alpha(\mathbf{x}\,|\,j)\hat{a}_j \tag{2.2}$$

The definition (2.2) applies to every admissible value of d, but in the present special case we must set $d=0$. If one assumes that there are no normal modes of zero frequency ($\Omega_j>0$ for $j=1,\ldots,3n$), one can identify $|\xi\rangle$ with the ground state of the phonon system. This identification is no longer valid for $d\neq 0$; see Section 3.1 in Banach and Piekarski (1993).

Let $\mathscr{H}$ denote the Hilbert space of all phonon states. The $\mathscr{H}$ is obtained as the completion of the pre-Hilbert space that accommodates the states $|\mathfrak{H}\rangle$ with a finite (but otherwise arbitrary) number of phonons. If $d=0$, we can verify formally that $\mathscr{H}$ is a Fock space (Emch, 1972). The construction of $\mathscr{H}$ for $d\neq 0$ is described in Banach and Piekarski (1993, Section 3.1). Suppose now that $\hat{N}_0(\Delta)$ is an operator on $\mathscr{H}$ whose expectation value with respect to density matrices $\hat{\rho}$ characterizes the number of phonons "localized in" Δ at time $t=0$. The question then is, using $\mathscr{H}$, is it possible to establish the connection between $\hat{E}_0(\Delta)$ and $\hat{N}_0(\Delta)$? Within the context of relativistic quantum mechanics, Amrein (1969, Section X) has shown how to determine the number-of-particles operator for *any* given system of projection operators $\hat{E}_0(\Delta)$. Clearly, we may illustrate the general considerations of Amrein by applying them to the projection defined by (2.1); the result of our calculations is as follows:

$$\hat{N}_0(\Delta) = \hat{N}_0^{(s)}(\Delta) := \sum_{\mathbf{x}\in\Delta} \hat{\mathbf{Y}}^+(\mathbf{x}) \circ \hat{\mathbf{Y}}(\mathbf{x}) \tag{2.3}$$

This result, in turn, is physically expected. Mathematically, however, it is intimately linked to the fact that $d=0$.

We want to close this subsection by pointing out that the restriction of $\hat{N}_0(\Delta)$ to $\mathscr{H}^{(1)}$ can be identified with $\hat{E}_0(\Delta)$ and that the operator $\hat{N}_t(\Delta)$ which represents the number of phonons "localized in" Δ at time t is given by

$$\hat{N}_t(\Delta)=\exp\left(\frac{i}{\hbar}\hat{H}_B t\right)\hat{N}_0(\Delta)\exp\left(-\frac{i}{\hbar}\hat{H}_B t\right) \tag{2.4a}$$

where

$$\hat{H}_B:=\sum_{j=d+1}^{3n}\hbar\Omega_j\left(\tfrac{1}{2}+\hat{a}_j^+\hat{a}_j\right) \tag{2.4b}$$

$$d=0 \tag{2.4c}$$

Obviously, to get $\hat{N}_t(\Delta)$ for weakly localizable phonons, we must first modify the definition of $\hat{N}_0(\Delta)$ and then abandon the condition (2.4c) in (2.4b).

2.2. The Case of Weakly Localizable Phonons

Since the method of obtaining $\hat{N}_t(\Delta)$ for $d\neq 0$ coincides with the construction as it appears in the theory of strongly localizable phonons, we shall confine ourselves to giving the final answer, amplified by short comments that are required for the clarification of the formal statements. In the problem of localizability considered here, the projection operators $\hat{E}_0(\Delta)$ acting on $\mathscr{H}^{(1)}$ at time $t=0$ are of the form (Banach and Piekarski, 1993)

$$\hat{E}_0(\Delta):=\sum_{\alpha,\mathbf{x}}\chi_\Delta(\mathbf{x})\mathfrak{Z}_\alpha(\mathbf{x};\Delta)\hat{Y}_\alpha^+(\mathbf{x})|\xi\rangle \tag{2.5a}$$

where

$$\mathfrak{Z}_\alpha(\mathbf{x};\Delta):=\mathfrak{Z}_\alpha(\mathbf{x})-\sum_{p\in\Gamma_\Delta}\sum_{\mathbf{x}'\in\Delta}[\mathbf{e}^\Delta(\mathbf{x}'|p)\circ\mathfrak{Z}(\mathbf{x}')]e_\alpha^\Delta(\mathbf{x}|p) \tag{2.5b}$$

$$\Gamma_\Delta:=\{1,2,\ldots,d_\Delta\} \tag{2.5c}$$

The integer d_Δ satisfying the inequality $d_\Delta\leq\min(d,3n_\Delta)$, where n_Δ represents the number of elements in Δ, will in general depend upon the choice of the subset Δ of D (e.g., $d_D=d$). It follows from our previous discussion (Banach and Piekarski, 1993, Section 4.2) that the real vectors $\mathbf{e}^\Delta(\mathbf{x}|p)$, $p\in\Gamma_\Delta$, are linear combinations of $\mathbf{e}(\mathbf{x}|j)$, $j\in\Gamma_D=\{1,2,\ldots,d\}$. We should recall also that

$$\sum_{\mathbf{x}\in\Delta}\mathbf{e}^\Delta(\mathbf{x}|p)\circ\mathbf{e}^\Delta(\mathbf{x}|p')=\delta_{p,p'} \tag{2.6}$$

With the use of the explicit formula (2.5a) and the universal formalism of Amrein (1969), it is not difficult to obtain the operator $\hat{N}_0(\Delta)$ corresponding to the number of phonons "localized in" Δ at time $t=0$ [precisely speaking, the expectation value of $\hat{N}_0(\Delta)$ on a state $\hat{\rho}$ gives us the average number of phonons that belong to the atoms (points) whose equilibrium positions are characterized by the members of Δ]:

$$\hat{N}_0(\Delta)=\hat{N}_0^{(w)}(\Delta):=\sum_{\mathbf{x}\in\Delta}\hat{\mathbf{Y}}^{+}(\mathbf{x};\Delta)\circ\hat{\mathbf{Y}}(\mathbf{x};\Delta) \tag{2.7a}$$

$$\hat{Y}_\alpha(\mathbf{x};\Delta):=\hat{Y}_\alpha(\mathbf{x})-\sum_{p\in\Gamma_\Delta}\sum_{\mathbf{x}'\in\Delta}[\mathbf{e}^{\Delta}(\mathbf{x}'|p)\circ\hat{\mathbf{Y}}(\mathbf{x}')]e_\alpha^{\Delta}(\mathbf{x}|p) \tag{2.7b}$$

We infer from (2.7) that in the case of weakly localizable phonons the operator $\hat{N}_0^{(s)}(\Delta)$ of equation (2.3) should not be regarded as being the true correlate of the number of phonons in Δ at time $t=0$. Indeed, a glance at (2.7) shows that it is impossible to write the correct operator $\hat{N}_0^{(w)}(\Delta)$ for weakly localizable phonons as a single sum over Δ, because, as noted in Banach and Piekarski (1993, Sections 4.2 and 4.4), the restrictions of $\hat{N}_0^{(w)}(\Delta_1)$ and $\hat{N}_0^{(w)}(\Delta_2)$ to $\mathscr{H}^{(1)}$ do not commute for every pair Δ_1,Δ_2 of subsets of D. [The restriction of $\hat{N}_0^{(w)}(\Delta)$ to $\mathscr{H}^{(1)}$ is equal to the rhs of (2.5a).] However, we see by (2.3) and (2.7) that

$$\langle\mathfrak{H}|\hat{N}_0^{(w)}(\Delta)|\mathfrak{H}\rangle\leq\langle\mathfrak{H}|\hat{N}_0^{(s)}(\Delta)|\mathfrak{H}\rangle \tag{2.8}$$

where $|\mathfrak{H}\rangle\in\mathscr{H}$; equality holds if $\Delta=D$ or if $\hat{N}_0^{(w)}(\Delta)|\mathfrak{H}\rangle=m|\mathfrak{H}\rangle$, $m=0,1,\ldots$.

The inequality (2.8) resembles quite closely a result first established by Amrein for phonons [see Amrein (1969), condition (121), p. 186], differing, however, in that Amrein interprets Δ as a Borel subset of Euclidean three-space $\mathbb{R}^3$.

The evolution in time of $\hat{N}_0(\Delta)$ is characterized by (2.4a) and (2.4b).

3. THE PHONON ANALOGUE OF THE KLIMONTOVICH PHASE SPACE OPERATOR

3.1. Discussion of the Problem for $d=0$

Given the number-of-particles operator $\hat{N}_t(\Delta)$ for a phonon system, we can try to find some connection between the results about $\hat{N}_t(\Delta)$ and the predictions of the theory based upon the universal ideas of Wigner (1932) and Klimontovich (1975). Namely, it is tempting to introduce the operators

$\hat{f}(j, \mathbf{x}, t)$ acting on $\mathscr{H}$ such that

$$\sum_{j=1}^{3n} \sum_{\mathbf{x}\in\Delta} \hat{f}(j, \mathbf{x}, t) = \hat{N}_t(\Delta) \tag{3.1a}$$

$$\sum_{\mathbf{x}\in D} \hat{f}(j, \mathbf{x}, t) = \hat{a}_j^+(t)\hat{a}_j(t) \tag{3.1b}$$

where [Banach and Piekarski (1993), equations (2.14b)]

$$\hat{a}_j(t) = \exp(-i\Omega_j t)\hat{a}_j, \qquad \hat{a}_j^+(t) = \exp(i\Omega_j t)\hat{a}_j^+ \tag{3.1c}$$

Since $\hat{N}_t(\Delta)$ has a well-defined quantum mechanical meaning and $a_j^+(t)\hat{a}_j(t)$ is an operator corresponding to the number of phonons of a particular kind j, we shall refer to the expectation value of $\hat{f}(j, \mathbf{x}, t)$ on a state $\hat{\rho}$, denoted by $\mathrm{Tr}\,\hat{\rho}\hat{f}(j, \mathbf{x}, t)$ or simply by $f(j, \mathbf{x}, t)$, as the phonon analogue of the Wigner distribution function (Wigner, 1932).

It is natural to ask now whether one might be able to determine $\hat{f}(j, \mathbf{x}, t)$ explicitly. We have already noted in the Introduction that $\hat{f}(j, \mathbf{x}, t)$ is not an observable. Therefore, the best that we can hope to do is to define $\hat{f}(j, \mathbf{x}, t)$ in terms of $e_\alpha(\mathbf{x}\,|\,j)$ and

$$\hat{Y}_\alpha(\mathbf{x}, t) := \sum_{j=1}^{3n} e_\alpha(\mathbf{x}\,|\,j)\hat{a}_j \tag{3.2}$$

which has many features analogous to those of the classical operator. For concreteness sake, let us examine the following proposition:

$$\hat{f}(j, \mathbf{x}, t) := \sum_{\mathbf{x}'\in D} [\mathbf{e}(\mathbf{x}'\,|\,j) \circ \hat{\mathbf{Y}}^+(\mathbf{x}', t)][\mathbf{e}(\mathbf{x}\,|\,j) \circ \hat{\mathbf{Y}}(\mathbf{x}, t)] \tag{3.3a}$$

$$j \in \{1, 2, \ldots, 3n\}, \qquad \mathbf{x}\in D \tag{3.3b}$$

By substituting (3.2) into (3.3a) we arrive at

$$\hat{f}(j, \mathbf{x}, t) = \sum_{j'=1}^{3n} [\mathbf{e}(\mathbf{x}\,|\,j) \circ \mathbf{e}(\mathbf{x}\,|\,j')]\hat{a}_j^+(t)\hat{a}_{j'}(t) \tag{3.4}$$

Although the operator (3.3a) does not have the property of being Hermitian, straightforward calculation shows that our proposition renders (3.1a) valid for every Δ and that equation (3.1b) is also satisfied when $j = 1, 2, \ldots, 3n$. [Just as in the case of particles existing in $\mathbb{R}^3$, we could try to modify the definition of $\hat{f}(j, \mathbf{x}, t)$ by replacing $\mathbf{x}'$ by $\mathbf{x} - \frac{1}{2}\mathbf{x}'$ and $\mathbf{x}$ by $\mathbf{x} + \frac{1}{2}\mathbf{x}'$ on the rhs of (3.3a). This modification is not possible for discrete systems, however, because in general $\mathbf{x} + \frac{1}{2}\mathbf{x}'$ does not belong to D if $\mathbf{x}$ and $\mathbf{x} - \frac{1}{2}\mathbf{x}'$ are members of D.] Clearly, the proposition (3.3a) is not the only way to reconcile the conditions (3.1a) and (3.1b). Instead, we may introduce the operator of the form

$$\hat{F}_c(j, \mathbf{x}, t) := c\hat{f}(j, x, t) + (1-c)\hat{f}^{+}(j, \mathbf{x}, t) \tag{3.5}$$

where c is a real or complex number; the $\hat{F}_c(j, \mathbf{x}, t)$ is Hermitian if $c=\frac{1}{2}$. We easily verify that equations (3.1a) and (3.1b) do not provide a unique determination of c.

Now that we have set down the preliminaries, we shall try to obtain the equation of motion satisfied by $\hat{f}(j, \mathbf{x}, t)$ in the harmonic approximation. After a bit of algebraic manipulation which employs only the definition of $\hat{Y}_\alpha(\mathbf{x}, t)$ and the orthonormality of $e_\alpha(\mathbf{x}\,|\,j)$, we find

$$\hat{a}_j^{+}(t)\hat{a}_{j'}(t) = \sum_{\mathbf{x}\in D} \hat{f}(j, j', \mathbf{x}, t) \tag{3.6a}$$

where

$$\hat{f}(j, j', \mathbf{x}, t) := \sum_{\mathbf{x}'\in D} [\mathbf{e}(\mathbf{x}'\,|\,j) \circ \hat{\mathbf{Y}}^{+}(\mathbf{x}', t)][\mathbf{e}(\mathbf{x}\,|\,j') \circ \hat{\mathbf{Y}}(\mathbf{x}, t)] \tag{3.6b}$$

Hence

$$\hat{f}(j, j', \mathbf{x}, t) \neq \hat{f}(j, \mathbf{x}, t) \qquad \text{when} \quad j \neq j' \tag{3.7a}$$

and

$$\hat{f}(j, j', \mathbf{x}, t) = \hat{f}(j, \mathbf{x}, t) \qquad \text{when} \quad j = j' \tag{3.7b}$$

Here, equation (3.7b) is intended to serve as an indication that the generalized operator $\hat{f}(j, j', \mathbf{x}, t)$ should be used in place of $\hat{f}(j, \mathbf{x}, t)$.

Indeed, in view of (3.4), (3.6), (3.7a), and

$$\partial_t(\hat{a}_j^{+}(t)\hat{a}_{j'}(t)) = i(\Omega_j - \Omega_{j'})\hat{a}_j^{+}(t)\hat{a}_{j'}(t)$$

we could never hope to discover a closed equation of motion for $\hat{f}(j, \mathbf{x}, t)$. However, by exactly the same argument as we have just gone through, we can see that there is a closed equation of motion obeyed by $\hat{f}(j, j', \mathbf{x}, t)$:

$$\partial_t \hat{f}(j, j', \mathbf{x}, t) = i \sum_{j''=1}^{3n} \sum_{\mathbf{x}'\in D} (\Omega_j - \Omega_{j''}) \times [\mathbf{e}(\mathbf{x}\,|\,j') \circ \mathbf{e}(\mathbf{x}\,|\,j'')]\hat{f}(j, j'', \mathbf{x}', t) \tag{3.8}$$

In deriving (3.8) from (3.6b), we have used the alternative expression for $\hat{f}(j, j', \mathbf{x}, t)$ of the form

$$\hat{f}(j, j', \mathbf{x}, t) = \sum_{j''=1}^{3n} [\mathbf{e}(\mathbf{x}\,|\,j') \circ \mathbf{e}(\mathbf{x}\,|\,j'')]\hat{a}_j^{+}(t)\hat{a}_{j''}(t) \tag{3.9}$$

Although equation (3.8) is quite complicated in structure considering the simplicity of the Hamiltonian involved, we can in principle solve this equation; the expectation value of $\hat{f}(j, j', \mathbf{x}, t)$ on a state $\hat{\rho}$ is determined by $\mathrm{Tr}\, \hat{\rho}\, \hat{f}(j, j'', \mathbf{x}', 0)$. One way or another, equations (3.8), (3.7b), and (3.1a) are necessary to form the mathematical basis of all the techniques for characterizing the behavior of the number-of-phonons operator $\hat{N}_t(\Delta)$.

Having made these comments about the indirect physical meaning of $\hat{f}(j, j', \mathbf{x}, t)$, we shall study now the connection between $\hat{f}(j, j', \mathbf{x}, t)$ and the operator $\mathscr{E}_t(\Delta)$ corresponding to the energy "localized in" Δ at time t. Recalling the universal idea of Amrein (1969, Section IX), we first mention that if $\hat{f}(j, j', \mathbf{x}, t)$ is to stand in any relation to $\hat{\mathscr{E}}_t(\Delta)$, this relation can never reduce to the statement that $\hat{\mathscr{E}}_t(\Delta)$ for $\Delta \neq D$ be simply a sum over $\{1, 2, \ldots, 3n\} \times \Delta$ of the product of $\hbar\Omega_j$ and $\hat{f}(j, j, \mathbf{x}, t)$. As a matter of fact, if Δ_1 and Δ_2 are disjoint subsets of D and $|3\rangle \in \mathscr{H}^{(1)}$ is an eigenvector of $\hat{E}_t(\Delta_1)$, then the expectation value of $\hat{\mathscr{E}}_t(\Delta_2)$ on a normalized one-phonon state $|3\rangle$ is not equal to zero. Indeed, the operator $\hat{\mathscr{E}}_t(\Delta)$ is given by [Amrein (1969), equation (89)]

$$\hat{\mathscr{E}}_t(\Delta) := \sum_{\mathbf{x} \in \Delta} \hat{\mathbf{G}}^+(\mathbf{x}, t) \circ \hat{\mathbf{G}}(\mathbf{x}, t) \tag{3.10a}$$

where

$$\hat{G}_\alpha(\mathbf{x}, t) := \sum_{j=1}^{3n} (\hbar\Omega_j)^{1/2} e_\alpha(\mathbf{x} \mid j) \hat{a}_j(t) \tag{3.10b}$$

Hence, using (3.10b) and (3.6a), we conclude that

$$\hat{\mathscr{E}}_t(\Delta) = \hbar \sum_{j=1}^{3n} \sum_{j'=1}^{3n} \sum_{\mathbf{x} \in \Delta} \sum_{\mathbf{x}' \in D} (\Omega_j \Omega_{j'})^{1/2} \times [\mathbf{e}(\mathbf{x} \mid j) \circ \mathbf{e}(\mathbf{x} \mid j')] \hat{f}(j, j', \mathbf{x}', t) \tag{3.11}$$

3.2. Discussion of the Problem for $d \neq 0$

Now we consider the case of weakly localizable phonons. Equation (2.7a) can be taken as the starting point for the determination of the phonon analogue of the Wigner distribution function, using a procedure very similar to that of Section 3.1. It is therefore completely within the spirit of the previous arguments to introduce the operators

$$\hat{f}_\Delta(j, j', \mathbf{x}, t) \qquad (j, j' = d+1, \ldots, 3n; \mathbf{x} \in D)$$

acting on $\mathscr{H}$ such that

$$\sum_{j=d+1}^{3n} \sum_{\mathbf{x} \in \Delta} \hat{f}_\Delta(j, j, \mathbf{x}, t) = \hat{N}_t(\Delta) \tag{3.12a}$$

$$\sum_{\mathbf{x} \in D} \hat{f}_D(j, j, \mathbf{x}, t) = \hat{a}_j^+(t) \hat{a}_j(t) \tag{3.12b}$$

The new feature in our proposition [as compared with equations (3.1a) and (3.1b)] is, of course, the dependence of $\hat{f}_\Delta(j, j', \mathbf{x}, t)$ upon Δ.

We gain a better insight into the nature and origin of this dependence if we write the number-of-phonons operator $\hat{N}_t(\Delta)$ in terms of $\hat{a}_j(t)$:

$$\hat{N}_t(\Delta) = \sum_{\mathbf{x}\in\Delta} \hat{\mathbf{Y}}^+(\mathbf{x}, t; \Delta) \circ \hat{\mathbf{Y}}(\mathbf{x}, t; \Delta) \tag{3.13a}$$

$$\hat{\mathbf{Y}}(\mathbf{x}, t; \Delta) = \sum_{j=d+1}^{3n} \boldsymbol{\lambda}_\Delta(\mathbf{x}\,|\,j)\hat{a}_j(t) \tag{3.13b}$$

$$\boldsymbol{\lambda}_\Delta(\mathbf{x}\,|\,j) := \mathbf{e}(\mathbf{x}\,|\,j) - \sum_{p\in\Gamma_\Delta} \sum_{\mathbf{x}'\in\Delta} [\mathbf{e}^\Delta(\mathbf{x}'\,|\,p) \circ \mathbf{e}(\mathbf{x}'\,|\,j)]\mathbf{e}^\Delta(\mathbf{x}\,|\,p) \tag{3.13c}$$

Should we want to conjecture that every operator $\hat{f}_\Delta(j, j, \mathbf{x}, t)$ on the lhs of (3.12) does not depend upon Δ, we would, as the careful analysis of (3.13c) suggests, require implicitly that the vector $\boldsymbol{\lambda}_\Delta(\mathbf{x}\,|\,j)$ be equal to $\mathbf{e}(\mathbf{x}\,|\,j)$; we know, however, from several explicit examples [see, e.g., the discussion in Banach and Piekarski (1993, Section 5)] that this requirement can be violated if $d \neq 0$; we therefore conclude that the operators $\hat{f}_\Delta(j, j', \mathbf{x}, t)$ are not necessarily independent of Δ. The results below reinforce this statement.

Before proceeding further, we first observe that if

$$\hat{\mathbf{Y}}(\mathbf{x}, t; \Delta) := \exp\left(\frac{i}{\hbar} \hat{H}_B t\right) \hat{\mathbf{Y}}(\mathbf{x}; \Delta) \exp\left(-\frac{i}{\hbar} \hat{H}_B t\right) \tag{3.14}$$

is written in the form (3.13b), then by using the orthonormality properties of $e_a(\mathbf{x}\,|\,j)$ and the identity [the $\mathbf{e}^\Delta(\mathbf{x}\,|\,p)$, $p\in\Gamma_\Delta$, is a linear combination of $\mathbf{e}(\mathbf{x}\,|\,j)$, $j = 1, \ldots, d$ (Banach and Piekarski, 1993)]

$$\sum_{\mathbf{x}\in D} \mathbf{e}(\mathbf{x}\,|\,j) \circ \mathbf{e}^\Delta(\mathbf{x}\,|\,p) = 0 \qquad (p\in\Gamma_\Delta, j = d+1, \ldots, 3n) \tag{3.15}$$

it is easy to show that

$$\hat{a}_j(t) = \sum_{\mathbf{x}\in D} \mathbf{e}(\mathbf{x}\,|\,j) \circ \hat{\mathbf{Y}}(\mathbf{x}, t; \Delta) \tag{3.16a}$$

where

$$j = d+1, \ldots, 3n \tag{3.16b}$$

Directly from $\Gamma_D = \{1, 2, \ldots, d\}$ and $\mathbf{e}^D(\mathbf{x}\,|\,p) = \mathbf{e}(\mathbf{x}\,|\,p)$ we also conclude that (Banach and Piekarski, 1993)

$$\boldsymbol{\lambda}_D(\mathbf{x}\,|\,j) = \mathbf{e}(\mathbf{x}\,|\,j), \qquad j = d+1, \ldots, 3n \tag{3.17}$$

Since our method of obtaining $\mathbf{e}^{\Delta}(\circ|p)$, $p\in\Gamma_\Delta$, delivers the three-component function $\mathbf{e}(\circ|j)_{|\Delta}$, $j\in\Gamma_D$, as an exhibited linear combination of $\mathbf{e}^{\Delta}(\circ|p)$, $p\in\Gamma_\Delta$, we finally see that (Banach and Piekarski, 1993)

$$\sum_{\mathbf{x}\in\Delta} \mathbf{e}(\mathbf{x}|j)\circ\hat{\mathbf{Y}}(\mathbf{x},t;\Delta)=0, \qquad j\in\Gamma_D \tag{3.18}$$

With these preliminaries by way of introduction, we are now ready to study the properties of the following expression for $\hat{f}_\Delta(j,j',\mathbf{x},t)$:

$$\begin{aligned}\hat{f}_\Delta(j,j',\mathbf{x},t) &:= \sum_{\mathbf{x}'\in D} [\mathbf{e}(\mathbf{x}'|j)\circ\hat{\mathbf{Y}}^{+}(\mathbf{x}',t;\Delta)][\mathbf{e}(\mathbf{x}|j')\circ\hat{\mathbf{Y}}(\mathbf{x},t;\Delta)]\\ &= \sum_{j''=d+1}^{3n} [\mathbf{e}(\mathbf{x}|j')\circ\boldsymbol{\lambda}_\Delta(\mathbf{x}|j'')]\hat{a}_j^{+}(t)\hat{a}_{j''}(t)\end{aligned} \tag{3.19a}$$

$$j,j'=d+1,\ldots,3n, \qquad \mathbf{x}\in D \tag{3.19b}$$

From (3.13a), (3.17), (3.18), and

$$\sum_{j=d+1}^{3n} e_\alpha(\mathbf{x}|j)e_\beta(\mathbf{x}'|j)=\delta_{\alpha,\beta}\delta_{\mathbf{x},\mathbf{x}'}-\sum_{j=1}^{d} e_\alpha(\mathbf{x}|j)e_\beta(\mathbf{x}'|j) \tag{3.20}$$

we may easily prove that the operators $\hat{f}_\Delta(j,j',\mathbf{x},t)$ as given by (3.19) satisfy the conditions (3.12a) and (3.12b).

Next, using the relation [this relation is a consequence of equation (3.15) and the definition (3.13c) of $\boldsymbol{\lambda}_\Delta(\mathbf{x}|j)$]

$$\sum_{\mathbf{x}\in D} \mathbf{e}(\mathbf{x}|j)\circ\boldsymbol{\lambda}_\Delta(\mathbf{x}|j')=\delta_{j,j'} \tag{3.21}$$

in which $j,j'\in\{d+1,\ldots,3n\}$, one can show that

$$\begin{aligned}\partial_t\hat{f}_\Delta(j,j',\mathbf{x},t) &= i\sum_{j''=d+1}^{3n}\sum_{\mathbf{x}'\in D}(\Omega_j-\Omega_{j''})\\ &\quad\times[\mathbf{e}(\mathbf{x}|j')\circ\boldsymbol{\lambda}_\Delta(\mathbf{x}|j'')]\hat{f}_\Delta(j,j'',\mathbf{x}',t)\end{aligned} \tag{3.22}$$

In this way, we get to the closed equation of motion obeyed by $\hat{f}_\Delta(j,j',\mathbf{x},t)$.

By appeal to the same device as proposed in Section 3.1 it is also possible to find the connection between the operator $\hat{\mathscr{E}}_t(\Delta)$ corresponding to the energy "localized in" Δ at time t and $\hat{f}_\Delta(j,j',\mathbf{x},t)$. However, we shall not discuss here this aspect of the theory of weakly localizable phonons.

To sum up: Equations (3.8) and (3.22) are derived by neglecting the anharmonic effects. The analysis of the $d\neq 0$ case is no more complicated in principle, but it involves some algebraic complexities. The main difference between the two cases is that for $d=0$ one has to replace $\boldsymbol{\lambda}_\Delta(\mathbf{x}|j'')$ by $\mathbf{e}(\mathbf{x}|j'')$ in equation (3.22) and then interpret the operators $\hat{f}_\Delta(j,j',\mathbf{x},t)$ as being insensitive to the choice of the subset Δ of D.

4. FINAL REMARKS

In this and the companion paper we have treated only a very simple molecular model: a system composed of n atoms bound to one another by elastic forces. Although the theory of this model is consistent with the specific principles governing the behavior of lattice vibrations in perfect crystals, it may be formulated completely without ever using them, and without ever specifying the symmetry properties of an equilibrium configuration of n atoms. As a matter of fact, we may say that if we study the definition of a notion of localizability for phonons arising from the harmonic vibrations of a system of atoms about their equilibrium positions, then (in the absence of external forces) this definition is influenced primarily by the precise form of the eigenvectors associated with all normal modes of zero frequency. In considering these eigenvectors it is not necessary to assume that there exists a group of symmetry operations which transforms the equilibrium configuration of atoms into itself. However, any idea based upon the introduction of normal modes of zero frequency must at least include the possibility, altogether natural for an inertial frame of reference, that the potential energy of the system may remain invariant under arbitrary infinitesimal translations and rotations. (By way of digression, the conservation of total momentum and total moment of momentum arises because of invariance of the Hamiltonian against infinitesimal translations and rotations.)

Although mathematically meager, our method has the distinct advantage of offering a precise explanation of the statement that, in certain cases of conceptual interest, the phonons are only weakly localizable. It allows us to investigate, with some justifiable confidence, the particle aspects of phonons for discrete systems described by a finite number of degrees of freedom. The extension of this last observation to the system consisting of an infinite number of atoms is, of course, a problem of considerable complexity. One obvious reason for this is that, with the important exception of a perfect crystal subject to the Born–von Karman cyclic boundary conditions (Born and von Karman, 1913), we can draw no conclusions about the "thermodynamic limit" $n \Rightarrow \infty$ [unless we make some arbitrary assumptions regarding the unknown dependence of $\mathbf{e}(\mathbf{x}\,|\,j)$ upon n]. (See also our comments at the end of this section.)

In the systematic development of the theory of either strongly or weakly localizable phonons, the axioms are formulated in terms of projection operators $\hat{E}_t(\Delta)$. It turns out that these operators have properties which stand in close analogy to those first discovered by Jauch and Piron (1967) within the context of consequent relativistic theory of elementary particles of mass zero. The construction of $\hat{E}_t(\Delta)$ enables us to use the universal method of Amrein (1969) in order to obtain the explicit expression for the number-of-phonons operator $\hat{N}_t(\Delta)$. Moreover, our approach renders the resulting formula rigorously proved, not merely formal. From this point of view, we conclude that since the theory is consistent with the Jauch–Piron quantum description of localization (in a discrete space D), the operator $\hat{N}_t(\Delta)$ is to be considered as a guide to introduce (in a certain sense) the simplest and most natural phonon analogue of the Wigner distribution function (Wigner, 1932).

Once the basic expression of $\hat{f}_\Delta(j, j', \mathbf{x}, t)$ in terms of $e_\alpha(\mathbf{x}\,|\,j)$ and $\hat{Y}_\alpha(\mathbf{x}, t; \Delta)$ has been established, we may derive the closed equation of motion satisfied by $\hat{f}_\Delta(j, j', \mathbf{x}, t)$. Such an equation arises because the anharmonic contributions to the Hamiltonian $\hat{H}$ have been completely left out. Clearly, to say more about the t evolution of $\hat{f}_\Delta(j, j', \mathbf{x}, t)$ than (3.22) asserts, we must first specify the equilibrium configuration of a system of n atoms and then develop the properties of Ω_j and $e_\alpha(\mathbf{x}\,|\,j)$; moreover, we must enter into the details regarding the meaning of j. We could try to exhibit some aspects of this program. However, to erect the general structure of the theory of localizable phonons, we need not descend beyond the elementary formalism proposed, e.g., in Banach and Piekarski (1993).

If one restricts one's attention to the perfect crystal subject to the Born–von Karmán cyclic boundary conditions, one can think of a symbol j as being a pair $(\mathbf{k}, s)$, where $\mathbf{k}$ is a discrete wave vector varying within the first Brillouin zone and s is an integer running from 1 to r (r denotes the number of atoms per unit cell). As mentioned at the end of the Introduction, our approach to localizable phonons can easily be modified to cover also the crystal case, with naturally the obvious exception that in solid-state physics it is the custom to introduce the complex eigenvectors of the dynamical matrix (Jensen, 1964; Jensen and Nielsen, 1969). Now, by referring to the kinetic theory of phonon excitations in dielectric crystals (Gurevich, 1980) we expect that when $j = (\mathbf{k}, s)$, then under some kind of passage to the continuum limit the equation of motion for the expectation value of either $\hat{f}$ or $\hat{f}_\Delta$ will be very similar to the "collisionless' part of the Boltzman–Peierls equation (Peierls, 1955; Gurevich, 1980). Such is indeed the case, but this preliminary paper does not allow space for the more complete treatment of these problems.

Finally we note that if we attempt to construct the projection operators $\hat{E}_t(\Delta)$ for an infinite perfect crystal ($n \Rightarrow \infty$), then a slight modification of the present method can justly be regarded as a method for formally approximating $\hat{E}_t(\Delta)$ by a sequence of projection operators $\hat{E}_t^{(n)}(\Delta)$; these operators correspond to a family of crystals with an increasing number of atoms. We shall not exhibit the specimens of this calculation here; we want only to mention that the resulting set of projection operators $\hat{E}_t(\Delta)$ forms a generalized system of imprimitivities describing weakly localizable phonons.

To summarize, in the conventional presentation there is a clear-cut distinction between the Jauch–Piron quantum theory of localization in space and the Wigner function formalism. Actually, however, the application of the ideas of our two papers bridges the gap between the two points of view. Thus, it would also seem natural to apply our ideas to the construction of the Wigner distribution function for other particle systems, e.g., relativistic particles.

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