Center-of-Mass Corrections in Nuclear Levels of Non-normal Parity*

N. FREED† AND PAUL GOLDHAMMER‡
Department of Physics, University of Nebraska, Lincoln, Nebraska
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A simplified method of constructing shell-model wave functions for states of nonnormal parity is applied to the $1p$ shell. The center-of-mass motion is confined to the $1s$ state for oscillator orbitals, as it is for ground states.

THE observation of low-lying energy levels in the $1p$ shell with parity opposite to that of the ground-state configuration has motivated numerous theoretical studies.[1–4] These studies are usually performed within the context of the intermediate coupling calculations, in which the Hamiltonian is taken to be

$$H=-(\hbar^2/2m)\sum_i \nabla_i^2+\sum_{i<j} V_{ij}+a\sum_i \mathbf{l}_i\cdot\mathbf{s}_i \qquad (1)$$

where V_{ij} is a central two-body interaction operator, and the strength of the spin-orbit operator a must be varied throughout the shell (in addition, a must differ for $1p$ and $1d$ orbitals). The Hamiltonian is then diagonalized with respect to the states generated by those configurations obtained from the promotion of one orbital out of the ground-state configuration $(1s)^4(1p)^{A-4}$ of an oscillator well:

$$(1s)^4(1p)^{A-5}(1d), \qquad (2a)$$

$$(1s)^4(1p)^{A-5}(2s), \qquad (2b)$$

and

$$(1s)^3(1p)^{A-3}. \qquad (2c)$$

Elliott and Skyrme[5] have pointed out that all of the states generated by these configurations should not be included in the calculation. The nuclear shell model supplies basis functions in which all particle motion is referred to the fixed center of an oscillator well, and therefore the center of mass of the nucleons oscillates about this center. For ground-state configurations, such as $(1s)^4(1p)^{A-4}$, this motion is confined to the $1s$ state.[5,6] Excited configurations, like those in Eq. (2), contain states which involve a spurious excitation of the center of mass. Such unphysical states must be removed from the set of shell-model basis functions before even qualitative agreement with the observed nuclear spectra may be obtained.

The removal of such spurious states is not easy in practice, and causes severe technical difficulties. Frequently the problem is left to a high-speed computer. In this note we describe a method of constructing basis states free of spurious center-of-mass excitation which has the advantage of being extremely simple formally.

All of the configurations in Eq. (2) have a $(1s)^3(1p)^{A-5}$ "core" of orbitals in common. One may then construct (using oscillator orbitals φ_{nlm}) two-nucleon wave functions for the particles outside the core[7]:

$$\psi_{L=0,M=0}{}^{1s2s}=2^{-1/2}[\varphi_{100}(1)\varphi_{200}(2)+\varphi_{100}(2)\varphi_{200}(1)]$$
$$=(3\pi^3)^{-1/2}(q_1^2+q_2^2-3)\exp[-\tfrac{1}{2}(q_1^2+q_2^2)], \qquad (3a)$$

$$\psi_{L=2,M=2}{}^{1s1d}=2^{-1/2}(\varphi_{100}(1)\varphi_{122}(2)+\varphi_{100}(2)\varphi_{122}(1))$$
$$=(4\pi^3)^{-1/2}[(q_{1x}+iq_{1y})^2+(q_{2x}+iq_{2y})^2]\times\exp[-\tfrac{1}{2}(q_1^2+q_2^2)], \qquad (3b)$$

$$\psi_{L=0,M=0}{}^{1p1p}=\sum_m C_{m-m0}{}^{110}\varphi_{1,1,-m}(1)\varphi_{11m}(2)$$
$$=2(3\pi^3)^{-1/2}\mathbf{q}_1\cdot\mathbf{q}_2\exp[-\tfrac{1}{2}(q_1^2+q_2^2)], \qquad (3c)$$

and

$$\psi_{L=2,M=2}{}^{1p1p}=\varphi_{111}(1)\varphi_{111}(2)$$
$$=\pi^{-3/2}(q_{1x}+iq_{1y})(q_{2x}+iq_{2y})\exp[-\tfrac{1}{2}(q_1^2+q_2^2)]. \qquad (3d)$$

Introducing relative and center-of-mass coordinates for the two particles:

$$\mathbf{q}_\pm=(1/\sqrt{2})(\mathbf{q}_1\pm\mathbf{q}_2) \qquad (4)$$

we form the linear combinations

$$\Phi_{00}(1,2)=(1/\sqrt{2})(\psi_{00}{}^{1s2s}-\psi_{00}{}^{1p1p})$$
$$=(6\pi^3)^{-1/2}(2q_-{}^2-3)\exp[-\tfrac{1}{2}(q_+{}^2+q_-{}^2)]$$
$$=\varphi_{100}(\mathbf{q}_+)\varphi_{200}(\mathbf{q}_-) \qquad (5)$$

and

$$\Phi_{22}(1,2)=(1/\sqrt{2})(\psi_{22}{}^{1s1d}-\psi_{22}{}^{1p1p})$$
$$=(2\pi^3)^{-1/2}(q_{x-}+iq_{y-})^2\exp[-\tfrac{1}{2}(q_+{}^2+q_-{}^2)]$$
$$=\varphi_{100}(\mathbf{q}_+)\varphi_{122}(\mathbf{q}_-). \qquad (6)$$

Properly antisymmetric basis functions of the A-particle system can then be written in LS-coupling as

$$\Psi_{LM}{}^{2s}=\{\psi_{LM}[(1s)^3(1p)^{A-5}],\Phi_{00}(1,2)\}_{LM} \qquad (7)$$

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† Present address: Institute of Theoretical Physics, University of Lund, Lund, Sweden.
‡ Present address: University of Kansas, Lawrence, Kansas.
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for the $2s$ excitation, and

$$\Psi_{LM}{}^{1d}=\sum_{L'}(L[\![L'2)\times\{\psi_{L'M'}[(1s)^3(1p)^{A-5}]_8\,\Phi_{2m}(1_8 2)\}_{LM} \quad (8)$$

for the $1d$ excitation. The $(L[\![L'2)$ are coefficients of fractional parentage, and the curly brackets denote antisymmetric vector coupled wave functions. The spin and isobaric spin quantum numbers are not written explicitly, but their incorporation into Eqs. (7) and (8) is always implied through the orbital angular momentum (in other words L symbolically stands for $LSJT$).

It is easy to demonstrate that spurious center-of-mass excitations are absent from the shell model wave functions in Eqs. (7) and (8). Following closely the analysis of Elliott and Skyrme,[5] we may write either (7) or (8) in the form:

$$\Psi_{LM}=P_{A-3}(\mathbf{q}_i)\exp[-\tfrac{1}{2}\sum q_i{}^2], \quad (9)$$

where $P_{A-3}(\mathbf{q}_i)$ is a polynomial of degree $A-3$ in the coordinates $\mathbf{q}_i$ and is antisymmetric under the simultaneous interchange of orbital, spin, and isobaric spin coordinates of any two nucleons. The identities ($\mathbf{Q}=\sum\mathbf{q}_i/A$):

$$\sum_i q_i{}^2=\sum_i(\mathbf{q}_i-\mathbf{Q})^2+AQ^2 \quad (10)$$

and

$$P_{A-3}(\mathbf{q}_i-\mathbf{Q})=P_{A-3}(\mathbf{q}_i) \quad (11)$$

must be established to complete the proof. Equation (10) is obvious. Equation (11) may be proved by expanding $P_{A-3}(\mathbf{q}_i-\mathbf{Q})$ into a power series in Q:

$$P_{A-3}(\mathbf{q}_i-\mathbf{q})=P_{A-3}(q_i)+\mathbf{Q}\cdot P_{A-4}(q_i)+\cdots. \quad (12)$$

In order that Eq. (12) retain its homogeneity, one of the oscillator orbitals in $P_{A-4}(\mathbf{q}_i)$ must be demoted to a lower energy state. The $\varphi_{200}(\mathbf{q}_-)$ and $\varphi_{12m}(\mathbf{q}_-)$ orbitals are now invariant under $\mathbf{q}_i\rightarrow\mathbf{q}_i-\mathbf{Q}$ so we must demote a $1p$ orbital. The $1s$ shell is filled, however, with three $1s$ nucleons and $\varphi_{100}(\mathbf{q}_+)$; thus we must have $P_{A-4}(\mathbf{q}_i)\equiv 0$ and in a like manner

$$P_{A-n}(\mathbf{q}_i)\equiv 0 \quad \text{if} \quad n>3. \quad (13)$$

The wave functions in Eqs. (7) and (8) are therefore free of spurious center-of-mass excitation, and appropriate for shell-model calculations.

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Nuclear Spectroscopy With a Soft Core Potential*

YESHWANT R. WAGHMARE
Department of Physics, University of California, San Diego, La Jolla, California

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Nuclear spectroscopic calculations with a potential of the type $v(r)=v_0[(r^n-c^n/r^n)]\exp(-r^2/r_0{}^2)$ are made for the core radius $c=0.4$ F and potential range $r_0=2.06$ F. For simplicity of calculation, $n=2$ is assumed. The calculations are made for f, p, and g-shell nuclei. It is shown that in the case of Zr^{90} the configuration dependence of the effective two-body interaction can be replaced by a singular potential. The configuration interaction in this nucleus is found to depress the ground state 0^+ by ~ 0.4 MeV and raise the excited 0^+ level by the same amount. For the f and p shells, the level splittings in Ti^{50}, Ni^{58}, and Be^{10} are analyzed. The calculations show that the triplet forces are small for these configurations.

I. INTRODUCTION

IT has been shown by many authors that the nucleon-nucleon interaction inside a nucleus is strongly attractive and is believed to have a hard core at small distances of order 0.4–0.5 F. One, therefore, cannot use a perturbation approach. Also, the actual wave functions of the individual nucleons are modified due to the strong internucleonic force. In calculations one should therefore use such modified wave functions in order to calculate various quantities. However, if one uses the perturbation theory one could also use another approach. Instead of using the modified form of the wave functions, one could use the unperturbed shell-model wave functions and the modified form of the two-body Hamiltonian. Very little is known about the exact nature of the nucleon-nucleon interaction. However, some elegant theories[1–3] which would provide better understanding of the nature of nuclear forces are now available. In the past few years, the Brueckner[1] many-body theory has been extensively used in deducing various quantities concerned with the Weizsäcker mass formula. This theory is based upon the assumption of the two-particle correlations. A "reaction matrix" for a two-body potential is evaluated

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