Soluble Many-Body Problem for Particles in a Coulomb Potential*

M. MOSHINSKY†
Instituto de Física, Universidad de México, México, D.F., México
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Use is made of the accidental degeneracy of the energy levels in a Coulomb potential to construct a correlated wave function for a system of n particles in this potential.

In the atomic and nuclear shell models one considers a system of particles moving in a common potential and interacting through two-body interactions. As the problem cannot be solved exactly, the customary procedure is to start from a system of independent particles in the common potential and consider the interactions through perturbation or variational techniques.

If the common potential is of the Coulomb type, the negative energy levels have an accidental degeneracy due to the invariance of the problem with respect to a four-dimensional rotation[1] group (R_4). In this paper we shall make use of this invariance to find a set of integrals of motion for particles in a Coulomb field that diagonalize a certain type of interaction. We shall also obtain the exact eigenfunctions associated with these integrals of motion and so have a new starting point for atomic shell theory calculations.

We begin by briefly reviewing some well-known[1] considerations on the Coulomb potential which have been recently summarized by Biedenharn.[2]

The Hamiltonian

$$H=(p^2/2m)-(Ze^2/r), \tag{1}$$

commutes with the angular momentum $\mathbf{L}'$ and the Runge-Lenz[2] vector $\mathbf{A}'$ defined by

$$\mathbf{L}'=\mathbf{r}\times\mathbf{p},\quad \mathbf{A}'=(2Ze^2m)^{-1}(\mathbf{L}'\times\mathbf{p}-\mathbf{p}\times\mathbf{L}')+r^{-1}\mathbf{r}. \tag{2a,b}$$

From (2b) we obtain

$$\mathbf{A}'\times\mathbf{A}'=i[-2\hbar(Z^2e^4m)^{-1}H]\mathbf{L}', \tag{3}$$

so that defining

$$\mathbf{A}\equiv[-2\hbar^2(Z^2e^4m)^{-1}H]^{-\frac{1}{2}}\mathbf{A}',\quad \mathbf{L}\equiv\hbar^{-1}\mathbf{L}' \tag{4}$$

we get

$$\mathbf{A}\times\mathbf{A}=i\mathbf{L},\quad [L_i,A_j]=i\epsilon_{ijk}A_k,\quad \mathbf{L}\times\mathbf{L}=i\mathbf{L}. \tag{5}$$

From the commutation relations (5) we see that the components of $\mathbf{L}$, $\mathbf{A}$ could be considered as the operators associated with the six infinitesimal rotations in a four-dimensional space.[2]

The linear combinations

$$\mathbf{M}\equiv\tfrac{1}{2}(\mathbf{L}+\mathbf{A}),\quad \mathbf{N}\equiv\tfrac{1}{2}(\mathbf{L}-\mathbf{A}) \tag{6}$$

will be particularly useful as they satisfy the commutation relations

$$[\mathbf{M},\mathbf{N}]=[H,\mathbf{M}]=[H,\mathbf{N}]=0,\quad \mathbf{M}\times\mathbf{M}=i\mathbf{M},\quad \mathbf{N}\times\mathbf{N}=i\mathbf{N}. \tag{7}$$

Furthermore, from (4) and (6) we have

$$2(\mathbf{M}^2+\mathbf{N}^2)+1=\mathbf{L}^2+\mathbf{A}^2+1=-Z^2e^4m(2\hbar^2H)^{-1},\quad \mathbf{M}^2-\mathbf{N}^2=\mathbf{L}\cdot\mathbf{A}. \tag{8a,b}$$

Now let us pass to the problem of n particles in a Coulomb potential. We shall indicate by H_s, $\mathbf{M}_s$, $\mathbf{N}_s$, $\mathbf{L}_s$ the operators given above when associated with particle $s=1, 2, \cdots n$, and define the operators

$$H^{(p)}=\sum_{s=1}^{p}H_s,\quad \mathbf{M}^{(p)}=\sum_{s=1}^{p}\mathbf{M}_s,\quad \mathbf{N}^{(p)}=\sum_{s=1}^{p}\mathbf{N}_s,\quad \mathbf{L}^{(p)}=\mathbf{M}^{(p)}+\mathbf{N}^{(p)}, \tag{9}$$

where $p=1, 2, \cdots, n$.

From (9) we construct the following set of scalar operators:

$$H^{(1)}, (\mathbf{M}^{(1)})^2, (\mathbf{N}^{(1)})^2, \cdots, H^{(p)}, (\mathbf{M}^{(p)})^2, (\mathbf{N}^{(p)})^2, \cdots, H^{(n)}, (\mathbf{M}^{(n)})^2, (\mathbf{N}^{(n)})^2. \tag{10}$$

Each triplet of operators $H^{(p)}$, $(\mathbf{M}^{(p)})^2$, $(\mathbf{N}^{(p)})^2$ commute because of (7). Furthermore, as $\mathbf{M}^{(q)}$ for $q>p$ is

$$\mathbf{M}^{(q)}=\mathbf{M}^{(p)}+\sum_{s=p+1}^{q}\mathbf{M}_s, \tag{11}$$

we see that $\mathbf{M}^{(q)}$ commutes with the operators of index p in (10) as the second part in (11) contains only operators of particles $s=p+1, \cdots, q$. Therefore $(\mathbf{M}^{(q)})^2$ [and by the same reasoning $(\mathbf{N}^{(q)})^2, H^{(q)}$] commutes with all operators of index $p\leq q$, and so all operators (10) commute.

Two operators in (10) $(\mathbf{M}^{(1)})^2$, $(\mathbf{N}^{(1)})^2$ are not independent as from (2) $\mathbf{L}\cdot\mathbf{A}=0$ for a single particle, so from (8b) $(\mathbf{M}^{(1)})^2=(\mathbf{N}^{(1)})^2$ and both are related with $H^{(1)}$ by (8a). We take them out of (10) and replace them by $(\mathbf{L}^{(n)})^2$, $L_z^{(n)}$ that commute with all scalar operators.

We obtained then $3n$ commuting operators of which $H^{(n)}$, the Hamiltonian of n particles in a Coulomb field, is one. We have therefore a set of integrals of motion for this problem different from the independent-particle set H_s, $\mathbf{L}_s^2$, L_{zs}. The set of integrals of motion of the previous paragraph diagonalizes a symmetric scalar

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[1] V. Fock, Z. Physik **98**, 145 (1935); V. Bargmann, *ibid.* **99**, 576 (1936).
[2] L. C. Biedenharn, J. Math. Phys. **2**, 433 (1961).

interaction of the form

$$V=f[(\mathbf{L}^{(n)})^2,(\mathbf{M}^{(n)})^2,(\mathbf{N}^{(n)})^2], \qquad (12)$$

where f is an arbitrary function. From the commutation relations (5) and (7) the eigenvalues v of this interaction will be

$$v=f[\lambda^{(n)}(\lambda^{(n)}+1),\ \mu^{(n)}(\mu^{(n)}+1),\ \nu^{(n)}(\nu^{(n)}+1)], \qquad (13)$$

with $\lambda^{(n)}$, $2\mu^{(n)}$, $2\nu^{(n)}$ restricted to integer values.

We shall refer to the eigenfunctions of the integrals of motion (10) that have a definite total angular momentum as correlated wave functions. To find them we only need the coefficients with whose help we could transform an eigenfunction of the operators

$$\mathbf{M}_1^2,\ \mathbf{N}_1^2,\ \mathbf{L}_1^2,\ L_{z1};\quad \mathbf{M}_2^2,\ \mathbf{N}_2^2,\ \mathbf{L}_2^2,\ L_{z2} \qquad (14a)$$

into an eigenfunction of the operators

$$\mathbf{M}_1^2,\ \mathbf{N}_1^2,\ \mathbf{M}_2^2,\ \mathbf{N}_2^2;\quad (\mathbf{M}^{(2)})^2,\ (\mathbf{N}^{(2)})^2,\ (\mathbf{L}^{(2)})^2,\ L_z^{(2)}. \qquad (14b)$$

These coefficients will be the Wigner coefficients of the R_4 group obtained by Biedenharn[2] which can essentially be given in terms of 9-j coefficients, as, from (7) and (9), passing from (14a) to (14b) is a problem in the recoupling of angular momenta.[3]

As an illustration we shall give the explicit form of the correlated wave function for a system of two particles. For a single particle $\mathbf{M}^2=\mathbf{N}^2$ and so the corresponding eigenvalues are equal, i.e., $\mu=\nu$. We can then denote the single-particle ket as

$$|\mu\mu\lambda m\rangle\equiv \mathcal{R}_{2\mu+1\ \lambda}(r)Y_{\lambda m}(\theta,\varphi), \qquad (15)$$

where Y is a spherical harmonic and $\mathcal{R}$ is the radial wave function for a particle in a Coulomb field of charge $-Ze$ and total quantum number $2\mu+1$. If we now designate with the indices 1, 2 the kets (15) for particles 1, 2, the two-particle correlated wave function takes the form

$$|\mu_1\mu_2,\mu^{(2)}\nu^{(2)}\lambda^{(2)}m^{(2)}\rangle=\sum_{\lambda_1 m_1}\sum_{\lambda_2 m_2}\Bigg\{[(2\lambda_1+1)(2\lambda_2+1)(2\mu^{(2)}+1)(2\nu^{(2)}+1)]^{\frac{1}{2}} \times\begin{Bmatrix}\mu_1 & \mu_2 & \mu^{(2)}\\ \mu_1 & \mu_2 & \nu^{(2)}\\ \lambda_1 & \lambda_2 & \lambda^{(2)}\end{Bmatrix}\langle\lambda_1\lambda_2 m_1 m_2|\lambda^{(2)}m^{(2)}\rangle|\mu_1\mu_1\lambda_1 m_1\rangle|\mu_2\mu_2\lambda_2 m_2\rangle\Bigg\}, \qquad (16)$$

where $\langle|\rangle$ is an ordinary Wigner coefficient and $\{\ \}$ is a 9-j coefficient.

In a similar way, by adding a particle at a time, we could construct the n-particle correlated wave function, which could be given afterwards any desired symmetry characterization; e.g., it could be antisymmetrized if the spin part of the wave function has all spins up.

We could then use correlated wave functions as a starting point in atomic shell-model calculations. The author does not know how advantageous this starting point is for realistic electron interactions, but he would like to point out that an equivalent problem to the one discussed here, for the three-dimensional harmonic oscillator, has contributed to our understanding of nuclear collective motions from the standpoint of the nuclear shell model.[4,5]

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[5] V. Bargmann and M. Moshinsky, Nuclear Phys. **18**, 697 (1960); **23**, 177 (1961).