

Exact solutions to the center of mass problem in a model theory

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(Received 15 October 1979; revised manuscript received 19 June 1980)

A model theory, standard time-independent perturbation theory in a harmonic oscillator shell model basis, is used to investigate various aspects of the center of mass problem. In this model it is shown that the center of mass problem can be solved by projection techniques, but that the way in which one projects is crucial. The appropriate projection functions are found to be $\text{const} \times R^{-3/2}$ for wave function projection and 1 for density projection. The former illustrates, among other things, that the center of mass problem cannot be solved by simply eliminating the spurious components of the wave function. The latter agrees with the Gartenhaus-Schwartz prescription. Also, explicit center of mass corrections are calculated.

[NUCLEAR STRUCTURE Methods for treating center of mass effects tested in]
a model theory.]

I. INTRODUCTION

Due to the great simplicity provided by independent motion, most nuclear theories are based upon the independent particle model. One consequence of such an approach to nuclear theory is that it introduces a violation of translational invariance; that is, the center of mass (c.m.) motion is not in a free state as required by the symmetry of the Hamiltonian. As a result such theories do not directly give predictions for the intrinsic properties of nuclei. This difficulty has long been recognized and is generally referred to as the c.m. problem.

In the literature there exist a number of quite different methods for treating the c.m. problem. The reason for this variety is that the problem can be attacked at different levels. First, at the more fundamental level, there exist dynamical methods¹⁻¹⁰ in which the treatment of the c.m. motion is built right into the theory one is using. This can be done by modifying the standard shell model approach, for example, by adding an auxiliary c.m. potential^{1,2} or restricting the calculation to the space of nonspurious states.⁵ In the second, static approach,¹¹⁻¹⁹ one attacks the c.m. problem at a later stage by restoring translational invariance after the wave function has already been developed. The most well known methods of this type are the Gartenhaus-Schwartz transformation¹¹ and wave function projection.^{12,13} The dynamic and static approaches are quite complementary. The dynamic one gives the best (often exact) solution to the c.m. problem, but its application tends to be restricted or very difficult. Most dynamical methods are incompatible with most theories used in actual calculations. The static approach, on the other hand, can be

universally applied, but since restoring translational invariance only removes the symptom of the problem, one has little idea of what such solutions to the c.m. problem mean physically. Often one simply neglects this difficulty and considers the result to be approximate. However, in any nontrivial situation, different static methods give different results.^{13,15,17} Unless the dynamics is considered in some way (usually it is not), there is no way of knowing if one method produces a better solution than another. One is thus left with an ambiguous result, which is not very satisfactory.

In the present investigation of the c.m. problem, we test and compare various methods for treating c.m. effects by applying them to a model theory for which the c.m. problem can be solved exactly. The theory is standard time-independent perturbation theory in a harmonic oscillator (HO) shell model (SM) basis, for which it is extremely easy to understand the origins of the c.m. problem and to see what the effect of applying a particular method will be. Since the fact that the dynamical methods can solve the c.m. problem is almost trivial, our main interest is in studying the effect of the static methods. The most practical aspect of this work is that it provides a testing ground for projection methods which can give some justification for their use more widely.

Our main results are that for perturbation theory the c.m. problem can be solved by either wave function or density projection and that the choice of the projection function is crucial. The correct density projection method agrees with the Gartenhaus-Schwartz prescription (see Appendix A). These results, along with the explicit calculations of the c.m. corrections for the rms radius and the binding energy, are presented in

Sec II. Section III contains a discussion of the results.

II. CENTER OF MASS CORRECTIONS IN PERTURBATION THEORY

In this section we present the solution to the c.m. problem for time-independent perturbation theory in the HOSM basis.

Nonrelativistically, the nuclear Hamiltonian is given by

$$H = T + V, \quad (1)$$

where T represents the sum of the kinetic energies of the nucleons and V the (purely relative) potential interaction between them. Introducing a single-particle potential U it is common to rewrite (1) as

$$H = H_0 + \Delta V, \quad (2)$$

with

$$H_0 = T + U, \quad (3)$$

$$\Delta V = V - U. \quad (4)$$

Since H_0 represents an independent-particle model, the corresponding Schrödinger equation can be solved exactly. This provides a basis for calculating the effects of the residual interacting ΔV . In perturbation theory²⁰ this is done by solving a modified Schrödinger, or perturbation, equation

$$(H_0 + \lambda \Delta V)\psi_\lambda = E_\lambda \psi_\lambda, \quad (5)$$

where

$$\psi_\lambda = \sum_{n=0}^{\infty} \lambda^n \psi_{(n)}, \quad (6)$$

$$E_\lambda = \sum_{n=0}^{\infty} \lambda^n E_{(n)}, \quad (7)$$

successively to each order in λ . Using the normalization condition

$$\langle \psi_\lambda | \psi_\lambda \rangle = 1, \quad (8)$$

this gives an explicit set of equations for $\psi_{(n)}$ and $E_{(n)}$ in terms of the eigensolutions of H_0 . These expressions, which are required in order to actually carry out a calculation in perturbation theory, are well known. They are, however, not required in the following, and therefore will not be presented here. To a given order, say, the p th, physical quantities are calculated by keeping all terms in the expressions for the quantities of order λ^n with $n \leq p$ and then setting $\lambda = 1$; for example,

$$\psi_p = \sum_{n=0}^p \psi_{(n)}, \quad (9)$$

$$E_p = \sum_{n=0}^p E_{(n)} = \langle \psi | H_0 | \psi \rangle_p + \langle \psi | \Delta V | \psi \rangle_{p-1}, \quad (10)$$

$$\begin{aligned} \langle \psi' | 0 | \psi \rangle_p &= \sum_{n=0}^p \langle \psi' | 0 | \psi \rangle_{(n)} \\ &= \sum_{m+n=p} \langle \psi'_{(m)} | 0 | \psi_{(n)} \rangle, \end{aligned} \quad (11)$$

where we have introduced the notation that a subscript p indicates the prediction for a quantity in p th order and (p) for the p th order correction for this quantity [$A_{(p)} = A_p - A_{p-1}$].

In the HOSM basis the single-particle potential is defined to be

$$U = \sum_{i=1}^A \frac{m}{2} \omega^2 r_i^2, \quad (12)$$

where m is the nucleon mass, \vec{r}_i the coordinate of nucleon i , and A the number of nucleons in the nucleus, which separates into a purely c.m. [dependent only on the c.m. coordinate $\vec{R} = (1/A) \times \sum_{i=1}^A \vec{r}_i$] plus a purely intrinsic (dependent only on $\vec{r}_i - \vec{R}$) piece. We indicate this by the superscripts c.m. and int, respectively:

$$U = U^{\text{int}} + U^{\text{c.m.}}. \quad (13)$$

As a consequence H_0 and ΔV also separate:

$$H_0 = H_0^{\text{int}} + H_0^{\text{c.m.}}, \quad (14)$$

$$\Delta V = \Delta V^{\text{int}} + \Delta V^{\text{c.m.}}, \quad (15)$$

where, since $V^{\text{c.m.}} = 0$,

$$\Delta V^{\text{c.m.}} = -U^{\text{c.m.}}. \quad (16)$$

As a consequence of this separability a corresponding intrinsic theory can be defined by replacing H_0 and ΔV in (5) by their intrinsic counterparts, i.e.,

$$(H_0^{\text{int}} + \lambda \Delta V^{\text{int}})\chi_\lambda = E_\lambda^{\text{int}} \chi_\lambda, \quad (17)$$

where we have used the symbol χ for the corresponding intrinsic wave function.

For convenience in the following we also introduce the analogous c.m. perturbation theory defined by

$$(H_0^{\text{c.m.}} + \lambda \Delta V^{\text{c.m.}})\phi_\lambda = E_\lambda^{\text{c.m.}} \phi_\lambda. \quad (18)$$

Since $\Delta V^{\text{c.m.}} = -U^{\text{c.m.}}$ this equation is the same as that for the c.m. motion in the HOSM, but with $U^{\text{c.m.}}$ replaced by $(1 - \lambda)U^{\text{c.m.}}$. Equation (18) can thus be solved analytically: the wave functions and energies are the same as in the harmonic oscillator model but with ω replaced by $(1 - \lambda)^{1/2}\omega$. For example, the solution for the 0s state is

$$\phi_\lambda(R) = \left(\frac{A}{\pi b^2}\right)^{3/4} (1 - \lambda)^{3/8} \exp\left[-\frac{1}{2}(1 - \lambda)^{1/2}AR^2/b^2\right], \quad (19)$$

$$E_{\lambda}^{\text{c.m.}} = \frac{3}{2}(1 - \lambda)^{1/2}\omega, \quad (20)$$

where $b \equiv (m\omega)^{-1/2}$. By expanding in λ one can thus easily obtain $\phi_{(n)}$ and $E_{(n)}^{\text{c.m.}}$. We note that the $\phi_{(n)}$ have the form $P_n(AR^2/b^2)\exp(-\frac{1}{2}AR^2/b^2)$, where P_n is a polynomial of order n and thus form a linearly independent (but nonorthogonal) set.

From Eqs. (17) and (18) it follows that

$$\psi_{\lambda} = \chi_{\lambda}\phi_{\lambda}, \quad (21)$$

$$E_{\lambda} = E_{\lambda}^{\text{int}} + E_{\lambda}^{\text{c.m.}} \quad (22)$$

provide a solution to Eq. (5). If one starts from a separable unperturbed state $\psi_0 = \chi_0\phi_0$ one then finds that $\psi_{(p)}$ and $E_{(p)}$ can be expressed as

$$\psi_{(p)} = \sum_{n=0}^p \chi_{(p-n)}\phi_{(n)}, \quad (23)$$

$$E_{(p)} = E_{(p)}^{\text{int}} + E_{(p)}^{\text{c.m.}}, \quad (24)$$

and thus using (9) and (10),

$$\psi_p = \sum_{n=0}^p \chi_{p-n}\phi_{(n)} = \chi_p\phi_{(0)} + \chi_{p-1}\phi_{(1)} + \cdots + \chi_0\phi_{(p)}, \quad (25)$$

$$E_p = E_p^{\text{int}} + E_p^{\text{c.m.}}. \quad (26)$$

Thus the desired intrinsic wave functions and energies are contained within the wave functions and energies obtained from the original, shell model based calculation in a well defined way. Furthermore the two are connected by the simple physics of the c.m. perturbation theory described by (18). Essentially it is the knowledge of this physics which allows one to extract the intrinsic physics and thus solve the c.m. problem. This is our central result, which we shall use to discuss various aspects of the c.m. problem and in particular to compare different methods for treating c.m. effects. In the following we shall assume that the unperturbed state ψ_0 is a non-spurious state (for example the ground state), i.e., ϕ_0 is the 0s state wave function.

We first consider the c.m. problem for the wave function, that is, how to extract χ_p from ψ_p . Since χ_p is contained in the first term on the right hand side of (25), the main problem is to eliminate the rest of the terms. This, for example, can be done by

(i) explicit construction: knowledge of ψ_n and $\phi_{(n)}$ for $n \leq p$ is sufficient information to extract χ_p from (25);

(ii) the Bolsterli-Feenberg-Lipkin method,^{1,2} i.e., replacing ΔV by $\Delta V + U^{\text{c.m.}} = \Delta V - \Delta V^{\text{c.m.}} = \Delta V^{\text{int}}$. In this case the higher order terms in ϕ simply do not appear in the wave function and one has

$$\psi_p^{\text{BFL}} = \chi_p\phi_0; \quad (27)$$

(iii) wave function projection,¹³ i.e., eliminating the c.m. dependence by integrating over \vec{R} ,

$$\chi_p = \int d\vec{R} W(\vec{R})\psi_p, \quad (28)$$

with

$$\int d\vec{R} W(\vec{R})\phi_{(n)}(\vec{R}) = \delta_{n0}, \quad n \leq p. \quad (29)$$

Since the $\phi_{(n)}$ form an independent set, a projection function $W(\vec{R})$ which satisfies (29) can always be constructed. Furthermore, using the generating function for the $\phi_{(n)}$, that is, ϕ_{λ} , one can obtain the projection function which is valid to all orders by requiring that

$$\int d\vec{R} W(\vec{R})\phi_{\lambda}(\vec{R}) = 1. \quad (30)$$

From the structure of ϕ_{λ} (19) it is clear that the integral will be independent of λ if $W \sim R^{-3/2}$. Working out the normalization, one finds

$$W(\vec{R}) = [2^{7/4}\pi^{1/4}\Gamma(\frac{3}{4})]^{-1}R^{-3/2}. \quad (31)$$

We now turn to the problem of extracting intrinsic matrix elements,

$$\langle \chi' | O^{\text{int}} | \chi \rangle_p = \sum_{m+n=p} \langle \chi'_{(m)} | O^{\text{int}} | \chi_{(n)} \rangle. \quad (32)$$

The most obvious way to obtain these matrix elements of course is to calculate them directly with the intrinsic wave functions. To do this, however, one must not only extract the intrinsic wave functions but also perform an integration over relative coordinates, which can be quite tedious. Two more direct ways of obtaining $\langle \chi' | O^{\text{int}} | \chi \rangle$ follow.

(i) The first is density projection,¹⁵ i.e., elimination of the c.m. dependence by integrating the product of wave functions which occurs in the matrix element (instead of each individually) over \vec{R} ,

$$\langle \chi' * \chi \rangle = \int d\vec{R} D(\vec{R})(\psi' * \psi). \quad (33)$$

This prescription is neither more nor less fundamental than wave function projection, but it simplifies the procedure for calculating matrix elements considerably. In this case, the projection prescription, i.e., the integration over \vec{R} , allows one to convert the integral over relative coordinates to one over single-particle coordinates:

$$\langle \chi' | O^{\text{int}} | \chi \rangle = \langle \psi' | D(\vec{R})O^{\text{int}} | \psi \rangle. \quad (34)$$

In perturbation theory this prescription reads

$$\begin{aligned} \langle \chi' | O^{int} | \chi \rangle_p &= \langle \psi' | D(\vec{R}) O^{int} | \psi \rangle_p \\ &= \sum_{k+l+m+n \leq p} \langle \chi'_{(k)} | O^{int} | \chi_{(l)} \rangle \\ &\quad \times \langle \phi_{(m)} | D | \phi_{(n)} \rangle \\ &= \sum_{n=0}^p \langle \chi' | O^{int} | \chi \rangle_{p-n} \langle \phi | D | \phi \rangle_{(n)}, \end{aligned} \quad (35)$$

and thus the desired projection function must satisfy

$$\langle \phi | D | \phi \rangle_{(n)} = \delta_{n0}, \quad n \leq p, \quad (36)$$

a condition similar to that found for the wave function projection function (29). In this case the projection function which is valid for all orders is simply

$$D(\vec{R}) = 1, \quad (37)$$

as can be verified by noting that with this choice (36) reduces to the normalization condition (8). We note that this result agrees with that obtained by Gartenhaus and Schwartz¹¹ (see Appendix A).

(ii) The second is explicit calculation of the c.m. corrections for the matrix elements. As noted above the c.m. problem can be solved (for the theory considered here) simply by using intrinsic operators when calculating matrix elements. Usually, however, the "full" operators have been used instead. There are two reasons for this; intrinsic operators are more complicated, and unless one wished to use the Gartenhaus-Schwartz prescription, there is no particular reason to use intrinsic operators.

In the theory considered here the calculation of c.m. corrections is quite an easy task. Basically, they are given by the expectation value of the c.m. part of the full operator which can easily be determined by using the generating function ϕ_λ . For example, the operator for the mean square radius, $\bar{r}^2 = (1/A) \sum_{i=1}^A r_i^2$, has the form

$$\bar{r}^2 = \bar{r}^{2int} + R^2, \quad (38)$$

from which it directly follows that

$$\langle \bar{r}^2 \rangle_p^{int} = \langle \bar{r}^2 \rangle_p - \langle R^2 \rangle_p. \quad (39)$$

The correction, $\langle R^2 \rangle_p$, can be determined by expanding

$$\begin{aligned} \langle R^2 \rangle_\lambda &\equiv \langle \phi_\lambda | R^2 | \phi_\lambda \rangle = \frac{3}{2} \frac{b^2}{A} (1-\lambda)^{-1/2} \\ &= \sum_{n=0}^{\infty} \lambda^n \langle R^2 \rangle_{(n)}. \end{aligned} \quad (40)$$

This gives

$$\langle \bar{r}^2 \rangle_p^{int} = \langle \bar{r}^2 \rangle_p - \frac{3}{2} \frac{b^2}{A} \beta_p, \quad (41)$$

with

$$\beta_p = \frac{(2p+1)!!}{(2p)!!}, \quad (42)$$

i.e., $\beta_0 = 1$, $\beta_1 = \frac{3}{2}$, $\beta_2 = \frac{15}{8}$, $\beta_3 = \frac{35}{16}$, An even simpler example is the c.m. correction for the energy, which can be obtained directly from (20) and (26):

$$E_p^{int} = E_p - \frac{3}{2} \omega \beta'_p, \quad (43)$$

with

$$\beta'_p = \frac{(2p-1)!!}{(2p)!!}, \quad (44)$$

i.e., $\beta'_0 = 1$, $\beta'_1 = \frac{1}{2}$, $\beta'_2 = \frac{3}{8}$, $\beta'_3 = \frac{5}{16}$,

III. DISCUSSION

Our main results concern projection [see Eqs. (28), (31), (33), (37)]. The projection functions which are valid to all orders were found to be extremely simple. They are independent of all parameters of the theory and therefore essentially determined by dimensional considerations. As a result the same projection prescriptions can be directly applied to the results obtained with other theories: there is no need to "choose the appropriate oscillator parameter," etc.

As far as we know, the result we have obtained for wave function projection [see Eq. (28) and (31)] is new. It is interesting to note that choosing $W(R) = \phi_0(R)$, which would eliminate the spurious components of the wave function, would not give the correct solution. Thus, the argument that a particular method eliminates spurious states^{11,12,21} does not really provide any justification that the method gives the correct intrinsic results. The result for density projection [see Eqs. (34) and (37)] agrees with Gartenhaus-Schwartz transformation. It thus provides a non-trivial justification of this widely used prescription (see Appendix A).

The results for the explicit c.m. corrections [see Eqs. (41)-(44)] are primarily of academic interest. They illustrate the convergence problems associated with the c.m. motion approaching a plane wave if one went to very high orders in perturbation theory. Also they can be used for rough estimates for the corrections for other theories in a similar way that the pure HOSM has been used in the past. For example, since Brueckner-Hartree-Fock theory includes all second order perturbation corrections to the energy, the result for the c.m. corrections [Eq. (43)] with $p=2$ would be more appropriate than the correction for the pure HOSM, corresponding to $p=1$.²²

ACKNOWLEDGMENT

The author would like to thank J. H. Koch for critically reading the manuscript. This work is part of the research program of the Institute for Nuclear Physics Research (IKO), made possible by financial support from the Foundation for Fundamental Research on Matter (FOM) and the Netherlands Organization for the Advancement of Pure Research (ZWO).

APPENDIX A

In this appendix we briefly discuss the Gartenhaus-Schwartz (GS) prescription for treating c.m. effects. We do this in order to illustrate that this method is, in effect, only a projection prescription, and thus that our proof that this method is correct for a specific theory is by no means trivial. Due to the way in which it was derived this prescription has caused much confusion, which in turn has given rise to a series of critiques on this subject.^{19, 23-25} Some of these go so far as to imply, in contrast to what we find here, that this prescription is not correct. Below we summarize the main features of the GS paper.¹¹

The basic motivation, which Gartenhaus and Schwartz use as the starting point to develop their method for treating c.m. effects, is that the wave function should be translationally invariant. In order to accomplish this they introduce a unitary transformation whose effect (the precise form of the GS operator is not required for the present purposes) on the wave function is

$$\psi(\vec{r}_1 - \vec{R}, \dots, \vec{r}_A - \vec{R}, \vec{R}) \rightarrow \alpha^{3/2} \psi(\vec{r}_1 - \vec{R}, \dots, \vec{r}_A - \vec{R}, \alpha \vec{R}). \quad (\text{A1})$$

By taking the limit $\alpha \rightarrow 0$ such a translationally invariant wave function can thus be obtained. Aside from possible normalization difficulties this is equivalent to wave function projection [see Eq. (28)] with $W(\vec{R}) \sim \delta(\vec{R})$. Rather than taking this limit directly Gartenhaus and Schwartz note that one can first construct the desired matrix element; then redefining the c.m. coordinate \vec{R} , $\vec{R} \rightarrow \alpha^{-1} \vec{R}$, one has

$$\langle \psi' | O | \psi \rangle \rightarrow \langle \psi' | \tilde{O} | \psi \rangle, \quad (\text{A2})$$

where the operator \tilde{O} is the same as O but with

the replacements $\vec{R} \rightarrow \alpha^{-1} \vec{R}$ and for the conjugate c.m. momentum $\vec{P} \rightarrow \alpha \vec{P}$. Since the former gives difficulties in the limit $\alpha \rightarrow 0$, Gartenhaus and Schwartz postulate that O should be independent of \vec{R} ; the limit $\vec{P} \rightarrow 0$ then makes the operator \tilde{O} purely intrinsic. This gives the GS prescription, which is (a) that intrinsic matrix elements can be calculated in the normal way with shell model based wave functions but using an intrinsic operator, and (b) a method for constructing the intrinsic operator. The former is identical with density projection [Eq. (34)] with $D(\vec{R}) = 1$.

What has caused the most confusion about the GS method is that on the surface it appears to be equivalent with two generally incompatible prescriptions, namely, wave function projection with $W(\vec{R}) \sim \delta(\vec{R})$ and density projection with $D(\vec{R}) = 1$. The resolution of this contradiction, pointed out by Friar¹⁵ and by Palumbo,²³ is that if (A1) is used in a matrix element, the limit $\alpha \rightarrow 0$ does not correspond to wave function projection. The point is that the latter really requires not $\alpha \rightarrow 0$ but $\alpha \vec{R} \rightarrow 0$, and since in a matrix element one integrates over all \vec{R} automatically, the limit $\alpha \vec{R} \rightarrow 0$ cannot be attained. In other words (A1) with $\alpha \rightarrow 0$ only gives translational invariance within a bounded region, $R < R_0 = \text{const}$. Thus, if one calculates matrix elements, the integration over \vec{R} should also be bounded. After making the replacement $\vec{R} \rightarrow \alpha^{-1} \vec{R}$ this bound becomes $R < \alpha R_0$ and, in the limit $\alpha \rightarrow 0$, \vec{R} is restricted to the origin. One thus obtains density projection with $D(\vec{R}) \sim \delta(\vec{R})$, which is perfectly consistent with the wave function projection prescription above.

We thus conclude that while the GS method in the sense (a) above gives one possible prescription for treating c.m. effects, it is inconsistent with what GS originally considered to be the desired solution to the c.m. problem. Concerning (b), the question of how to construct intrinsic operators, in this paper we take the point of view that intrinsic matrix elements are simply not defined unless the intrinsic operator is already known, and thus this problem, *per se*, does not occur. We only note that if one makes the very natural assumption that intrinsic operators should be used, the GS transformation, since it is unitary, does not affect matrix elements at all.

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