Lorentz Invariant Localized States*

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Newton and Wigner have previously discussed the definition of "localized states" in terms of invariance conditions. However, their localization conditions are not Lorentz covariant. The present work presents a modified set of invariance postulates which includes a Lorentz invariance condition. It is shown that for spinless systems there do exist states satisfying the modified set of postulates; these states are calculated explicitly. The procedure appears to preclude the existence of Lorentz covariant "position operators."

INTRODUCTION

A RELATIVISTIC elementary system has been defined[1] as a set of states which forms an irreducible representation space for the inhomogeneous Lorentz group. The concept of an elementary particle is somewhat more restrictive since one requires not only that its states form an elementary system, but also that in some sense it shall not be useful to consider the particle as a composite of other particles.[2]

The principles of relativistic quantum mechanics for elementary systems readily provide expressions for the operators corresponding to the energy-momentum four-vector and the angular-momentum tensor. Other operators, such as "position operators," are not so easily defined. Thus it has been proposed in NW that operators corresponding to other physical observables should be defined in terms of general, invariant theoretic principles.

POSTULATES FOR LOCALIZED STATES

Invariance principles have been proposed by Newton and Wigner for the definition of "localized states" which may be interpreted as eigenstates of position operators. It has been postulated that states "localized" at the point x, y, z at the time t should satisfy the following conditions:

(a) The set S of all such states forms a linear manifold invariant under all those spatial rotations, spatial inversions, and time inversions which leave invariant the point of localization. (Linearity, symmetry.)

(b) If a state from S is subjected to any finite spatial displacement, it will become orthogonal to all states of S. (Orthogonality.)

(c) All infinitesimal operators of the Lorentz group are applicable to all states of S. (Regularity.[3])

We will refer to these as the NW postulates.

It is found that for all elementary systems of nonzero mass and arbitrary integral or half-integral spin there exist linear manifolds of states localized at each space-time point. For massless particles, localized states exist only for spins 0 and $\frac{1}{2}$. In each case the localized states belong to the continuous spectrum of three Hermitian operators (components of the "position operator") whose eigenvalues are the coordinates of the point of localization. These operators satisfy the proper commutation relations for position operators.

Unfortunately this definition of "localization" is not Lorentz invariant. (This was already recognized in NW.) A state which satisfies the localization postulates in one coordinate system will not satisfy the postulates when viewed from another coordinate system in uniform relative motion. Moreover, the three components of the position operator are apparently not part of any simple covariant quantity.

LORENTZ INVARIANT LOCALIZATION

The present paper proposes an alternative set of localization postulates which includes a Lorentz invariance condition.[4] States localized at the point x, y, z at the time t must satisfy the following conditions:

(a) The set S of all such states forms a linear manifold invariant under all those spatial rotations, spatial inversions, and time inversions which leave invariant the point of localization. (Linearity, symmetry.)

(b) The set S is invariant under all Lorentz accelerations. (Lorentz invariance.)

(c) The eigendifferentials formed by the superposition of states localized in a small finite region are normalizable. (Normalizability.)

(d) The set S contains no subset which satisfies the conditions (a), (b), and (c). (Irreducibility.)

We will call these the LI (Lorentz invariant) postulates. In this paper, application of these postulates is limited to the simplest physical case, elementary systems of *nonzero mass and zero spin.*

Since no set of localized states determined by the NW postulates is Lorentz invariant, at least one of the NW postulates must be omitted in formulating the new (LI) set of postulates. We have chosen to relax

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[1] T. D. Newton and E. P. Wigner, Rev. Mod. Phys. 21, 400 (1949); hereafter referred to as NW.

[2] Two recent articles which deal with the usefulness of the concept of elementary particle are those of G. F. Chew, Phys. Today 17, No. 4, 30 (1964), and W. Heisenberg, address at the Niels Bohr Commemoration meeting (unpublished).

[3] The regularity condition, as stated here, is not sufficiently explicit; it is discussed in detail in the original paper (NW).

[4] T. O. Philips, dissertation, Princeton University, 1963 (unpublished).

the requirement of orthogonality. An unfortunate consequence of this procedure will be our inability to define Hermitian position operators.

Spinless states will be represented by wave functions $\psi(p_1p_2p_3)$ defined on the positive mass shell. We use the usual form of the scalar product

$$(\psi,\varphi)=\int\psi(p_1p_2p_3)^*\varphi(p_1p_2p_3)d^3p/p_0, \quad (1)$$

where

$$p_0=+(|\mathbf{p}|^2+m^2)^{1/2} \quad \text{and} \quad d^3p=dp_1dp_2dp_3.$$

We denote by S_0 a set of states localized at the origin at $t=0$ according to the LI postulates. States localized at other space-time points can be obtained using the displacement operator

$$T(a)\psi(\mathbf{p})=\exp(-ia\cdot p)\psi(\mathbf{p}), \quad (2)$$

where the Lorentz-invariant product is

$$a\cdot p=a^0p^0-\mathbf{a}\cdot\mathbf{p}.$$

Any set of $2j+1$ functions of the form

$$\varphi_{jm}(\mathbf{p})=Y_{jm}(\theta,\varphi)f(p), \quad m=-j, -j+1, \cdots, +j, \quad (3)$$

with j a fixed non-negative integer, satisfies the linearity and symmetry conditions for states localized at the origin. Here p, θ, φ are the spherical polar coordinates of (p_1,p_2,p_3), and the Y_{jm} are the normalized spherical harmonics. The function $f(p)$ is arbitrary, but may be assumed real without loss of generality; this is a direct consequence of the requirement of time-reversal invariance. A manifold such as that of Eq. (3) exists for each non-negative integer j and each choice of the function $f(p)$. The set S_0 must therefore consist of one or more sets of the form in Eq. (3).

THE LORENTZ INVARIANCE CONDITION

Before we can apply the Lorentz invariance condition, we must obtain a representation of the infinitesimal operators of Lorentz accelerations. Since any homogeneous Lorentz transformation may be written as the product of a rotation and a Lorentz acceleration along one particular axis, we need consider only the infinitesimal generator L_3 of Lorentz accelerations along the x_3 axis. In spherical coordinates this infinitesimal operator is

$$L_3=p_0\partial/\partial p_3=p_0[(\cos\theta)\partial/\partial p-(\sin\theta)p^{-1}\partial/\partial\theta]. \quad (4)$$

When L_3 is applied to states φ_{jm} of the form in Eq. (3), we obtain

$$L_3\varphi_{jm}(\mathbf{p})=N_{jm}Y_{j-1,m}(\theta,\varphi)p_0[f'(p)+(j+1)p^{-1}f(p)] +N_{j+1,m}Y_{j+1,m}(\theta,\varphi)p_0[f'(p)-jp^{-1}f(p)] \quad (5)$$

with

$$N_{jm}=[(j^2-m^2)/(2j+1)(2j-1)]^{1/2}.$$

Note that from states φ_{jm} with angular factors Y_{jm}, application of the operator L_3 generates states with angular factors $Y_{j-1,m}$ and $Y_{j+1,m}$.

If the state φ_{jm} is in S_0, the Lorentz invariance condition requires that $(L_3)^n\varphi_{jm}$ be in S_0 for any n. This means that S_0 may in general contain an infinite number of linearly independent states with different angular factors Y_{jm}. Note that the choice of $f(p)$ for the functions with a particular j completely determines the set S_0, since all other states in S_0 are generated by repeated application of the operator L_3. (We are here implicitly applying the irreducibility condition.)

Many different sets of functions may be generated by the application of L_3 to sets of the form (3). We will sort all possible sets into three classes. Each class will then be investigated to discover which sets (if any) satisfy the normalizability condition.

Class I. The linear manifolds being considered are spanned by a basis consisting of states with angular factors Y_{jm}. Class I will consist of those sets for which there exists a finite maximum value of j (which we denote by J). For this to obtain, the set must include a state

$$\varphi_{Jm}=\text{constant}\times Y_{Jm}(\theta,\varphi)p^J. \quad (6)$$

Then the state $L_3\varphi_{Jm}$ is found to have an angular dependence $Y_{J-1,m}$; the term which would contain $Y_{J+1,m}$ vanishes. Repeated application of L_3 generates a set with $j=0, 1, \cdots, J$. One set of this type exists for every non-negative integer J.

Class II. This class consists of those sets with a nonzero minimum value of j (which we denote by J'). For this to obtain the set must include a state

$$\varphi_{J'm}=\text{constant}\times Y_{J'm}(\theta,\varphi)p^{-J'-1}. \quad (7)$$

Then the state $L_3\varphi_{J'm}$ has an angular dependence $Y_{J'+1,m}$. Repeated application of L_3 generates a set with $j=J', J'+1, J'+2, \cdots$, with *no* finite maximum value of j. One set of this type exists for every positive integer J'.

Class III. One can arbitrarily choose a function with angular dependence Y_{00}:

$$\varphi_{00}=f(p). \quad (8)$$

Repeated application of L_3 generates a set of states satisfying the Lorentz invariance condition. For certain choices of $f(p)$ this will be a Class I set with no values of j larger than some finite maximum value J. Class III will consist of all sets generated starting from any *other* choices of $f(p)$; for such sets j takes on all non-negative integral values.

EIGENDIFFERENTIALS OF LOCALIZED STATES

Let $\psi(\mathbf{p};\mathbf{x})$ represent a state localized at the point $\mathbf{x}$ at time $t=0$. In particular suppose that the state

$$\psi(\mathbf{p};0)=f(p)Y_{jm}(\theta,\varphi) \quad (9)$$

is localized at the origin at $t=0$. Using the translation operator (2), we obtain the state localized at an arbitrary point $\mathbf{x}$ (at $t=0$):

$$\psi(\mathbf{p};\mathbf{x})=e^{i\mathbf{x}\cdot\mathbf{p}}\psi(\mathbf{p};0)=e^{i\mathbf{x}\cdot\mathbf{p}}f(p)Y_{jm}(\theta,\varphi). \quad (10)$$

Eigendifferentials will be formed as the superposition of states localized in the sphere $S(\epsilon,\mathbf{x})$, which has radius ϵ and center $\mathbf{x}$. The radius ϵ is arbitrarily small but finite. We define these eigendifferentials by the expression

$$\bar{\psi}(\mathbf{p};\mathbf{x})=\frac{3}{4\pi\epsilon^3}\int_{S(\epsilon,\mathbf{x})}\psi(\mathbf{p};\mathbf{x}')d^3x'. \quad (11)$$

After substituting (10) into (11) and performing the integration, we obtain

$$\bar{\psi}(\mathbf{p};\mathbf{x})=N(\epsilon p)\psi(\mathbf{p};\mathbf{x}), \quad (12a)$$

where

$$N(z)=3z^{-3}(\sin z-z\cos z)=3z^{-1}j_1(z); \quad (12b)$$

$j_1(z)$ is a spherical Bessel function. In the limit $|z|\ll 1$

$$N(z)\sim 1-\tfrac{1}{10}z^2+O(z^4).$$

Using the form (10) for the localized states and the form (12a) for the eigendifferentials, we can calculate the norm of the eigendifferentials:

$$\|\bar{\psi}\|^2=\int_0^\infty p^2N(\epsilon p)^2f(p)^2dp/p_0. \quad (13)$$

This norm is independent of the point $\mathbf{x}$ at which $\bar{\psi}$ is formed. In order that the normalization condition (c) of the LI postulates be satisfied, the integral (13) must converge. If $f(p)$ has the asymptotic expansions

$$|f(p)|\sim p^n \quad \text{for} \quad p\to\infty \quad (14a)$$

and

$$|f(p)|\sim p^l \quad \text{for} \quad p\to 0, \quad (14b)$$

we can find necessary conditions upon n and l such that the integral converges:

$$\text{(a) } n<1, \quad \text{and} \quad \text{(b) } l>-\tfrac{3}{2}. \quad (15)$$

With regard to these conditions we consider the three classes of sets defined above.

Class I. For a given J, the states with the angular factors Y_{jm}, $j\leqq J$, have a radial dependence which is the sum of terms of the form

$$p_0{}^{J-j}p^j, \quad p_0{}^{J-j-2}p^{j+2}, \quad p_0{}^{J-j-4}p^{j+4}, \ldots.$$

Asymptotically as $p\to\infty$ each of these terms behaves as p^J. Condition (15a) is satisfied only for $J=0$. In this case there is a single state

$$\varphi(\mathbf{p})=\text{constant} \quad (16)$$

which has a normalizable eigendifferential. Thus only for $J=0$ may a Class I set be considered a set of localized states for spinless systems.

Class II. For a given integer J' the states with the angular factors Y_{jm}, $j\geqq J'$, have a radial dependence which is the sum of terms of the form

$$p_0{}^{j-J'}p^{-j-1}, \quad p_0{}^{j-J'-2}p^{-j+1}, \quad p_0{}^{j-J'-4}p^{-j+3}, \ldots.$$

As $p\to 0$ the most strongly divergent term is p^{-j-1}; thus condition (15b) is satisfied only for $j=0$. But all Class II sets contain states with $j>0$. Thus no Class II set may be considered as a set of localized states.

Class III. It has not been possible to prove rigorously that all sets of Class III violate the requirement that all eigendifferentials be normalizable. However, this violation can be demonstrated for a variety of choices of the function $f(p)$ in (8). For example, all functions of the form

$$f(p)=p^me^{-\gamma p}, \quad m=\text{integer}, \quad \gamma\geqq 0,$$

fail to satisfy the normalizability condition. We conjecture that this will be the case for *all* choices of $f(p)$ which generate sets of Class III. This would then mean that no Class III set may be considered a set of localized states.

We could also choose to eliminate the sets of Class III by means of an additional postulate: A set S of localized states must have a finite basis. Such a postulate would also eliminate sets of Class II. However in the case of Class II, and we believe also in the case of Class III, the additional postulate is superfluous.

THE LORENTZ INVARIANT LOCALIZED STATE

If the conjecture concerning Class III is correct, there is a single uniquely defined state which is localized at the origin at time $t=0$:

$$\psi(\mathbf{p};0)=(2\pi)^{-3/2}. \quad (17a)$$

It is easily seen that this state is Lorentz invariant, since $L_3\psi(\mathbf{p};0)=0$. It should be recalled that this is a state of a system with zero spin. In configuration space this localized state has the form, at $t=0$ (up to a normalization factor),

$$\Psi(\mathbf{x})=(m/r)K_1(mr), \quad (17b)$$

where $r=|\mathbf{x}|$. This state can be compared with the corresponding localized state found using the NW postulates:

$$\psi_{\mathrm{NW}}(\mathbf{p})=(2\pi)^{-3/2}(p^2+m^2)^{1/4}, \quad (18a)$$

$$\Psi_{\mathrm{NW}}(\mathbf{x})=(m/r)^{5/4}K_{5/4}(mr). \quad (18b)$$

For the LI localized state (17) the eigendifferential centered at the point $\mathbf{x}$ is

$$\bar{\psi}(\mathbf{p};\mathbf{x})=(2\pi)^{-3/2}N(\epsilon p)e^{i\mathbf{x}\cdot\mathbf{p}}; \quad (19)$$

the scalar product between two eigendifferentials $\bar{\psi}_1$ and $\bar{\psi}_2$, centered at $\mathbf{x}$ and $\mathbf{y}$, respectively, is

$$(\bar{\psi}_1,\bar{\psi}_2)=(2\pi)^{-3}m^2 \times\int_{S(\epsilon,\mathbf{x})} d^3x'\int_{S(\epsilon,\mathbf{y})} d^3y'\frac{K_1(m|\mathbf{x}'-\mathbf{y}'|)}{m|\mathbf{x}'-\mathbf{y}'|}. \quad (20)$$

Since the Bessel function $K_1(z)$ is always positive for $z>0$, this scalar product is positive and nonzero for arbitrarily large distances $|\mathbf{x}-\mathbf{y}|$ between the spheres in which the eigendifferentials are formed. Thus Lorentz-invariant localization, as we have formulated it, does not lead to orthogonal localized states.

The nonorthogonality of the eigendifferentials means that there is no self-adjoint operator ("position operator") which has the localized state (17) in its continuous spectrum. This constitutes an unfortunate consequence of the decision to drop the orthogonality requirement included in the NW postulates.

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Many-Body Perturbation Theory Applied to Atoms*

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Many-body perturbation theory as formulated by Brueckner and Goldstone is applied to atoms to obtain corrections to Hartree-Fock wave functions and energies. Calculations are made using a complete set of single-particle Hartree-Fock wave functions which includes both the continuum and an infinite number of bound states. It is shown how one may readily perform the sums over an infinite number of bound excited states. In order to demonstrate the usefulness of many-body perturbation theory in atomic problems, calculations are made for a wide variety of properties of the neutral beryllium atom. The calculated $2s$-$2s$ correlation energy is -0.0436 atomic unit for $l=1$ excitations. The calculated dipole and quadrupole polarizabilities are 6.93×10^{-24} cm^3 and 14.1×10^{-40} cm^5, respectively. The calculated dipole and quadrupole shielding factors are 0.972 and 0.75. Results are given for oscillator strengths, photoionization cross sections, and the Thomas-Reiche-Kuhn sum rule, which is 4.14 as compared with 4.00, the theoretical value.

I. INTRODUCTION

MANY-BODY perturbation theory as developed by Brueckner[1] and Goldstone[2] has proven very useful in the study of many-particle systems. As shown by Brueckner, the appropriate form of perturbation theory as the number of particles becomes large is Rayleigh-Schrödinger theory modified so as to eliminate the "unlinked clusters." The principal applications of the Brueckner-Goldstone linked cluster expansion (BG expansion) to many-fermion systems have thus far been investigations of nuclear structure[3] and of the electron gas.[4] However, the BG theory, which corrects both wave functions and energies, should also prove very useful in calculations of atomic structure and in other fields. In applying this theory to atoms, where the interparticle forces are well known, one also gains information as to its general applicability to finite systems.

A previous application of BG theory to the calculation of correlation energies in the neutral beryllium atom yielded excellent results.[5] However, it was found necessary to calculate high orders in the expansion. This difficulty was related to the set of single-particle Hartree-Fock states which were used. The purpose of this paper is to investigate the use of a different basis set for the expansion and to show the usefulness of perturbation calculations using this set. The states used are the ground-state Hartree-Fock orbitals and single-particle excitations calculated in the Hartree-Fock potential field of the nucleus and $N-1$ of the N ground-state orbitals. The use of this set is justified in Sec. II. In Sec. III it is shown how sums over an infinite number of bound excited states may be carried out. In Sec. IV the $l=1$ correlation energy among the two $2s$ electrons of Be is calculated. In Sec. V calculations are given for the dipole and quadrupole polarizabilities and shielding factors for Be. In Sec. VI many oscillator strengths and the photoionization cross section curve are calculated. Section VII contains the conclusions.

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