Center-of-Mass Motion in the Nuclear Shell Model

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The methods for treating center-of-mass motion in the nuclear shell model are reviewed. The existence of inherent difficulties of principle is pointed out for any method which attempts to remove center-of-mass effects from a shell-model wave function without considering the relation of the shell-model wave function to the Hamiltonian of the real nucleus.

I. INTRODUCTION

It is now well known that center-of-mass motion is not properly treated in the nuclear shell model. The shell model Hamiltonian is not translation-invariant and the shell-model wave functions are not eigenfunctions of the total linear momentum. A number of attempts have been made to develop formalisms for treating center-of-mass motion rigorously within the framework of the shell model[1–8]; however, difficulties of principle are encountered when these methods are applied to any case other than the simple harmonic oscillator shell model.

The principal difficulty is that the "removal of spurious center-of-mass effects from a given shell-model wave function" *is in general not a well-defined problem and has no unique solution.* A variety of methods can be proposed for "projecting out a translationally invariant part" of the shell-model wave function. These methods all consider a single individual wave function at a time and do not take into account any properties of the real nuclear Hamiltonian other than translation invariance. Different methods lead to different results in all cases except that of harmonic oscillator wave functions where all methods seem to be equivalent. There seems to be no basis *a priori* to choose between these methods. An understanding of which method (if any) gives correct results will probably come only with a better understanding of why the shell model works at all for nuclei; i.e., with the introduction of some connection between the shell-model wave function and the real nuclear Hamiltonian.

Another difficulty encountered in these methods is that the translationally invariant wave functions obtained from different shell-model wave functions are not generally orthogonal to one another.

II. CENTER-OF-MASS FLUCTUATIONS

A wave function describing a real nucleus should be an eigenfunction of the total momentum operator describing center-of-mass motion as a plane wave. This is not the case for shell-model wave functions, which must therefore describe some other kind of center-of-mass motion. To investigate the kind of center-of-mass motion which shell-model wave functions do describe, we can calculate expectation values of powers of the coordinate and the momentum of the center of mass using these wave functions. The results show that the position of the center of mass fluctuates about the origin of the coordinate system and that neither the amplitude nor the kinetic energy of these fluctuations can be considered as small. In fact, the latter is of the same order of magnitude as the energy of the particle excitations in the nucleus. These fluctuations are not present in real nuclei and their dynamical effects must be removed if the shell-model wave functions are to be used for calculating properties of real nuclei.

In the harmonic oscillator shell model it is possible to describe these fluctuations in a simple way. The center of mass, instead of moving as a free particle, moves as if it were "tied by a spring" to the center of the potential; i.e., like a particle in a harmonic oscillator well. Elliott and Skyrme[2] have pointed out that this leads to two spurious effects not present in a real nucleus: 1. For every state of internal motion of the system there exists a spectrum of higher excited states of center-of-mass oscillation in an oscillator well, 2. In states where the center-of-mass oscillator is in its lowest state there is a zero-point motion of the center of mass. They have classified all states in which the center of mass is excited as "spurious states" which should be rejected and they have given a prescription for eliminating the dynamical effects of the zero-point motion.

In all cases other than that of the harmonic oscillator potential the problem is much more complicated and the question arises whether it is at all possible to remove the dynamic effects of center-of-mass motion in an unambiguous way. We shall see that this is not possible except in the case of the harmonic oscillator.

III. CONSTRUCTION OF MOMENTUM EIGENFUNCTIONS

Let us now examine how one might remove center-of-mass effects from a shell-model wave function. For

[1] H. A. Bethe and M. E. Rose, Phys. Rev. **51**, 283 (1937).
[2] J. P. Elliott and T. H. R. Skyrme, Proc. Roy. Soc. (London) **A232**, 561 (1955).
[3] Lipkin, de-Shalit, and Talmi, Nuovo cimento **2**, 773 (1955).
[4] F. Villars (unpublished).
[5] T. Tamura, Nuovo cimento **4**, 713 (1956).
[6] H. J. Lipkin, Suppl. Nuovo cimento **4**, 1147 (1956).
[7] R. E. Peierls and J. Yoccoz, Proc. Phys. Soc. (London) **A70**, 381 (1957); R. E. Peierls, *Proceedings of the Rehovoth Conference on Nuclear Structure* (North-Holland Publishing Company, Amsterdam, 1958), p. 135; J. J. Griffin and J. A. Wheeler, Phys. Rev. **108**, 311 (1957).
[8] S. Gartenhaus and C. Schwartz, Phys. Rev. **108**, 482 (1957).

each state of internal excitation of a real nucleus there is a continuous "translational spectrum" of states all having the same internal structure and a different total momentum. Since it is only the internal structure which is of interest in nuclear spectroscopy, nothing is lost by considering only a single state in each translational spectrum, namely that corresponding to a total linear momentum zero. We shall therefore consider how to construct a function of total momentum zero from a shell-model wave function.

The essential features of the problem become evident if the shell-model wave function ψ_{SM} is expressed in terms of coordinates of the particles in the center-of-mass system instead of in the laboratory system. We can thus write ψ_{SM} as a function of the center-of-mass coordinate $\mathbf{X}$ and a set of relative coordinates q^α. Since the coordinates of the particles relative to the center of mass are not all independent, the q^α must be a set of independent functions of these relative coordinates and the number of the q^α will be just $3A-3$ if the number of particles in the system is A. The exact definition of the q^α is rather messy in practice but it is sufficient for our purposes to note that they can be defined in principle. Thus

$$\psi_{\mathrm{SM}}=\psi_{\mathrm{SM}}(\mathbf{X},q^\alpha). \qquad (1)$$

We now wish to construct from ψ_{SM} a function ψ_0 having total momentum zero: ψ_0 must satisfy the relation

$$\mathbf{P}\psi_0=-i\hbar\partial\psi_0/\partial\mathbf{X}=0. \qquad (2)$$

This simply means that ψ_0 should not depend upon $\mathbf{X}$, but only upon the relative coordinates q^α. We therefore wish to remove the dependence upon $\mathbf{X}$ from the shell-model wave function ψ_{SM}. This can be done in a variety of ways. For example,

$$\psi_0(q^\alpha)=\int_{-\infty}^{+\infty}G(\mathbf{X})\psi_{\mathrm{SM}}(\mathbf{X},q^\alpha)d\mathbf{X} \qquad (3)$$

is a wave function independent of $\mathbf{X}$ for any arbitrary choice of the function $G(\mathbf{X})$. The methods which have been proposed for treating center-of-mass motion are all based upon prescriptions for constructing zero-momentum wave functions. These prescriptions are usually stated in terms of the particle coordinates in the laboratory system, rather than in terms of the coordinates $(\mathbf{X},q^\alpha)$. They therefore appear to be quite different from one another and from the relation (3). However, when the shell-model wave functions are written in terms of the coordinates $(\mathbf{X},q^\alpha)$, it becomes evident that each prescription is equivalent to a relation of the type (3), with some particular choice for the function $G(\mathbf{X})$. For example, the prescription used in the method of generator coordinates,[7]

$$\psi_0(q^\alpha)=\int\psi_{\mathrm{SM}}((\mathbf{X}-\mathbf{a}),q^\alpha)d\mathbf{a}, \qquad (4a)$$

is clearly equivalent to taking $G(\mathbf{X})=1$ in Eq. (3). The prescription used by Gartenhaus and Schwartz,[8]

$$\psi_0(q^\alpha)=\lim_{\Lambda\to\infty}\exp[-i\Lambda(\mathbf{P}\cdot\mathbf{X}+\mathbf{X}\cdot\mathbf{P})/2]\psi_{\mathrm{SM}}(\mathbf{X},q^\alpha) \qquad (4b)$$

appears to be very different from Eq. (3). However, noting that

$$\exp[-i\Lambda(\mathbf{P}\cdot\mathbf{X}+\mathbf{X}\cdot\mathbf{P})/2]\psi_{\mathrm{SM}}(\mathbf{X},q^\alpha)=\psi_{\mathrm{SM}}(\mathbf{X}e^{-\Lambda},q^\alpha),$$

we see that the relation (4b) is equivalent to taking $G(\mathbf{X})=\delta(\mathbf{X})$ in Eq. (3).

It is evident that in general the functions $\psi_0(q^\alpha)$ corresponding to different choices of the generating function $G(\mathbf{X})$ will be quite different. Since there seems to be no reason, *a priori*, to choose a particular $G(\mathbf{X})$,[9] we see that the problem of "removing center-of-mass effects" from a given shell-model wave function is not uniquely defined.

A second difficulty inherent in the definition of zero-momentum wave functions by a relation of the type (3) is that the set of all wave functions $\psi_0(q^\alpha)$ corresponding to a complete orthonormal set of shell-model wave functions must be a redundant set. Two zero-momentum wave functions ψ_0 corresponding to two orthogonal shell-model wave functions will in general not be orthogonal. The redundance is evident, since the relation (3) eliminates 3 degrees of freedom from the system without reducing the number of wave functions. This redundance may not cause difficulty in calculations of diagonal matrix elements of operators, such as electric or magnetic moments. However, one can question the meaning of off-diagonal matrix elements between two wave functions which may not be orthogonal to one another.

IV. HARMONIC OSCILLATOR SHELL MODEL

The one case which has been treated simply and successfully by all methods is that of harmonic oscillator wave functions. The simplicity results from the separability of center-of-mass motion in the harmonic oscillator case[1,2,6] which allows the shell-model wave functions to be written in the form

$$\psi_{\mathrm{SM}}(\mathbf{X},q^\alpha)=F(\mathbf{X})\varphi(q^\alpha), \qquad (5)$$

where the functions $F(\mathbf{X})$ and $\varphi(q^\alpha)$ constitute two

[9] In the treatment of rotational states in nuclei, certain problems are encountered which are analogous to the treatment of center-of-mass motion (translational states). It is therefore possible to carry over some of the arguments in this treatment directly to the rotational case by substituting the words "rotation" for "translation," "angular momentum" for "linear momentum," "collective angular coordinate" for "center-of-mass coordinate, etc." An important difference between the two cases, however, is that the collective coordinate is *not uniquely defined* in the rotational case. Thus, in using relations of the type (3) to generate functions of zero angular momentum, the choice $G(X)=1$ has the particular feature of being independent of the choice of collective coordinate X. The method of generator coordinates therefore allows the rotational problem to be treated without explicitly defining a collective coordinate. It is not clear whether this is an advantage or a disadvantage [H. J. Lipkin, *Proceedings of the Rehovoth Conference on Nuclear Structure* (North-Holland Publishing Company, Amsterdam, 1958)], p. 144.

independent sets of orthonormal functions. It is evident that a separable function of the type (5) will always give the same zero-momentum wave function in the relation (3) *regardless of the form of the generating function* $G(\mathbf{X})$ (apart from a constant factor which has no significance since the functions $\psi_0(q^\alpha)$ are not normalized), except for the case where $G(\mathbf{X})$ is orthogonal to $F(\mathbf{X})$ and the integral vanishes. Furthermore, two different orthogonal shell-model wave functions will generate two zero-momentum wave functions which are either orthogonal or identical, depending upon whether the internal parts $\varphi(q^\alpha)$ of the two functions are the same or different. The redundance can therefore be removed simply by rejecting the set of duplicate states as spurious. This can be done simply by setting $G(\mathbf{X})$ in (3) equal to the complex conjugate of one of the functions of the set $F(\mathbf{X})$ in (5), for example, that of the ground-state wave function. All the "spurious states" then give zero in the relation (3) since they contain functions $F(\mathbf{X})$ orthogonal to $G(\mathbf{X})$.

Once the zero-momentum wave functions are constructed, expectation values of operators can be calculated by any of the methods proposed, some being more elegant or easier to calculate than others. However, it is clear that for the oscillator case, all methods should give the same result.

Unfortunately, the harmonic oscillator case is the only case for which the separability (5) is valid. For any other case, such as, for example, the harmonic oscillator potential with an added spin-orbit interaction, the center-of-mass motion is no longer separable. Different methods of treating center-of-mass motion then give different results; different zero-momentum wave functions constructed in any one method are not orthogonal to one another and there is no simple way to define and to reject "spurious states."

V. CONCLUSIONS

The general solution of the center-of-mass problem for the nonseparable case does not seem to be possible using a relation of the type (3) which defines a zero-momentum eigenfunction for a given individual shell-model wave function without regard to the other shell-model wave functions. To construct an orthonormal set of zero-momentum wave functions, it seems to be necessary to treat together the whole set of shell-model wave functions, or at least a group of several of them. The particular direction to look for such a treatment is not at all clear. One way of doing it formally would be as follows:

Let the shell-model Hamiltonian be

$$H=\sum_i T_i+\sum_i V_i, \tag{6}$$

where T_i and V_i are the kinetic and potential energy of the ith particle. If the potential energy $\sum_i V_i$ is expressed in terms of the coordinates $(\mathbf{X},q^\alpha)$,

$$\sum_i V_i=U(\mathbf{X},q^\alpha), \tag{7}$$

we can define a "translationally invariant potential" by a relation analogous to (3):

$$U_0(q^\alpha)=\int G(\mathbf{X})U(\mathbf{X},q^\alpha)d\mathbf{X}. \tag{8}$$

The function $G(\mathbf{X})$ and the translationally invariant potential are of course not uniquely determined. We can now write down a Hamiltonian,

$$H'=\sum_i T_i+U_0(q^\alpha). \tag{9}$$

The Hamiltonian (9) is translationally invariant, and we can in principle write down all its eigenfunctions corresponding to a total momentum zero. In this way we have defined an orthonormal set of zero-momentum wave functions corresponding in some way to the set of shell-model wave functions. This does not seem to be a very practical solution, because of the difficulty of finding the eigenfunctions of (9), which will not be simple single-particle wave functions.

A striking feature of all these treatments of center-of-mass motion in the nuclear shell model is that they only consider the shell-model wave functions and are completely independent of the form of the Hamiltonian of the real nucleus. This might be justified on the grounds that it is known empirically that the use of shell-model wave functions gives results in reasonable agreement with experiment and that the only point considered here is that of the relatively small corrections for center-of-mass motion which do not have any direct bearing on the justification of the shell model from first principles. However, it is evident that there is no unique prescription for making these corrections without reference to the Hamiltonian of the real nucleus.

One possible approach would be to determine the function $G(\mathbf{X})$ in Eq. (3) by a variational method which would minimize the energy as calculated with the Hamiltonian of a real nucleus using two-body forces.[10]

This assumes that the shell-model wave function is an approximation to the real wave function, except for its description of center-of-mass motion. If the relation between the shell-model and the real wave functions is more complicated, such as proposed by Brueckner,[11] then it does not seem reasonable that the center-of-mass problem can be separated from the general problem of justifying the shell model.

VI. ACKNOWLEDGMENTS

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[10] I. Talmi (private communication). (This should not be confused with the variational approach presented in the method of generator coordinates.[7] The latter becomes trivial in the case of center-of-mass motion and merely requires that the functions generated be eigenfunctions of the total momentum if the real Hamiltonian is translationally invariant.)

[11] R. J. Eden, *Proceedings of the Rehovoth Conference on Nuclear Structure* (North-Holland Publishing Company, Amsterdam, 1958), p. 3.