International Journal of Theoretical Physics, Vol. 32, No. 1, 1993

Jauch–Piron System of Imprimitivities for Phonons. I. Localizability in Discrete Space

Zbigniew Banach[1] **and Sławomir Piekarski**[2]

Received January 31, 1992

This paper is devoted to a discussion of the 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 natural tools for the analysis of localizability are the projection operators $\hat{E}(\Delta)$ acting on the Hilbert space of one-phonon states, where Δ is an arbitrary subset of the set that consists of n vectors specifying the equilibrium positions of n atoms. The expectation value of $\hat{E}(\Delta)$ is the probability that the phonon belongs to the atoms whose equilibrium positions are characterized by the elements of Δ. For a strongly localizable phonon all of the projection operators $\hat{E}(\Delta)$ commute with one another, whereas in the case of a weakly localizable phonon the operators $\hat{E}(\Delta_1)$ and $\hat{E}(\Delta_2)$ do not commute when Δ_1 and Δ_2 overlap. With the aid of the Jauch–Piron quantum theory of localization in space, the present paper describes the method of obtaining $\hat{E}(\Delta)$ and also shows that if in the system of n atoms there exist normal modes of zero frequency, then the phonon is only weakly localizable. Given the explicit expression for $\hat{E}(\Delta)$, one can define the number-of-phonons operator as well as the quasiparticle analogue (given in a companion paper) of the Wigner distribution function.

1. INTRODUCTION

In quantum mechanics to each elementary question concerning the state of a system there corresponds a projection operator whose expectation value gives us the probability of obtaining a positive answer (von Neumann, 1955; Emch, 1972). In particular, many investigations of localizability for particles can be formulated in terms of projection operators $\hat{E}(\Delta)$, where Δ is some measurable subset of space. The $\hat{E}(\Delta)$ are supposed to describe a property of the particle, the property of being localized in Δ. Precisely speaking, if

[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.

0020-7748/93/0100-0001$07.00/0

the system is prepared in the normalized state $|\mathfrak{Z}\rangle$, then the probability of finding the particle in Δ is equal to the expectation value of $\hat{E}(\Delta)$, i.e., $\langle\mathfrak{Z}|\hat{E}(\Delta)|\mathfrak{Z}\rangle$.

For a wide class of elementary particles, the construction and analysis of the properties of $\hat{E}(\Delta)$ was initiated by Mackey (1953, 1958) and Wightman (1962) and has been generalized by Jauch and Piron (1967); the reader will also find an interesting discussion of this approach in the thesis by Amrein (1969). The most important results of these fundamental studies can be stated as follows: (i) if it is possible to localize the particle in an arbitrary finite region of space, then this particle is either *strongly* or *weakly* localizable; (ii) for strongly localizable systems all of the projection operators $\hat{E}(\Delta)$ commute with one another, whereas in the case of weakly localizable particles the operators $\hat{E}(\Delta_1)$ and $\hat{E}(\Delta_2)$ may not commute if Δ_1 and Δ_2 overlap; (iii) restricting attention to strongly localizable systems, the probability that the particle lies in Δ can be expressed in terms of a positive-definite probability density in $\mathbf{x}$ space; (iv) such a probability density no longer exists for weakly localizable systems.

As a matter of fact, the special application which guided the development of the general formalism proposed in the above-mentioned papers was the study of the properties of $\hat{E}(\Delta)$ for relativistic particles (Newton and Wigner, 1949). Our primary intent in the present paper is to show that, aside from its original usefulness and meaning, this formalism can also serve the purpose of characterizing the notion of localizability for phonons, i.e., quasiparticles arising from the collective vibrations of many-body systems (Knox and Gold, 1964; Birman, 1974; Lax, 1974).

To the best of our knowledge, in the literature the problems concerning the localization of phonons were first discussed by Jensen (1964) and Jensen and Nielsen (1969). These authors considered the harmonic vibrations of a system of n material points bound to each other by elastic forces. First, they formulated the eigenvalue problem under the assumption that in the system there exist no normal modes of zero frequency. Second, defining $3n$ annihilation and $3n$ creation operators, they investigated the possibility of introducing dynamical variables for a single phonon analogous to the variables of ordinary particles. Finally, they demonstrated that if the vector $\mathbf{x}$ specifies the equilibrium position of a material point and $\mathfrak{Z}(\mathbf{x})$ denotes the Schrödinger function of the phonon in the $\mathbf{x}$-representation, then $[\mathfrak{Z}^*(\mathbf{x}) \circ \mathfrak{Z}(\mathbf{x})]^{1/2}$ is the probability that when exactly one phonon is present it has the position $\mathbf{x}$. Summarizing, Jensen and Nielsen showed that in their model the phonons are strongly localizable.

On the other hand, for certain situations of conceptual interest (an inertial frame of reference, no external forces acting on the particles), the Hamiltonian of a system of n points is invariant under the infinitesimal translations and rotations (Knox and Gold, 1964, pp. 173–181), even for an arbitrary equilibrium configuration possessing no symmetry whatever, and thus, in this particular but important case, there exist at least six normal modes of zero frequency.[3] [A detailed analysis of the nature and origin of such modes is given, for example, in the book by Rajaraman (1982).] Consequently, to bring into consideration all admissible motions, displacements of the center of mass along the three coordinate axes and rotations about these axes must be included (treated as being normal modes of zero frequency).

In this paper a generalization of the results of Jensen (1964) and Jensen and Nielsen (1969) is proposed, which shows that if the eigenvalue problem has nontrivial solutions with vanishing eigenfrequencies, then the phonons are only weakly localizable. We present also the method of obtaining the projection operators $\hat{E}(\Delta)$, where Δ is an arbitrary subset of the set D that consists of n vectors $\mathbf{x}$ specifying the equilibrium positions of all material points. The expectation value of $\hat{E}(\Delta)$ gives us the probability that the phonon belongs to the points (atoms) whose equilibrium positions are characterized by the members of Δ. Among other things, we shall recognize that (i) in general the projection operators $\hat{E}(\Delta_1)$ and $\hat{E}(\Delta_2)$ do not commute and that (ii) $\sum_{\mathbf{x}\in\Delta} \hat{E}(\{\mathbf{x}\}) \leq \hat{E}(\Delta)$; equality holds if and only if all the frequencies of normal modes are positive.

The problem of constructing $\hat{E}(\Delta)$ is not only an academic game, intellectually challenging but of no importance. As shown in a companion paper (Banach and Piekarski, 1993), the existence of projection operators $\hat{E}(\Delta)$ acting on the Hilbert space $\mathscr{H}^{(1)}$ of one-phonon states enables us to obtain the operator $\hat{N}(\Delta)$ corresponding to the number of phonons "localized in" Δ. In fact, applying the results of Jauch and Piron (1967) about a generalized notion of localizability and using the method of Amrein (1969, Section X), we easily verify that the number-of-phonons operator $\hat{N}(\Delta)$ can be regarded as being an extension of $\hat{E}(\Delta)$ to the Fock space (von Neumann, 1955; Emch, 1972). Finally, given the explicit expression for $\hat{N}(\Delta)$, it would also seem particularly important to introduce phase space operators, actually quantum pseudofields in phase space, which are compatible with the definition of $\hat{N}(\Delta)$ and which have the property that their expectation values are phonon analogues (Banach and Piekarski, 1993) of the Wigner distribution functions (Wigner, 1932; Klimontovich, 1975). Such phase space operators could then be applied in a number of investigations, especially in studies concerning the derivation of the Boltzmann–Peierls equation (Beck *et al.*, 1974; Gurevich, 1980).

[3]We postulate that the points are not all collinear. Clearly, due to the possible extra properties of the system, i.e., the properties which cannot be predicted by symmetry, some additional normal modes with vanishing eigenfrequencies may occur accidentally.

By way of digression, the ideas of our two papers are very universal and will, for the most part, find almost immediate application in the context of other particle systems. Thus, for example, one would like to consider such objects as the Wigner distribution functions for relativistic particles. Consequently, one might like to show that these functions are consistent with, and can be obtained from, the Jauch–Piron description of localization in (continuum) space.

In connection with our system of n points bound to one another by elastic forces, we mention here that we take the origin of coordinates at the center of mass. The question then naturally arises whether there exists a group $\mathbb{G}$ of three-dimensional rotations R which transforms the equilibrium configuration of points (atoms) into itself. This preliminary paper does not allow space for a complete mathematical treatment of these problems, but our construction of $\hat{E}(\Delta)$ is valid for every admissible choice of $\mathbb{G}$; for example, in order to reflect some features of disordered and/or amorphous solids, we can assume that the system has no symmetry.

The layout of this paper is as follows. Section 2 introduces the two alternative forms of the Hamiltonian in the harmonic approximation. The analysis in Section 3 relates to the determination of the most general one-phonon states. We start from the description in terms of the traditional annihilation and creation operators and then pass directly to a space representation of the phonon. The objective of Section 4 is to construct the projection operators $\hat{E}(\Delta)$. This section closes with a short discussion of the properties of $\hat{E}(\Delta)$. Some elementary examples of normal modes of zero frequency appear in Section 5. We conclude the paper with final remarks of Section 6. The auxiliary technical material is included as an Appendix.

2. THE HAMILTONIAN OF THE SYSTEM

2.1. The Eigenvalue Problem

Following Wigner (Knox and Gold, 1964, pp. 173–181), we consider the harmonic vibrations of a system of n material points (atoms) bound to one another by elastic forces. Let D denote the set of n vectors $\mathbf{x}$ specifying the equilibrium positions of n points; we take the origin of coordinates at the center of mass. An atom will be labeled by $\mathbf{x}$. To the atom $\mathbf{x}$ belong a displacement vector $\mathbf{U}(\mathbf{x})$ and a momentum vector $\mathbf{P}(\mathbf{x})$, and we shall use subscripts $\alpha, \beta, \gamma, \ldots$ to denote their components $U_\alpha(\mathbf{x})$ and $P_\alpha(\mathbf{x})$ in a Cartesian coordinate system. The Hermitian operators corresponding to $\mathbf{U}(\mathbf{x})$ and $\mathbf{P}(\mathbf{x})$ will be denoted by $\hat{\mathbf{U}}(\mathbf{x})$ and $\hat{\mathbf{P}}(\mathbf{x})$, respectively. These operators satisfy the commutation relations of the form

$$[\hat{U}_\alpha(\mathbf{x}),\ \hat{U}_\beta(\mathbf{x}')]=0, \qquad [\hat{P}_\alpha(\mathbf{x}),\ \hat{P}_\beta(\mathbf{x}')]=0 \tag{2.1a}$$

$$[\hat{U}_\alpha(\mathbf{x}),\ \hat{P}_\beta(\mathbf{x}')]=i\hbar\ \delta_{\alpha,\beta}\ \delta_{\mathbf{x},\mathbf{x}'} \tag{2.1b}$$

In equation (2.1b) the symbols $\delta_{\alpha,\beta}$ and $\delta_{\mathbf{x},\mathbf{x}'}$ stand for the Kronecker deltas, and $\hbar$ is Planck's constant divided by 2π.

Restricting attention to the small vibrations of atoms about their equilibrium positions, we can introduce phonons on the basis of the harmonic approximation in which the system is described by the Hamiltonian

$$\hat{H}:=\sum_{\mathbf{x}} \frac{1}{2m_{\mathbf{x}}}\ \hat{\mathbf{P}}(\mathbf{x}) \circ \hat{\mathbf{P}}(\mathbf{x}) + \tfrac{1}{2} \sum_{\mathbf{x},\mathbf{x}'} \mathbf{\Phi}(\mathbf{x},\ \mathbf{x}') \circ [\hat{\mathbf{U}}(\mathbf{x}) \otimes \hat{\mathbf{U}}(\mathbf{x}')] \tag{2.2a}$$

where

$$\sum_{\mathbf{x}} (\circ\ \circ\ \circ) := \sum_{\mathbf{x}\in D} (\circ\ \circ\ \circ) \tag{2.2b}$$

Here $m_{\mathbf{x}}$ is the mass of the $\mathbf{x}$ atom, and the notation indicates that this mass depends on $\mathbf{x}$. The $[\mathbf{\Phi}]$ is the force constant matrix whose components in a Cartesian coordinate system will be denoted by $\Phi_{\alpha,\beta}(\mathbf{x}, \mathbf{x}')$. Clearly, the matrix $[\mathbf{\Phi}]$ is *positive-semidefinite*, *real*, and *symmetric* (Birman, 1974).

It is well known that the elastic vibrations of the system can be built up of *normal modes*. To bring into consideration all possible motions, we specify a complete set of *real* vectors $\mathbf{e}(\mathbf{x} \mid j)$, where j is an integer which runs from 1 to $3n$, obeying the following conditions:

$$\sum_{j} e_\alpha(\mathbf{x} \mid j) e_\beta(\mathbf{x}' \mid j) = \delta_{\alpha,\beta}\ \delta_{\mathbf{x},\mathbf{x}'} \tag{2.3a}$$

$$\sum_{\alpha,\mathbf{x}} e_\alpha(\mathbf{x} \mid j) e_\alpha(\mathbf{x} \mid j') = \delta_{j,j'} \tag{2.3b}$$

Irrespective of degeneracy, the three-component functions $\mathbf{e}(\circ \mid j)$ are defined as being "eigenvectors" of the so-called dynamical matrix $[\mathbf{K}]$:

$$K_{\alpha,\beta}(\mathbf{x},\ \mathbf{x}') := (m_{\mathbf{x}} m_{\mathbf{x}'})^{-1/2} \Phi_{\alpha,\beta}(\mathbf{x},\ \mathbf{x}') \tag{2.4}$$

Thus

$$\sum_{\beta,\mathbf{x}'} K_{\alpha,\beta}(\mathbf{x},\ \mathbf{x}') e_\beta(\mathbf{x}' \mid j) = \Omega_j^2 e_\alpha(\mathbf{x} \mid j) \tag{2.5}$$

The eigenvalues are denoted by Ω_j^2. They are real, because the matrix $[\mathbf{K}]$ is real and symmetric, and they are nonnegative, since the potential energy V of the system is assumed to be nonnegative. By convention, the *frequencies* Ω_j are such that $\Omega_j \geq 0$ for every j $(j=1, \ldots, 3n)$.

Of course, it may happen that one or more eigenfrequencies are zero. This happens, for example, when the potential energy V of the (finite) system is invariant under the infinitesimal translations and rotations; an arbitrary inertial frame of reference, no external forces acting on the particles (Knox and Gold, 1964, pp. 11, 174). (In Section 5, we discuss the important examples of normal modes of zero frequency.) In order to study the notion of localizability for the most general case, we postulate that

$$\Omega_j = 0 \qquad \text{if} \quad j = 1, \ldots, d \tag{2.6a}$$

and that

$$\Omega_j > 0 \qquad \text{if} \quad j = d+1, \ldots, 3n \tag{2.6b}$$

2.2. The Collective Operators

Applying the eigenvalues and eigenvectors of the dynamical matrix **[K]**, our next task is to introduce $3n-d$ different annihilation operators $\hat{a}_j$ and $3n-d$ different creation operators $\hat{a}_j^+$ through the definitions

$$\hat{a}_j := \sum_{\mathbf{x}} \left\{ \left(\frac{m_{\mathbf{x}} \Omega_j}{2\hbar} \right)^{1/2} [\mathbf{e}(\mathbf{x} \mid j) \circ \hat{\mathbf{U}}(\mathbf{x})] + i \left(\frac{1}{2\hbar m_{\mathbf{x}} \Omega_j} \right)^{1/2} [\mathbf{e}(\mathbf{x} \mid j) \circ \hat{\mathbf{P}}(\mathbf{x})] \right\} \tag{2.7a}$$

$$\hat{a}_j^+ := \sum_{\mathbf{x}} \left\{ \left(\frac{m_{\mathbf{x}} \Omega_j}{2\hbar} \right)^{1/2} [\mathbf{e}(\mathbf{x} \mid j) \circ \hat{\mathbf{U}}(\mathbf{x})] - i \left(\frac{1}{2\hbar m_{\mathbf{x}} \Omega_j} \right)^{1/2} [\mathbf{e}(\mathbf{x} \mid j) \circ \hat{\mathbf{P}}(\mathbf{x})] \right\} \tag{2.7b}$$

in which

$$j = d+1, \ldots, 3n \tag{2.7c}$$

The fact that in the present case $\Omega_j = 0$ when $j = 1, \ldots, d$ precludes using (2.7a) and (2.7b) to define $\hat{a}_j$ and $\hat{a}_j^+$ for $j = 1, \ldots, d$. Consequently, the remaining $2d$ degrees of freedom will be represented by the collective operators $\hat{U}_j$ and $\hat{P}_j$:

$$\hat{U}_j := \sum_{\mathbf{x}} (m_{\mathbf{x}})^{1/2} [\mathbf{e}(\mathbf{x} \mid j) \circ \hat{\mathbf{U}}(\mathbf{x})] \tag{2.8a}$$

$$\hat{P}_j := \sum_{\mathbf{x}} (m_{\mathbf{x}})^{-1/2} [\mathbf{e}(\mathbf{x} \mid j) \circ \hat{\mathbf{P}}(\mathbf{x})] \tag{2.8b}$$

$$j = 1, \ldots, d \tag{2.8c}$$

From (2.7) together with the canonical commutation relations (2.1) for $\hat{U}_\alpha(\mathbf{x})$ and $\hat{P}_\alpha(\mathbf{x})$ it follows that the operators $\hat{a}_j$ and $\hat{a}_j^+$ obey the commutation relations characterizing annihilation and creation operators for Bose particles:

$$[\hat{a}_j, \hat{a}_l] = [\hat{a}_j^+, \hat{a}_l^+] = 0 \tag{2.9a}$$

$$[\hat{a}_j, \hat{a}_l^+] = \delta_{j,l} \tag{2.9b}$$

To obtain (2.9), we have made use of the orthonormality rule (2.3b). In the same way, one can prove that $\hat{U}_j$ and $\hat{P}_j$ are canonically conjugate variables which commute with the $2(3n-d)$ annihilation and creation operators describing oscillatory motion:

$$[\hat{U}_j, \hat{U}_l] = 0, \qquad [\hat{P}_j, \hat{P}_l] = 0 \tag{2.10a}$$

$$[\hat{U}_j, \hat{P}_l] = i\hbar\delta_{j,l} \tag{2.10b}$$

$$[\hat{a}_j, \hat{U}_l] = [\hat{a}_j^+, \hat{U}_l] = 0 \tag{2.10c}$$

$$[\hat{a}_j, \hat{P}_l] = [\hat{a}_j^+, \hat{P}_l] = 0 \tag{2.10d}$$

Beginning from (2.3a), we easily find that

$$\hat{\mathbf{U}}(\mathbf{x}) = \sum_{j=1}^{d} (m_\mathbf{x})^{-1/2}\mathbf{e}(\mathbf{x} \mid j)\hat{U}_j + \sum_{j=d+1}^{3n} \left(\frac{\hbar}{2m_\mathbf{x}\Omega_j}\right)^{1/2} \mathbf{e}(\mathbf{x} \mid j)(\hat{a}_j + \hat{a}_j^+) \tag{2.11a}$$

$$\hat{\mathbf{P}}(\mathbf{x}) = \sum_{j=1}^{d} (m_\mathbf{x})^{1/2}\mathbf{e}(\mathbf{x} \mid j)\hat{P}_j - i \sum_{j=d+1}^{3n} \left(\frac{\hbar m_\mathbf{x}\Omega_j}{2}\right)^{1/2} \mathbf{e}(\mathbf{x} \mid j)(\hat{a}_j - \hat{a}_j^+) \tag{2.11b}$$

2.3. The Alternative Form of the Hamiltonian

If we substitute (2.11) into (2.2a), then by use of (2.3b), (2.5), and (2.6) we obtain

$$\hat{H} = \sum_{j=1}^{d} \tfrac{1}{2}\hat{P}_j^2 + \sum_{j=d+1}^{3n} \hbar\Omega_j(\tfrac{1}{2} + \hat{a}_j^+\hat{a}_j) \tag{2.12}$$

This completes the derivation of the alternative form of the Hamiltonian as given by (2.2a).

The result (2.12) shows that the Hamiltonian $\hat{H}$ of the system is compounded of two physically different parts, one of which arises from the existence of d independent eigenvectors with vanishing eigenfrequencies, and the second from the existence of oscillatory movement. Note that the first expression on the rhs of (2.12) has the form of the Hamiltonian for the free particle of unit mass located in the d-dimensional space $\mathbb{R}^d$. Since the "position–momentum" operators $(\hat{U}_j, \hat{P}_j)$ commute with the annihilation–creation operators $(\hat{a}_j, \hat{a}_j^+)$, the motion of this abstract particle can be treated separately.

In the Heisenberg picture, the state of the system is identified as the corresponding Schrödinger state at time $t=0$, and the evolution in time of the operator $\hat{A}$ acting on the Hilbert space of all quantum states is given by

$$\hat{A}(t)=\exp\left(\frac{i}{\hbar}\hat{H}t\right)\hat{A}\exp\left(-\frac{i}{\hbar}\hat{H}t\right) \tag{2.13}$$

In particular, by placing (2.12) into (2.13), we conclude that

$$\hat{U}_j(t)=\hat{U}_j+\hat{P}_j t, \qquad \hat{P}_j(t)=\hat{P}_j \tag{2.14a}$$

$$\hat{a}_j(t)=\exp(-i\Omega_j t)\,\hat{a}_j, \qquad \hat{a}_j^+(t)=\exp(i\Omega_j t)\,\hat{a}_j^+ \tag{2.14b}$$

3. DEFINITION OF THE ONE-PHONON STATES

3.1. The Schrödinger Function in the j Representation

Let $|\mathfrak{Z}_A\rangle$ and $|\mathfrak{Z}_B\rangle$ be the states used in the quantum mechanical description of the systems A and B whose Hamiltonians are given, respectively, by

$$\hat{H}_A := \sum_{j=1}^{d} \tfrac{1}{2}\hat{P}_j^2 \tag{3.1a}$$

and

$$\hat{H}_B := \sum_{j=d+1}^{3n} \hbar\Omega_j(\tfrac{1}{2}+\hat{a}_j^+\hat{a}_j) \tag{3.1b}$$

Clearly, since there is no interaction between A and B, the Hamiltonian of the composite system $A+B$ is equal to $\hat{H}_A+\hat{H}_B$. We can now choose for the state of $A+B$ the product of $|\mathfrak{Z}_A\rangle$ and $|\mathfrak{Z}_B\rangle$.

The ground state of B will be denoted by $|0_B\rangle$; this state is *unique* and obeys the *condition of stability*:

$$\hat{a}_j|0_B\rangle=0 \qquad \text{for} \quad j=d+1,\ldots,3n \tag{3.2}$$

The state $|0_B\rangle$ contains no phonon and is therefore interpreted as the *vacuum* of the theory. By far the Hilbert space most advantageous for the second quantization is the Fock space; we reserve the symbol $\mathscr{H}_B$ to denote it.

Characterizing $\mathscr{H}_B$, each state in $\mathscr{H}_B$ can be approximated as closely as we wish by a state obtained from $|0_B\rangle$ by acting on the vacuum with an appropriate polynomial in the creation operators $\hat{a}_j^+$.

Although our method accommodates every state of A, for simplicity we postulate that the "vector" $|\mathfrak{Z}_A\rangle$, *which is chosen once and for all*, obeys the following conditions:

$$\langle\mathfrak{Z}_A|\hat{U}_j|\mathfrak{Z}_A\rangle=0, \qquad j=1,\ldots,d \tag{3.3a}$$

$$\langle\mathfrak{Z}_A|\hat{P}_j|\mathfrak{Z}_A\rangle=0, \qquad j=1,\ldots,d \tag{3.3b}$$

Because the canonically conjugate operators $\hat{U}_j$ and $\hat{P}_j$ have continuous spectra ranging from minus to plus inifinity, a proof of the existence of the state $|\mathfrak{Z}_A\rangle$ satisfying (3.3) can be constructed using a slight variation of the ideas proposed, e.g., in Fong and Rowe (1968) and Bauer (1983); the $|\mathfrak{Z}_A\rangle$ is not unique, however.

Von Neumann's (1955) exposition of the principles of quantum mechanics shows that each observable on a system A or B is also one on the composite system $A+B$. Consequently, if we consider the particular state of $A+B$, namely, the state

$$|\xi\rangle:=|\mathfrak{Z}_A\rangle\otimes|0_B\rangle \tag{3.4}$$

then we easily verify that

$$\langle\xi|\hat{U}_j|\xi\rangle=0 \qquad \text{when} \quad j=1,\ldots,d \tag{3.5a}$$

$$\langle\xi|\hat{P}_j|\xi\rangle=0 \qquad \text{when} \quad j=1,\ldots,d \tag{3.5b}$$

$$\hat{a}_j|\xi\rangle=0 \qquad \text{when} \quad j=d+1,\ldots,3n \tag{3.5c}$$

Assuming that the states $|\mathfrak{Z}_A\rangle$ and $|0_B\rangle$ are normalized, we arrive at the following expression for the zero-point energy $E_0:=\langle\xi|\hat{H}|\xi\rangle$:

$$E_0=\langle\xi|\hat{H}_A|\xi\rangle+\tfrac{1}{2}\sum_{j=d+1}^{3n}\hbar\Omega_j \tag{3.6}$$

From $|\xi\rangle$ a complete space $\mathscr{H}$ of states can be obtained by successive application of the creation operators $\hat{a}_j^+$. Of course, if $|\mathfrak{H}\rangle$ lies in $\mathscr{H}$, then there exists exactly one element $|\mathfrak{H}_B\rangle$ of $\mathscr{H}_B$ such that $|\mathfrak{H}\rangle=|\mathfrak{Z}_A\rangle\otimes|\mathfrak{H}_B\rangle$. Now, let us observe that equations (3.5a) and (3.5b) are still valid when we replace $|\xi\rangle$ by $|\mathfrak{H}\rangle$ in these equations. Furthermore, by appeal to (2.10d) we see that for normalized states $|\mathfrak{H}\rangle$ the $\langle\mathfrak{H}|\hat{H}_A|\mathfrak{H}\rangle$ is equal to $\langle\xi|\hat{H}_A|\xi\rangle$. Generalizing, we may say that the replacement of $|\xi\rangle$ by $|\mathfrak{H}\rangle$ does not affect any of the expectation values of the operators represented in terms of $\hat{U}_j$ and $\hat{P}_j$ alone. Here and henceforth, *we shall call the state* $|\mathfrak{H}\rangle$ *belonging to* $\mathscr{H}$ *the phonon state.*

The most general one-phonon state is

$$|\mathfrak{Z}\rangle := \sum_{j=d+1}^{3n} \mathfrak{Z}_j \hat{a}_j^+ |\xi\rangle \tag{3.7a}$$

where

$$\sum_{j=d+1}^{3n} |\mathfrak{Z}_j|^2 = 1 \tag{3.7b}$$

It will be convenient to use the symbol $\mathscr{H}^{(1)}$ to signify the Hilbert space spanned by the one-phonon states. We shall refer to $\mathfrak{Z}_j$ as the Schrödinger function of the phonon in the j representation; generally, the $\mathfrak{Z}_j$ is complex.

3.2. Transition to a Space Description of Phonons

We can now transform to the $\mathbf{x}$ representation by introducing the function

$$\mathfrak{Z}_\alpha(\mathbf{x}) := \sum_{j=d+1}^{3n} \mathfrak{Z}_j e_\alpha(\mathbf{x} \mid j) \tag{3.8}$$

which defines the position-space Schrödinger function belonging to $\mathfrak{Z}_j$. Directly from (3.8) and (2.3b) we find that $\mathfrak{Z}_\alpha(\mathbf{x})$, $\alpha = 1, 2, 3$, are complex-valued fields subject to the *constraints*

$$\sum_{\alpha,\mathbf{x}} e_\alpha(\mathbf{x} \mid j)\mathfrak{Z}_\alpha(\mathbf{x}) = 0, \qquad j = 1, \ldots, d \tag{3.9}$$

In view of (2.3) it is straightforward to facilitate conversions between $\mathfrak{Z}_j$ and $\mathfrak{Z}_\alpha(\mathbf{x})$:

$$\mathfrak{Z}_j = \sum_{\alpha,\mathbf{x}} e_\alpha(\mathbf{x} \mid j)\mathfrak{Z}_\alpha(\mathbf{x}), \qquad j = d+1, \ldots, 3n \tag{3.10}$$

By substituting (3.10) into (3.7a), we arrive at

$$|\mathfrak{Z}\rangle = \sum_{\alpha,\mathbf{x}} \mathfrak{Z}_\alpha(\mathbf{x}) \hat{Y}_\alpha^+(\mathbf{x}) |\xi\rangle \tag{3.11a}$$

where

$$\hat{Y}_\alpha(\mathbf{x}) := \sum_{j=d+1}^{3n} e_\alpha(\mathbf{x} \mid j)\hat{a}_j \tag{3.11b}$$

In order to underline the formal similarities between the present theory and the theory of Mandel (1964, 1966), we shall call $\hat{Y}_\alpha(\mathbf{x})$ the *detection operator.*

It can easily be shown that if $|\mathfrak{Z}\rangle$ and $|\mathfrak{Q}\rangle$ are members of $\mathscr{H}^{(1)}$, then

$$\langle \mathfrak{Z} | \mathfrak{Q} \rangle = \sum_{j=d+1}^{3n} \mathfrak{Z}_j^* \mathfrak{Q}_j = \sum_{\alpha,\mathbf{x}} \mathfrak{Z}_\alpha^*(\mathbf{x}) \mathfrak{Q}_\alpha(\mathbf{x}) \tag{3.12}$$

Let $\mathbb{L}^2$ be a Hilbert space of complex-valued, three-component functions on D with the inner product given by the third expression in (3.12), and define the closed subspace L^2 of $\mathbb{L}^2$ by saying that its elements satisfy the constraints (3.9). Introduce a mapping on L^2 with range $\mathscr{H}^{(1)}$ by letting the three-component function $\mathfrak{Z}_\alpha(\mathbf{x})$ have image $|\mathfrak{Z}\rangle \in \mathscr{H}^{(1)}$, where $|\mathfrak{Z}\rangle$ is obtained from $\mathfrak{Z}_\alpha(\mathbf{x})$ by putting (3.10) into (3.7a). The mapping is clearly linear, and (3.12) ensures that the mapping is one-to-one. Also, it is obvious that each vector $|\mathfrak{Z}\rangle \in \mathscr{H}^{(1)}$ is the image of some member of L^2. In summary, the mapping is a one-to-one linear norm-preserving mapping of L^2 onto $\mathscr{H}^{(1)}$.

The above facts help to explain why it is not possible, in the particular but conceptually important case when there exist normal modes of zero frequency ($d \neq 0$), to leave out the constraints (3.9) in the definition of the position-space Schrödinger function. Also, we conclude that the function $\mathfrak{Z}_\alpha(\mathbf{x}) = \delta_{\alpha,\beta}\delta_{\mathbf{x},\mathbf{x}'}$ is a Schrödinger function (for the description of a phonon in the fully localized state) if and only if $d=0$.

4. THE GENERALIZED SYSTEM OF IMPRIMITIVITIES

4.1. The Projection Operators $\hat{E}(\Delta)$ for a Strongly Localizable Phonon

As explained in the Introduction, the notion of localizability for a phonon can be formulated in terms of projection operators $\hat{E}(\Delta)$ acting on $\mathscr{H}^{(1)}$, where Δ is an arbitrary subset of D at a given time t. The projection operator $\hat{E}(\Delta)$ corresponds to a property of the phonon, the property of being localized in Δ. Precisely speaking, if $|\mathfrak{Z}\rangle$ denotes a normalized one-phonon state, then the expectation value of $\hat{E}(\Delta)$, i.e., $\langle \mathfrak{Z} | \hat{E}(\Delta) | \mathfrak{Z} \rangle$, is the probability that the phonon belongs to the atoms whose equilibrium or average positions are characterized by the elements of Δ. [In view of (2.10c), (2.10d), and (2.14a) one can see that assuming only that $\langle \xi | \hat{U}_j(t) | \xi \rangle$ and $\langle \xi | \hat{P}_j(t) | \xi \rangle$ vanish initially is enough to guarantee the fulfilment of the relations $\langle \mathfrak{Z} | \hat{U}_j(t) | \mathfrak{Z} \rangle = 0$ and $\langle \mathfrak{Z} | \hat{P}_j(t) | \mathfrak{Z} \rangle = 0$ for all $t>0$ and all $|\mathfrak{Z}\rangle \in \mathscr{H}^{(1)}$.]

We first consider the case in which the normal modes of zero frequency fail to exist ($d=0$). For $d=0$, since the $\mathfrak{Z}_\alpha(\mathbf{x})$ are not subject to the constraints (3.9), the projection operators $\hat{E}(\Delta)$ take the form

$$\hat{E}(\Delta)|\mathfrak{Z}\rangle := \sum_{\alpha,\mathbf{x}} \chi_\Delta(\mathbf{x}) \mathfrak{Z}_\alpha(\mathbf{x}) \hat{Y}_\alpha^+(\mathbf{x}) |\xi\rangle \tag{4.1a}$$

where $\chi_\Delta(\mathbf{x})=1$ if $\mathbf{x}\in\Delta$, and 0 if $\mathbf{x}\in D\backslash\Delta$. Alternatively, we may regard $\hat{E}(\Delta)$ as being the linear mapping of $\mathbb{L}^2$ into itself ($\mathbb{L}^2=L^2$) and thus write

$$[\hat{E}(\Delta)\mathfrak{Z}](\mathbf{x})=\chi_\Delta(\mathbf{x})\mathfrak{Z}(\mathbf{x}) \tag{4.1b}$$

Because of (4.1), we can identify localizability with the existence of a real-valued, positive function $\sum_\alpha |\mathfrak{Z}_\alpha(\mathbf{x})|^2$ on D such that

$$\langle\mathfrak{Z}|\hat{E}(\Delta)|\mathfrak{Z}\rangle=\sum_{\mathbf{x}\in\Delta}\left[\sum_\alpha |\mathfrak{Z}_\alpha(\mathbf{x})|^2\right] \tag{4.2}$$

when $\Delta\subset D$ and $|\mathfrak{Z}\rangle\in\mathscr{H}^{(1)}$. Also, from (4.1) it is not difficult to conclude that all of the $\hat{E}(\Delta)$ commute with one another.

As is by now well known (Wightman, 1962; Jauch and Piron, 1967; Amrein, 1969), one can think of the requirement that the identity (4.2) exists as a precise way of stating that the position operator

$$\hat{\mathbf{x}}:=\sum_{\mathbf{x}}\mathbf{x}[\hat{\mathbf{Y}}^+(\mathbf{x})\circ\hat{\mathbf{Y}}(\mathbf{x})] \tag{4.3}$$

for a single phonon exists (Jensen, 1964; Jensen and Nielsen, 1969) and that its components $\hat{x}_\alpha$ are simultaneously observables. Consequently, we can say that the definition (4.1a) relates to the phonon which is localizable in the ordinary sense (strongly localizable) (Wightman, 1962).

Equation (4.1a) is valid for a given (but otherwise arbitrary) time. Of course, the projection operator $\hat{E}_t(\Delta)$ for $t>0$ is associated with the projection operator $\hat{E}_0(\Delta)$ for $t=0$ by

$$\hat{E}_t(\Delta)=\exp\left(\frac{i}{\hbar}\hat{H}_Bt\right)\hat{E}_0(\Delta)\exp\left(-\frac{i}{\hbar}\hat{H}_Bt\right) \tag{4.4}$$

A systematic analysis of the properties of strongly localizable phonons can be found in the paper by Jensen and Nielsen (1969). If $d=0$, their approach explains in what sense it is true that, to study the notion of localizability for phonons, it is not necessary to use the concepts beyond those already appearing in the treatment of ordinary particles, i.e., classical particles of positive mass.

4.2. The Projection Operators $\hat{E}(\Delta)$ for a Weakly Localizable Phonon

Let us glance back now at the case in which one or more eigenfrequencies are zero ($d\neq 0$). In analogy with the discussion in Subsection 4.1, our purpose here is to show how the projection operators $\hat{E}(\Delta)$ for $d\neq 0$ should in fact be chosen. At first sight, it is tempting to try to characterize these operators by (4.1). Why does this not describe the phonon as a localizable system? The answer is that the $\hat{E}(\Delta)$ carry vectors obeying the constraints

(3.9) into vectors which do not obey them, so $\hat{E}(\Delta)$ is not a well-defined operator in the manifold of states, and, just as in the case of photons (Wightman, 1962; Jauch and Piron, 1967; Amrein, 1969), the conventional approach based upon (4.1b) by no means suffices to provide a precise tool for the analysis of localizability.

So as to be able to arrive at the projection operators $\hat{E}(\Delta)$ acting on a proper subspace L^2 of $\mathbb{L}^2$, by use of linear combinations of $\mathbf{e}(\circ \mid j)$, $1 \leq j \leq d$, we first introduce for each $\Delta \subset D$ a set of real vectors $\mathbf{e}^\Delta(\mathbf{x} \mid p)$, $\mathbf{x} \in D$, such that if p and p' are integers running from 1 to d_Δ ($d_\Delta \leq d$), then

$$\sum_{\mathbf{x} \in \Delta} \mathbf{e}^\Delta(\mathbf{x} \mid p) \circ \mathbf{e}^\Delta(\mathbf{x} \mid p') = \delta_{p,p'} \tag{4.5}$$

1. As a step toward constructing[4] $\mathbf{e}^\Delta(\mathbf{x} \mid p)$, let $\mathbf{e}(\circ \mid j)_{\mid \Delta}$, $1 \leq j \leq d$, denote the restriction of $\mathbf{e}(\circ \mid j)$, $1 \leq j \leq d$, to Δ, and consider the set of *linearly independent* three-component functions $\{\mathbf{e}(\circ \mid j_p)_{\mid \Delta}; p \in \Gamma_\Delta\}$, $\Gamma_\Delta := \{1, 2, \ldots, d_\Delta\}$, such that $d_\Delta \leq d$, $j_p \in \{1, 2, \ldots, d\}$, and every function $\mathbf{e}(\circ \mid j)_{\mid \Delta}$, $1 \leq j \leq d$, can be written as a linear combination of $\mathbf{e}(\circ \mid j_p)_{\mid \Delta}$, $p \in \Gamma_\Delta$. In view of these statements, we easily conclude that the functions $\mathbf{e}(\circ \mid j_p)_{\mid \Delta}$ exist and that if n_Δ signifies the number of elements in Δ, then the following conditions are automatically satisfied:

$$d_\Delta \leq \min(d, 3n_\Delta) \tag{4.6a}$$

$$d_D = d, \qquad \Gamma_D = \{1, 2, \ldots, d\} \tag{4.6b}$$

We now want to say that, although the choice of the subset $\{\mathbf{e}(\circ \mid j_p)_{\mid \Delta}; p \in \Gamma_\Delta\}$ of the set $\{\mathbf{e}(\circ \mid j)_{\mid \Delta}; j \in \Gamma_D\}$ is not in general unique, the number d_Δ depends only on Δ.

2. The next stage in the derivation of $\mathbf{e}^\Delta(\mathbf{x} \mid p)$ is to obtain the relations

$$\mathbf{e}^\Delta(\circ \mid p) = \sum_{p'=1}^{p} c^\Delta_{p,p'} \mathbf{e}(\circ \mid j_{p'})_{\mid \Delta}, \qquad p \in \Gamma_\Delta \tag{4.7}$$

in which the real numbers $c^\Delta_{p,p'}$, $c^\Delta_{p,p} > 0$, are uniquely determined by substituting (4.7) into (4.5) and then solving the resulting system of equations with respect to $c^\Delta_{p,p'}$. This is a standard procedure of orthogonalization (Sansone, 1959; Szegö, 1939).

3. Finally, after calculating $c^\Delta_{p,p'}$ and replacing $\mathbf{e}(\circ \mid j_{p'})_{\mid \Delta}$ by $\mathbf{e}(\circ \mid j_{p'})$ in equation (4.7), we can regard $\mathbf{e}^\Delta(\circ \mid p)$, $p \in \Gamma_\Delta$, as being a three-component

[4]The reader who is not interested in the details regarding the construction of $\mathbf{e}^\Delta(\mathbf{x} \mid p)$ may omit points 1–3. For the definition of $\hat{E}(\Delta)$ in terms of $\mathbf{e}^\Delta(\mathbf{x} \mid p)$ see equations (4.9a) and (4.9b).

function on D. Clearly, using (4.6b) and (2.3b), we find that

$$\mathbf{e}^{D}(\circ \mid p) = \mathbf{e}(\circ \mid p), \qquad p = 1, 2, \ldots, d \tag{4.8}$$

This observation completes our description of the construction of $\mathbf{e}^{\Delta}(\circ \mid p)$, $p \in \Gamma_{\Delta}$.

In the problem of localizability considered here, the projection operators $\hat{E}(\Delta)$ acting on $\mathscr{H}^{(1)}$ take the form

$$\hat{E}(\Delta) \mid \mathfrak{Z} \rangle := \sum_{\alpha, \mathbf{x}} \chi_{\Delta}(\mathbf{x}) \mathfrak{Z}_{\alpha}(\mathbf{x}; \Delta) \hat{Y}_{\alpha}^{+}(\mathbf{x}) \mid \xi \rangle \tag{4.9a}$$

where

$$\mathfrak{Z}_{\alpha}(\mathbf{x}; \Delta) := \mathfrak{Z}_{\alpha}(\mathbf{x}) - \sum_{p \in \Gamma_{\Delta}} \sum_{\mathbf{x}' \in \Delta} [\mathbf{e}^{\Delta}(\mathbf{x}' \mid p) \circ \mathfrak{Z}(\mathbf{x}')] e_{\alpha}^{\Delta}(\mathbf{x} \mid p) \tag{4.9b}$$

Directly from (4.9b) and (4.5) we can prove that

$$\sum_{\alpha} \sum_{\mathbf{x} \in \Delta} e_{\alpha}^{\Delta}(\mathbf{x} \mid p) \mathfrak{Z}_{\alpha}(\mathbf{x}; \Delta) = 0, \qquad p \in \Gamma_{\Delta} = \{1, 2, \ldots, d_{\Delta}\} \tag{4.10a}$$

$$\sum_{\alpha} \sum_{\mathbf{x} \in \Delta} e_{\alpha}(\mathbf{x} \mid j) \mathfrak{Z}_{\alpha}(\mathbf{x}; \Delta) = 0, \qquad j \in \Gamma_{D} = \{1, 2, \ldots, d\} \tag{4.10b}$$

Equation (4.10b) is a consequence of (4.10a), because our method of obtaining $\mathbf{e}^{\Delta}(\circ | p)$ delivers the three-component function $\mathbf{e}(\circ | j)_{|\Delta}, j \in \Gamma_D$ as an exhibited linear combination of $\mathbf{e}^{\Delta}(\circ \mid p)_{|\Delta}, p \in \Gamma_{\Delta}$. Further, while the procedure we have used in arriving at $\hat{E}(\Delta)$ is based upon a particular choice of the set $\{\mathbf{e}^{\Delta}(\circ \mid p); p \in \Gamma_{\Delta}\}$ obeying (4.5), the expression on the rhs of (4.9a) is completely independent of it, as elementary inspection shows.

Now, looking back at the properties of $\mathfrak{Z}_{\alpha}(\mathbf{x}; \Delta)$, we see that the projection operators $\hat{E}(\Delta)$ as given by (4.9) carry "vectors" $|\mathfrak{Z}\rangle$ satisfying the constraints (3.9) into "vectors" $\hat{E}(\Delta) | \mathfrak{Z} \rangle$ which also satisfy them, so $\hat{E}(\Delta)$ is now a well-defined projection operator in the manifold L^2 of one-phonon states ($L^2 \subset \mathbb{L}^2$, $L^2 \neq \mathbb{L}^2$); some traditional aspects of the theory of localizable systems, however, are lost in the process. Indeed, in the important case for which $d \neq 0$, one has instead of (4.2) a weaker relation, namely

$$\langle \mathfrak{Z} | \hat{E}(\Delta) | \mathfrak{Z} \rangle \leq \sum_{\mathbf{x} \in \Delta} \left(\sum_{\alpha} |\mathfrak{Z}_{\alpha}(\mathbf{x})|^2 \right) \tag{4.11}$$

Equality holds if and only if $\hat{E}(\Delta) | \mathfrak{Z} \rangle = | \mathfrak{Z} \rangle$. Consequently, the probability that the "event" corresponding to $\hat{E}(\Delta)$ will occur when the system is prepared in the normalized state $|\mathfrak{Z}\rangle \in \mathscr{H}^{(1)}$ cannot in general be identified with the simple expression[5] on the rhs of (4.11). We may understand this

[5]We remark once more that the expression on the lhs of (4.11) is the probability that the phonon belongs to the atoms whose equilibrium or average positions are characterized by the elements of Δ.

immediately by observing that here the projection operator $\hat{E}(\Delta)$ is not simply multiplication by the characteristic function $\chi_\Delta(\circ)$ of the set Δ. [For comparison, see equation (4.1b).]

We also mention that $\hat{E}(\Delta_1 \cap \Delta_2)=\hat{E}(\Delta_1)\hat{E}(\Delta_2)=\hat{E}(\Delta_2)\hat{E}(\Delta_1)$ if the sets Δ_1 and Δ_2 are disjoint or one of them is a subset of the other. At the same time, from (4.9) it follows that the operators $\hat{E}(\Delta_1)$ and $\hat{E}(\Delta_2)$ do not commute when Δ_1 and Δ_2 overlap. Since the property of $\hat{E}(\Delta)$ just mentioned resembles quite closely a result first established by Jauch and Piron (1967) and Amrein (1969) in the context of the theory of relativistic particles of mass zero, we shall adapt the original terminology of Jauch, Piron, and Amrein and say that the proposition (4.9) describes the phonon as a weakly localizable system.

One final word regarding $\hat{E}(\Delta)$. If one considers a subset Δ of the set D such that[6] $3n_\Delta \le d$ and $d_\Delta = 3n_\Delta$, then the "probability of finding the phonon in" Δ is equal to zero. This somewhat surprising fact, which is of interest when one or more eigenfrequencies are zero, does not describe of course any universal property of $\hat{E}(\Delta)$; rather, it reflects merely the particular choice of Δ in terms of which we decided at the outset to represent $\hat{E}(\Delta)$.

The general properties of $\hat{E}(\Delta)$ are summarized in Section 4.4.

4.3. The Unitary Representation of the Group $\mathbb{G}$ of Three-Dimensional Rotations

Let us take the origin of coordinates at the center of mass, and consider a situation in which the whole system has a symmetry, i.e., let there be a group $\mathbb{G}$ of three-dimensional rotations R transforming the equilibrium configuration of a system of n atoms into itself.

We wish to investigate the effect of $R \in \mathbb{G}$ on $|\mathfrak{Z}\rangle \in \mathscr{H}^{(1)}$. Therefore, for each $R \in \mathbb{G}$ we introduce the linear mapping $\hat{\mathfrak{g}}(R)\colon \mathscr{H}^{(1)} \Rightarrow \mathscr{H}^{(1)}$ defined by

$$\hat{\mathfrak{g}}(R)\,|\mathfrak{Z}\rangle := \sum_{\mathbf{x}} [R\mathfrak{Z}(R^{-1}\mathbf{x})] \circ \hat{\mathbf{Y}}^{+}(\mathbf{x})\,|\xi\rangle = \sum_{j=d+1}^{3n} \mathfrak{Z}_{j,R}\hat{a}_j^{+}\,|\xi\rangle \tag{4.12a}$$

where

$$\mathfrak{Z}_{j,R} := \sum_{j'=d+1}^{3n} \mathscr{B}_R(j,j')\mathfrak{Z}_{j'} \tag{4.12b}$$

$$\mathscr{B}_R(j,j') := \sum_{\mathbf{x}} \mathbf{e}(\mathbf{x}\,|\,j) \circ [R\mathbf{e}(R^{-1}\mathbf{x}\,|\,j')] \tag{4.12c}$$

[6] We recall that d_Δ signifies the number of three-component functions $\mathbf{e}^\Delta(\circ\,|\,p)$, $p=1,2,\ldots,d_\Delta$ $(d_\Delta \le d)$, satisfying (4.5) and n_Δ represents the number of elements in Δ.

In order to be sure that $\sum_\beta R_{\alpha,\beta}\mathfrak{Z}_\beta(R^{-1}\mathbf{x})$ satisfies the constraints (3.9) when $\mathfrak{Z}_\alpha(\mathbf{x})$ does, it is sufficient to establish the following property of $\mathscr{B}_R(j,j')$, $j,j'=1,2,\ldots,3n$:

Third Orthogonality Rule. If $j\neq j'$ and $\Omega_j\neq\Omega_{j'}$, then

$$\mathscr{B}_R(j,j')=0 \tag{4.13}$$

Proof. If we multiply each side of (2.5) by $e_{\beta''}(\mathbf{x}''\mid j)$ and then sum with respect to j, in view of (2.3a) we find that

$$K_{\alpha,\beta}(\mathbf{x},\mathbf{x}')=\sum_{j=1}^{3n}\Omega_j^2 e_\alpha(\mathbf{x}\mid j)e_\beta(\mathbf{x}'\mid j) \tag{4.14}$$

We may now put (4.14) into[7]

$$\sum_{\alpha'} R_{\alpha,\alpha'}K_{\alpha',\beta}(R^{-1}\mathbf{x},R^{-1}\mathbf{x}')=\sum_{\beta'}K_{\alpha,\beta'}(\mathbf{x},\mathbf{x}')R_{\beta',\beta} \tag{4.15}$$

then multiply both sides of (4.15) by $e_\alpha(\mathbf{x}\mid j)e_\beta(R^{-1}\mathbf{x}'\mid j')$, then sum the result with respect to $(\alpha,\beta,\mathbf{x},\mathbf{x}')$, then make use of (2.3b). Thus we obtain

$$(\Omega_j^2-\Omega_{j'}^2)\mathscr{B}_R(j,j')=0 \tag{4.16}$$

and so $\mathscr{B}_R(j,j')=0$ when $j\neq j'$ and $\Omega_j\neq\Omega_{j'}$. ■

We say that $\hat{\mathfrak{g}}(R)$, $R\in\mathbb{G}$, is the operator whose application to $|\mathfrak{Z}\rangle\in\mathscr{H}^{(1)}$ yields the one-phonon state $\hat{\mathfrak{g}}(R)|\mathfrak{Z}\rangle$ rotated by R. Now, directly from (4.12a) and (3.12) we conclude that $R\Rightarrow\hat{\mathfrak{g}}(R)$ is the unitary representation of $\mathbb{G}$ in $\mathscr{H}^{(1)}$.

Next, we should remark that if $R\in\mathbb{G}$, then there is a Hermitian operator $\hat{\Theta}(R)$ corresponding to R such that $\hat{\Theta}(R)|\xi\rangle=0$ and

$$\hat{\mathfrak{g}}(R)=\exp[-i\hat{\Theta}(R)] \tag{4.17}$$

The actual calculation of $\hat{\Theta}(R)$ rests heavily, indeed essentially, on the ideas proposed in Jensen and Nielsen (1969). Without going into any of the details of the derivation, which can easily be reconstructed from the original sources, here we only note that $\hat{\Theta}(R)$ is a linear-combination of $\hat{a}_j^+\hat{a}_{j'}$, $j,j'=d+1,\ldots,3n$:

$$\hat{\Theta}(R)=\sum_{j=d+1}^{3n}\sum_{j'=d+1}^{3n}\vartheta_{j,j'}(R)\hat{a}_j^+\hat{a}_{j'} \tag{4.18a}$$

$$\vartheta_{j,j'}^*(R)=\vartheta_{j',j}(R) \tag{4.18b}$$

[7]One can easily show that $\mathbf{K}(R\mathbf{x},R\mathbf{x}')=R\mathbf{K}(\mathbf{x},\mathbf{x}')R^{-1}$ for any $R\in\mathbb{G}$; see, e.g., the book by Lax (1974, p. 326).

Clearly, given (4.17) and (4.18), one will be justified in interpreting $\hat{\mathfrak{g}}(R)$ not only as a linear operator on $\mathscr{H}^{(1)}$, but also as a linear mapping of the Hilbert space $\mathscr{H}$ onto itself. (Concerning the precise definition of $\mathscr{H}$, see Section 3.1.) Moreover, because of the results of Jensen and Nielsen (1969), we have

$$R\hat{\mathbf{Y}}(R^{-1}\mathbf{x}) = \exp[i\hat{\Theta}(R)]\ \hat{\mathbf{Y}}(\mathbf{x})\ \exp[-i\hat{\Theta}(R)] \qquad (4.19a)$$

$$\hat{a}_{j,R} = \exp[i\hat{\Theta}(R)]\ \hat{a}_j\ \exp[-i\hat{\Theta}(R)] \qquad (4.19b)$$

where

$$\hat{a}_{j,R} := \sum_{j'=d+1}^{3n} \mathscr{B}_R(j, j')\hat{a}_{j'} \qquad (4.19c)$$

Some additional properties of the unitary representation $R \Rightarrow \hat{\mathfrak{g}}(R)$ of $\mathbb{G}$ in $\mathscr{H}$ are discussed in the Appendix.

4.4. The General Properties of Projection Operators $\hat{E}(\Delta)$

The idea of introducing $\hat{E}(\Delta)$, instead of trying to consider the set of states localized at a point (Newton and Wigner, 1949), was strongly advocated by Wightman (1962), Jauch and Piron (1967), and Amrein (1969), and it might be worthwhile to reproduce here their concise postulates. However, before we can formulate these postulates, we need some additional information about our notation.

The symbol $\varnothing$ will signify the empty subset of D. Let $R\Delta$ denote the set obtained from Δ by carrying out the rotation R. Suppose that $\hat{\mathbb{P}}_1$ and $\hat{\mathbb{P}}_2$ are projection operators acting on $\mathscr{H}^{(1)}$. The intersection of $\hat{\mathbb{P}}_1$ and $\hat{\mathbb{P}}_2$, denoted by $\hat{\mathbb{P}}_1 \cap \hat{\mathbb{P}}_2$, is defined as the projection of $\mathscr{H}^{(1)}$ onto the largest subspace contained in the ranges of both $\hat{\mathbb{P}}_1$ and $\hat{\mathbb{P}}_2$. If the ranges of $\hat{\mathbb{P}}_1$ and $\hat{\mathbb{P}}_2$ are two orthogonal subspaces of $\mathscr{H}^{(1)}$, we shall write $\hat{\mathbb{P}}_1 \perp \hat{\mathbb{P}}_2$. The projection operators on $\mathscr{H}^{(1)}$ with ranges $\varnothing$ and $\mathscr{H}^{(1)}$ will be denoted, respectively, $\hat{0}$ and $\hat{I}$.

With this notation in mind, the Jauch–Piron axioms for localizability in a "region" are as follows:

I. The following conditions hold:

$$\hat{E}(\varnothing) = \hat{0}, \qquad \hat{E}(D) = \hat{I} \qquad (4.20a)$$

II. If Δ_1 and Δ_2 are disjoint subsets of D, then

$$\hat{E}(\Delta_1) \perp \hat{E}(\Delta_2) \qquad (4.20b)$$

III. For any pair Δ_1, Δ_2 of subsets of D,

$$\hat{E}(\Delta_1 \cap \Delta_2) = \hat{E}(\Delta_1) \cap \hat{E}(\Delta_2) \qquad (4.20c)$$

IV. The following condition holds:

$$\hat{E}(R\Delta)\hat{\mathrm{g}}(R)=\hat{\mathrm{g}}(R)\hat{E}(\Delta) \tag{4.20d}$$

The physical significance of these axioms is as follows: Axiom I says that the system has probability 0 of being localized in $\varnothing$ and probability 1 of being somewhere; II states that the properties corresponding to $\hat{E}(\Delta_1)$ and $\hat{E}(\Delta_2)$ are simultaneously decidable for disjoint subsets Δ_1, Δ_2 of D; III expresses the fact that a system which is in both Δ_1 and Δ_2 is also in $\Delta_1 \cap \Delta_2$; IV implies that if $|\mathfrak{Z}\rangle \in \mathscr{H}^{(1)}$ is a state in which the system is localized in Δ, then $\mathrm{g}(R)|\mathfrak{Z}\rangle \in \mathscr{H}^{(1)}$ is a state in which the system is localized in $R\Delta$.

In the terminology of Jauch, Piron, and Amrein, Axioms I–IV state that the set of projection operators $\{\hat{E}(\Delta); \Delta \subset D\}$ is a *generalized system of imprimitivities* for the representation $R \Rightarrow \hat{\mathrm{g}}(R)$ of $\mathbb{G}$ with *base D*. In addition, we say that the above set of projection operators defines an *ordinary system of imprimitivities* if Axiom III can be replaced by the following.

III′. The following condition holds:

$$\hat{E}(\Delta_1 \cap \Delta_2)=\hat{E}(\Delta_1)\hat{E}(\Delta_2) \tag{4.20c′}$$

Now, it is not difficult to verify that the operators $\hat{E}(\Delta)$ as given by (4.9) satisfy I–IV. Consequently, for the phonon which is only weakly localizable, the resulting mathematical object is a generalized system of imprimitivities. Similarly, it is easy to show from (4.1) that, in the case of a strongly localizable phonon, one obtains the projection operators $\hat{E}(\Delta)$ obeying I, II, III′, and IV; the resulting structure is then an ordinary system of imprimitivities.

Our analysis here is not complete, of course, and for a general discussion of problems concerning the notion of imprimitivity see the detailed studies by Mackey (1953, 1958), Wightman (1962), Jauch and Piron (1967), and Amrein (1969).

5. EXAMPLES OF NORMAL MODES OF ZERO FREQUENCY

"It is well known that each motion of the system in which the center of [mass] remains stationary can be built up of normal modes. To bring into consideration *all* possible motions, displacements of the center of mass along the three coordinate axes and rotations about these axes must be included. (We assume that the points are not all collinear.) These displacements may be considered normal modes of zero frequency." This is the original statement of Wigner as translated by Knox and Gold (1964, p. 174).

Thus, following Wigner, let us assume now that, in an inertial frame of reference, the potential energy

$$V := \frac{1}{2} \sum_{\mathbf{x},\mathbf{x}'} \mathbf{\Phi}(\mathbf{x}, \mathbf{x}') \circ [\mathbf{U}(\mathbf{x}) \otimes \mathbf{U}(\mathbf{x}')] \tag{5.1}$$

is invariant under the (infinitesimal) translations and rotations of a system of n atoms (no external interactions). This leads to the specific symmetry properties of the force constant matrix $[\mathbf{\Phi}]$ (Madelung, 1978, p. 131):

$$\sum_{\mathbf{x}'} \Phi_{\alpha,\beta}(\mathbf{x}, \mathbf{x}') = 0 \tag{5.2a}$$

$$\sum_{\mathbf{x}'} \Phi_{\alpha,\beta}(\mathbf{x}, \mathbf{x}') x'_\gamma = \sum_{\mathbf{x}'} \Phi_{\alpha,\gamma}(\mathbf{x}, \mathbf{x}') x'_\beta \tag{5.2b}$$

Using (5.2), examination of the eigenvalue problem [cf. equation (2.5)] shows that there are six normal modes of zero frequency ($d = 6$). The eigenvectors corresponding to these modes are given by

$$e_\alpha(\mathbf{x} \mid j) = (m_\mathbf{x} M^{-1})^{1/2} e_\alpha(j), \qquad j = 1, 2, 3 \tag{5.3a}$$

$$e_\alpha(\mathbf{x} \mid j) = (m_\mathbf{x})^{1/2} \sum_\beta \varepsilon_{\alpha,\beta}(j) x_\beta, \qquad j = 4, 5, 6 \tag{5.3b}$$

where

$$M := \sum_\mathbf{x} m_\mathbf{x} \tag{5.3c}$$

$$\mathbf{e}(j) \circ \mathbf{e}(j') = \delta_{j,j'}, \qquad \varepsilon_{\alpha,\beta}(j) = -\varepsilon_{\beta,\alpha}(j) \tag{5.3d}$$

Remembering that the origin of coordinates is taken at the center of mass,

$$\sum_\mathbf{x} m_\mathbf{x} x_\alpha = 0, \qquad \alpha = 1, 2, 3 \tag{5.4}$$

we can easily prove that the orthonormality rule (2.3b) holds if $j = 1, 2, 3$ and $j' = 4, 5, 6$. In order to obtain the orthonormality rule (2.3b) for $j = 4, 5, 6$ and $j' = 4, 5, 6$, we must calculate $\varepsilon_{\alpha,\beta}(j)$ in (5.3b) by applying with respect to $\mathbf{e}(\mathbf{x} \mid j), j = 4, 5, 6$, a standard procedure called the Gram–Schmidt orthogonalization procedure (Szegö, 1939; Sansone, 1959). From (5.3d) it follows that conditions (2.3b) are automatically satisfied when $j, j' = 1, 2, 3$.

Let us consider a subset Δ of D such that $n_\Delta = 1$ or $n_\Delta = 2$. (We remark once more that n_Δ denotes the number of elements in Δ.) We know already that $\hat{E}(\Delta) = \hat{0}$ whenever $d_\Delta = 3n_\Delta$. Since in the present case $d_\Delta = 3$ if $n_\Delta = 1$ and $d_\Delta = 6 = d$ if $n_\Delta \geq 2$, we immediately conclude that the expectation value of $\hat{E}(\Delta)$ is equal to zero for every subset Δ of D obeying $n_\Delta = 1$ or $n_\Delta = 2$. These properties of $\hat{E}(\Delta)$ cast some light on the important *conceptual* difference between the strongly localizable phonon ($d = 0$) and the one which is only weakly localizable ($d \neq 0$). Indeed, for strongly localizable phonons we may easily show that $\hat{E}(\Delta) \neq \hat{0}$ if $\Delta \neq \varnothing$ and that for every Δ satisfying $n_\Delta = 1$ or $n_\Delta = 2$ there exists the normalized one-phonon state $|\mathcal{3}\rangle$ such that $\langle \mathcal{3} | \hat{E}(\Delta) | \mathcal{3} \rangle = 1$. At the same time, we are aware of the fact that all the differences between the results corresponding, respectively, to $d=0$ and $d \neq 0$ vanish asymptotically for large values of n_Δ and that if $n_\Delta \gg 1$, then the two formalisms can be used interchangeably. Therefore, just as in the case of photons (Amrein, 1969, esp. comments on p. 187), for many practical purposes one may employ the approximate but simple operator (4.1a).

6. FINAL REMARKS

As noted in the Introduction, the systematic construction of $\hat{E}(\Delta)$ enables us (Banach and Piekarski, 1993) to obtain the operator $\hat{N}(\Delta)$ corresponding to the number of phonons "localized in" Δ. In addition to these considerations, given the explicit expression for $\hat{N}(\Delta)$, it would also be of both conceptual and practical interest to introduce phase space operators, actually quantum pseudofields in phase space, which are compatible with the definition of $\hat{N}(\Delta)$ and which have the property that their expectation values are phonon analogues of the Wigner distribution functions (Wigner, 1932; Klimontovich, 1975). These operators could then be applied in a number of investigations, especially in studies concerning the quantum theory of transport phenomena.

Consequently, in a companion paper (Banach and Piekarski, 1993) our attention in large part focuses upon such questions as how one might formulate exactly an adequate notion of the Wigner distribution function in terms of which to characterize the evolution in time of the phonon system.

Finally, we mention that the Jauch–Piron system of imprimitivities can be used as an organizing principle for the development of the theory dealing with relativistic particles; for example, considering a gas of photons, one can define the one-particle Wigner distribution function which is consistent with the exact expression for the number-of-photons operator first obtained by Amrein (1969).

APPENDIX: THE TRANSFORMATION LAW FOR $\hat{U}(x)$ AND $\hat{P}(x)$

The operator $\hat{g}(R) = \exp[-i\hat{\Theta}(R)]$ acting on $\mathscr{H}$ has one more property[8] that is very important. Namely, if we make use of (2.11), (3.3), (4.19b), and

[8]The operator $\hat{g}(R)$ is introduced in Section 4.3.

(4.19c), we find that

$$\langle \mathfrak{H}|\ \exp[i\hat{\Theta}(R)]\ \hat{\mathbf{U}}(\mathbf{x})\ \exp[-i\hat{\Theta}(R)]\,|\mathfrak{H}\rangle = R\langle \mathfrak{H}\,|\,\hat{\mathbf{U}}(R^{-1}\mathbf{x})\,|\,\mathfrak{H}\rangle \quad \text{(A.1a)}$$

$$\langle \mathfrak{H}|\ \exp[i\hat{\Theta}(R)]\ \hat{\mathbf{P}}(\mathbf{x})\ \exp[-i\hat{\Theta}(R)]\,|\mathfrak{H}\rangle = R\langle \mathfrak{H}\,|\,\hat{\mathbf{P}}(R^{-1}\mathbf{x})\,|\,\mathfrak{H}\rangle \quad \text{(A.1b)}$$

where $|\mathfrak{H}\rangle$ is a member of $\mathscr{H}$. That such is indeed the case may be verified by direct if lengthy calculation. For completeness sake, we write down explicitly the basic formula that is needed in the proof of (A.1):

$$\begin{aligned} \hat{a}_{j,R} &:= \sum_{j'=d+1}^{3n} \mathscr{B}_R(j,j')\hat{a}_{j'} \\ &= \tfrac{1}{2} \sum_{j'=d+1}^{3n} [(\Omega_j\Omega_{j'}^{-1})^{1/2}\mathscr{B}_R(j,j')(\hat{a}_{j'}+\hat{a}_{j'}^{+}) \\ &\quad + (\Omega_{j'}\Omega_j^{-1})^{1/2}\mathscr{B}_R(j,j')(\hat{a}_{j'}-\hat{a}_{j'}^{+})] \end{aligned} \quad \text{(A.2)}$$

In obtaining (A.2) we have used only the fact that if $j \neq j'$ and $\Omega_j \neq \Omega_{j'}$, then $\mathscr{B}_R(j,j') = 0$. [This is the third orthogonality rule formulated in Section 4.3; see equation (4.13).]

The situation may therefore be summarized as follows. Let $|\mathfrak{H}\rangle$ be any member of $\mathscr{H}$. The important variables, namely, displacements and momenta, are given by $\langle \mathfrak{H}|\hat{\mathbf{U}}(\mathbf{x})|\mathfrak{H}\rangle$ and $\langle \mathfrak{H}|\hat{\mathbf{P}}(\mathbf{x})|\mathfrak{H}\rangle$, respectively. We say that a collection of these variables forms a pattern of motion. If one subjects the state $|\mathfrak{H}\rangle$ to a transformation R,

$$|\mathfrak{H}\rangle \Rightarrow \exp[-i\hat{\Theta}(R)]\,|\mathfrak{H}\rangle = \hat{\mathfrak{g}}(R)\,|\mathfrak{H}\rangle$$

then one arrives at the pattern of motion rotated by R, as one should.

REFERENCES

Amrein, W. O. (1969). *Helvetica Physica Acta*, **42**, 149–190.

Banach, Z., and Piekarski, S. (1993). The Jauch–Piron system of imprimitivities for phonons. II. The Wigner function formalism, *International Journal of Theoretical Physics*, this issue.

Bauer, M. (1983). *Annals of Physics* (New York), **150**, 1–21.

Beck, H., Meier, P. F., and Thellung, A. (1974). *Physica Status Solidi A*, **24**, 11–63.

Birman, J. L. (1974). Theory of crystal space groups and infra-red and Raman lattice processes of insulating crystals, in *Handbuch der Physik*, Vol. XXV/2b, S. Flügge, ed., Springer-Verlag, Berlin.

Emch, G. G. (1972). *Algebraic Methods in Statistical Mechanics and Quantum Field Theory*, Wiley-Interscience, New York.

Fong, R., and Rowe, E. G. P. (1968). *Annals of Physics* (New York), **46**, 559–576.

Gurevich, V. L. (1980). *Kinetika Fononnykh Sistem*, Nauka, Moscow.

Jauch, J. M., and Piron, C. (1967). *Helvetica Physica Acta*, **40**, 559–570.

Jensen, H. H. (1964). Phonons and phonon interaction, in *Aarhus Summer School Lectures*, T. A. Bak, ed., Benjamin, New York.

Jensen, H. H., and Nielsen, P. H. (1969). *Det Kongelige Danske Videnskabernes Selskab Matematisk-fysiske Meddelelser*, **37**, 1–28.

Klimontovich, Yu. L. (1975). *Kineticheskaya Teoriya Neidealjnogo Gaza i Neidealnoi Plazmy*, Nauka, Moscow.

Knox, R. S., and Gold, A. (1964). *Symmetry in the Solid State*, Benjamin, New York.

Lax, M. (1974). *Symmetry Principles in Solid State and Molecular Physics*, Wiley-Interscience, New York.

Mackey, G. W. (1953). *Annals of Mathematics*, **58**, 193–221.

Mackey, G. W. (1958). *Acta Mathematica*, **99**, 265–311.

Madelung, O. (1978). *Introduction to Solid-State Physics*, Springer-Verlag, Berlin.

Mandel, L. (1964). *Physical Review*, **136**, B1221–B1224.

Mandel, L. (1966). *Physical Review*, **144**, 1071–1077.

Newton, T. D., and Wigner, E. P. (1949). *Reviews of Modern Physics*, **21**, 400–406.

Rajaraman, R. (1982). *Solitons and Instantons. An Introduction to Solitons and Instantons in Quantum Field Theory*, North-Holland, Amsterdam.

Sansone, G. (1959). *Orthogonal Functions*, Interscience, New York.

Szegö, G. (1939). *Orthogonal Polynomials*, American Mathematical Society, Providence, Rhode Island.

von Neumann, J. (1955). *Mathematical Foundations of Quantum Mechanics*, Princeton University Press, Princeton, New Jersey.

Wightman, A. S. (1962). *Reviews of Modern Physics*, **34**, 845–872.

Wigner, E. P. (1932). *Physical Review*, **40**, 749–759.