

MONTE CARLO STUDIES OF NUCLEI AND QUANTUM LIQUID DROPS

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Received by OSTI

AUG 31 1989

The progress in application of variational and Green's function Monte Carlo methods to nuclei is reviewed. The nature of single-particle orbitals in correlated quantum liquid drops is discussed, and it is suggested that the difference between quasi-particle and mean-field orbitals may be of importance in nuclear structure physics.

1. INTRODUCTION

The ground-state energies and wave functions of nonrelativistic many-body systems interacting via given interparticle forces can be accurately calculated with the variational Monte Carlo (VMC) method. Moreover exact results can be obtained by improving upon the VMC with the Greens function Monte Carlo (GFMC) method.¹ Such exact calculations have been carried out for atomic Bose liquid ^4He and its drops.^{2,3} Even though fully converged exact GFMC calculations are not yet practical for Fermi systems, fairly accurate studies of ground states of electron gas⁴, atomic liquid ^3He and its drops^{5,6} have been carried out.

The Monte Carlo methods are rather simple to use when the interparticle forces depend only upon the positions of the particles. The nuclear forces, on the other hand, have strong tensor, spin and isospin dependent components. Nuclei are essentially bound by these noncentral forces; the central forces are too weak to give bound states. It is rather difficult to keep track of the spins and isospins of all the nucleons in a Monte Carlo calculation. Hence VMC and GFMC calculations have so far been possible only for the very light nuclei^{7,8,9} having $A \leq 5$. These are discussed in section II. VMC methods, using cluster expansions, are being developed to study heavier nuclei.¹⁰ We hope that in the near future these methods will obtain a useful level of accuracy, and they are discussed in section III.

Fermi liquid drops having ~ 100 particles interacting with central forces can be easily studied with Monte Carlo methods.⁶ In the last section we discuss the single-

P/89/7/101

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particle orbitals in a drop of atomic liquid ^3He containing seventy atoms¹¹, to illustrate the kind of problems of interest in the shell model that can be addressed by the Monte Carlo methods.

II. VARIATIONAL AND GREEN'S FUNCTION MONTE CARLO

The most general wave function of a nucleus can be expressed as a vector function $\Psi_n(\vec{R})$ where the $3A$ dimensional vector \vec{R} represents the coordinates $\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A$ of the A nucleons, and n labels their possible spin-isospin states.¹² Since any of the A nucleons can be the Z protons, there are $A!/N!Z!$ isospin states, and since the spin of any of the nucleons can be up or down there are 2^A spin states giving a total $M = 2^A A!/N!Z!$ spin-isospin states n . This number increases very rapidly with A . It is 24, 96, 320, 1280 and 7168 for ^3H , ^4He , ^5He , ^6Li and ^8He , and limits the use of methods requiring a complete vector function to light nuclei.

Let $\Phi(\vec{R})$ be an antisymmetric product of single-particle wave functions. In the VMC method¹² the variational wave function $\Psi_v(\vec{R})$ is generally taken to be:

$$\Psi_v(\vec{R}) = \left(\prod_{i<j<k} (1 + u_{ijk}) \right) \left(\prod_{i<j} F_{ij} \right) \Phi(\vec{R}), \quad (2.1)$$

where F_{ij} and $1 + u_{ijk}$ are pair and triplet correlation operators, and their products are symmetrized because they do not commute with each other. The expectation value of the Hamiltonian

$$H = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{i<j} v_{ij} + \sum_{i<j<k} V_{ijk}, \quad (2.2)$$

is calculated by averaging $\Psi^+(\vec{R}_i) H \Psi(\vec{R}_i) / \Psi^+(\vec{R}_i) \Psi(\vec{R}_i)$ over configurations \vec{R}_i generated by Metropolis Monte Carlo sampling of $\Psi^+(\vec{R}) \Psi(\vec{R})$. The Φ , F_{ij} and u_{ijk} are determined by minimizing the energy.

The exact ground state is obtained with the GFMC method⁹ from the equation:

$$\Psi_0 = \lim(\tau \rightarrow \infty) e^{-(H-E_0)\tau} \Psi_v. \quad (2.3)$$

Carlson⁹ has compared the VMC and GFMC results obtained with the Reid - v_8 interaction for ^3H and ^4He . The available VMC energies are ~6% above the exact GFMC energies, while the density and pair distribution functions given by the two methods are very similar. Wiringa¹³ has improved upon the variational wave functions and reduced the error in the energy to ~3%. He is also studying ^6Li and ^6He with VMC method.

Expectation values of many-body operators having intricate spin-isospin structure can be easily and exactly evaluated with the MC methods. For example, the realistic nuclear electromagnetic current operator, extracted by Riska¹⁴ from the

N-N interaction has two-body terms containing spin, isospin and gradient operators. Calculations of the magnetic and charge form factors for ^3H , ^3He and ^4He could be easily carried out with it by the MC method.¹⁵ The results obtained with the Argonne-v₁₄ two-nucleon¹⁶ and Urbana model VII three-nucleon interaction⁷, and Iachello Jackson and Lande nucleon form factors are in fair agreement with the experimental data as shown in figs. 1 and 2.

VMC calculations of ^3He and ^4He have been used to study models of the three-nucleon interaction⁷, effects of correlations on the Coulomb sum¹⁷ and the response functions of the trinucleons.^{18,19} These methods can also be used to study low-energy resonances⁸ and nuclear reactions.

III. CLUSTER EXPANSION MONTE CARLO

The Monte Carlo methods discussed in the previous section are impractical for heavier nuclei due to the large number of spin-isospin states, which is, for example, 843, 448, 320 in ^{16}O . Ideally, one would like to learn how to sample the spin-isospin space together with the $3A$ -dimensional coordinate space, and avoid using spin-isospin vectors. However, this has not yet become possible. The variance in sampling \vec{R} is not too large because when $\Psi_v(\vec{R})$ is close to the ground state the local energy $E(\vec{R})$:

$$E(\vec{R}) = \Psi_v^\dagger(\vec{R}) H \Psi_v(\vec{R}) / \Psi_v^\dagger(\vec{R}) \Psi_v(\vec{R}), \quad (3.1)$$

does not vary too much with \vec{R} ; when $\Psi_v(\vec{R}) = \Psi_0(\vec{R})$ the $E(\vec{R})$ equals E_0 at all values of \vec{R} and variance is zero. Many obvious ways to sample the spin-isospin space are impractical due to the large variance they produce. VMC calculations of ^{16}O , including effects of tensor forces, were first attempted by Carlson and Kalos.²⁰

Alternatively one could expand the energy in contributions of clusters containing a given number of particles linked via correlations or interactions. The Monte Carlo methods can be used to exactly calculate the contribution of clusters containing several particles. To calculate the contribution of four-body clusters, for example, we need to consider only four-body spin-isospin states which are ≤ 96 . We have attempted¹⁰ such a variational calculation for ^{16}O , using the Argonne-v₁₄ two-nucleon interaction and the Urbana-VII three-nucleon interaction. The preliminary results of this calculation are summarized in table I. The number in parenthesis gives the sampling error in the last digit. Note that the error in the total energy is generally less than that in either the kinetic or potential energies which tend to cancel.

The first four columns of table I give contributions of 1 to 4-body clusters. The column Σ gives the sum of 1 to 4-body-cluster contributions, while a crudely estimated sum of all clusters is listed in column "Est." The difference between "Est"

and Σ provides an estimate of the magnitude of five- and more-body contributions. The first four rows give contributions of kinetic, local pair-interactions (central, spin, isospin, tensor and Coulomb), non-local pair-interactions (spin-orbit, quadratic spin-orbit and L^2) and three-body interactions respectively. It appears that the convergence for kinetic and two-body interaction contributions is good, but that of $\langle V_{ijk} \rangle$ is not too good, and we can expect ~ -1 MeV per nucleon from five and more-body clusters. We should note that a variational calculation keeping V_{ijk} and only 1, 2 and 3-body terms was not possible; with a reasonable parameter space the energy calculated in this approximation had no minimum.

TABLE I
Cluster expansion of the energy of ^{16}O in MeV per nucleon.

| | 1 | 2 | 3 | 4 | Σ | Est. |
|----------------|---------|----------|---------|---------|----------|-------|
| Kinetic | 18.0(3) | 13.6(2) | -2.2(3) | 0.1(3) | 29.5(5) | 29.4 |
| v_{ij} -loc. | | -40.7(4) | 6.6(3) | -0.4(4) | -34.6(5) | -34.7 |
| v_{ij} -n.l. | | -0.3(1) | | | -0.3(1) | -0.3 |
| V_{ijk} | | | -2.6(1) | 1.5(1) | -1.1(1) | -1.6 |
| total | 18.0(3) | -27.9(3) | 1.7(3) | 1.2(3) | -6.5(3) | -7.2 |
| t(min) | 0.02 | 0.2 | 14.5 | 420 | | |

The last row gives the required computer (Cray 2-S single processor) time in minutes to do the calculation. It appears that in the future, with more efficient computers, we can sum up to 5-body clusters and perform such variational calculations with realistic forces. However it is not known if GFMC or similar exact calculations are possible using cluster expansions. The calculated density-distribution of ^{16}O (fig. 3) is in fair agreement with the empirical data. We note that the binding energy of ^{16}O , as estimated by this VMC calculation, with the Argonne v_{14} two-nucleon and Urbana model VII three nucleon interactions is $\sim 10\%$ too small. This difference could be due to the inaccuracy of this VMC calculation or due to deficiency of the model interactions used.

IV. SINGLE PARTICLE ORBITALS IN QUANTUM LIQUID DROPS

The nature of single-particle orbitals in a correlated Fermi system is one of the interesting aspects of the shell model that can be studied with the Monte Carlo method. Such studies have not yet been carried out for nuclei, however, we can use liquid ^3He drops as illustrative examples. Detailed studies of the properties of a drop of liquid ^3He containing seventy particles have been carried out with the VMC method.¹¹ The results of these studies are not exact due to the deficiencies of the

variational method, however, in the following discussion we neglect these deficiencies. In many ways this drop resembles a closed shell nucleus.

The simplest type of single-particle orbitals are obtained from a mean-field (MF) theory. As in the shell model one assumes that the N -particles in the drop occupy the lowest N orbitals $\phi_i(\vec{r})$ of a potential well $V(r)$ chosen such that

$$\sum_{i=1,N} \phi_i^2(\vec{r}) = \rho(r), \quad (4.1)$$

where $\rho(r)$ is the true density obtained from the VMC ground state Ψ_v . There are MF single-particle energies e_i associated with the ϕ_i however their physical significance is not obvious. The $\rho(r)$ and $V(r)$ of a liquid ${}^3\text{He}$ drop containing 70 particles is shown in fig. 4.

The density matrix $\rho(r,r')$ can be calculated from the VMC ground state Ψ_v :

$$\rho(\vec{r}_1, \vec{r}'_1) = N \int \Psi_v^*(\vec{r}_1, \vec{r}_2 \dots \vec{r}_N) \Psi(\vec{r}'_1, \vec{r}_2 \dots \vec{r}_N) d^3r_2 \dots d^3r_N, \quad (4.2)$$

and diagonalized¹¹ to obtain the so called natural orbitals (NO) $\psi_i(\vec{r})$ and their occupation numbers n_i :

$$\rho(\vec{r}, \vec{r}') = \sum_{i=1,\infty} n_i \psi_i^*(\vec{r}) \psi_i(\vec{r}'). \quad (4.3)$$

There are no single particle energies associated with these orbitals, however they provide a complete description of both the density distribution:

$$\rho(r) = \sum_i n_i \psi_i^2(\vec{r}), \quad (4.4)$$

and momentum distribution

$$\tilde{\rho}(\mathbf{k}) = \sum_i n_i |\tilde{\psi}(\mathbf{k})|^2. \quad (4.5)$$

The occupation numbers n_i of the natural orbitals are given in table II. We clearly see that there are seventy orbitals that are substantially occupied, while the others have relatively small occupation. Thus the basic assumption of the shell model seems to be applicable here.

The low energy states of drops having $N \pm 1$ particles can be identified as those having a quasi-particle or hole. The quasi-particle (QP) orbitals $\chi_h(\chi_p)$ are obtained from the VMC wave functions $\Psi_h(\Psi_p)$ of $N-1(N+1)$ drops, for example:

$$\sqrt{Z_h} \chi_h(\vec{r}_1) = \sqrt{N} \int \Psi_h^*(\vec{r}_2 \dots \vec{r}_N) \Psi_v(\vec{r}_1, \vec{r}_2 \dots \vec{r}_N) d^3r_2 \dots d^3r_N. \quad (4.6)$$

The $Z_{h,p}$ are quasi-particle pole strengths required to normalize the $\chi_{h,p}$ and the energies $(E_0 - E_n)$ and $(E_p - E_0)$ can be associated with the orbitals χ_h and χ_p . These orbitals can be easily and uniquely defined only for the low-energy states in the region of closed shell nuclei.

TABLE II

Occupation numbers of natural orbitals of the $N = 70$ Fermi-liquid ${}^3\text{He}$ drop.

| n,l | $n_{n,l}$ | n,l | $n_{n,l}$ | n,l | $n_{n,l}$ |
|-------|-----------|-------|-----------|-------|-----------|
| 1s | 0.54 | 1h | 0.059 | 1k | 0.024 |
| 1p | 0.58 | 2f | 0.074 | 2i | 0.022 |
| 1d | 0.60 | 3p | 0.081 | 3g | 0.028 |
| 2s | 0.63 | 1i | 0.048 | 4d | 0.038 |
| 1f | 0.69 | 2g | 0.062 | 5s | 0.039 |
| 2p | 0.77 | 3d | 0.071 | 1l | 0.018 |
| 1g | 0.75 | 4s | 0.074 | 2j | 0.016 |
| 2d | 0.84 | 1j | 0.033 | 3h | 0.013 |
| 3s | 0.85 | 2h | 0.033 | 4f | 0.019 |
| | | 3f | 0.039 | 5p | 0.022 |
| | | 4p | 0.045 | | |

In extended liquids the MF, NO and QP orbitals are just plane waves. In this case Z_F i.e. $Z_{h,p}$ for h or p close to k_F , is given by the discontinuity of the occupation probability²¹ $n(k)$ at k_F . Approximate values of Z_h for $h < k_F$ in nuclear matter, have been recently calculated by Benhar, Fabrocini and Fantoni²², and attempts to measure the Z_h in ${}^{208}\text{Pb}$ will be discussed by de Witt Huberts.²³

In quantum liquid drops having closed shells, the MF, NO and QP orbitals have the quantum numbers n, ℓ, m ignoring spin for simplicity. However, their radial wave functions are generally not identical as illustrated in figs. 5-7. Substantial differences occur when two or more states having the same ℓ, m are occupied in the shell model sense. In the $N=70$ drop the 1s, 2s, 3s; 1p, 2p; 1d, 2d; 1f and 1g states are occupied. Hence the 3s, 2p and 2d MF, NO and QP wave functions are rather different, while those for 1f and 1g are similar.

The MF and NO having $\ell = 0$ are compared in fig. 5. The essential difference between them is that the NO are highly localized for the hole states. They are quite similar to the localized MF states^{11,24} $\phi'_{n,0}$ which are linear combinations of the occupied $\phi_{n,0}$ (fig. 6). For example, the localized $\ell=0$ s-states are given by:

$$\phi'_{n,0} = \sum_{n'=1,3} a_{nn'} \phi_{n',0}; \quad n = 1,3, \quad (4.7)$$

where the $a_{nn'}$ are chosen so that $\phi'_{n,0}$ are maximally localized.

The QP orbital is uniquely defined for the 3s state; it can not be so easily defined for the other s-states because of their widths. It is in-between the MF and NO as shown in fig. 7. The density difference $\Delta\rho(r)$ between the $\rho(r)$ of $N=70$ and $N=69$ drops is also shown in fig. 7. It is similar²⁵ to the $\Delta\rho_c$ between ${}^{206}\text{Pb}$ and ${}^{205}\text{Tl}$, and is better explained with the QP orbital, than with the MF or NO.

A simple local density approximation provides a fairly accurate relation between the MF and QP orbitals.¹¹ It is:

$$\chi_h(\vec{r}) \propto \sqrt{Z_F[\rho(\vec{r})]} \phi_h(\vec{r}), \quad (4.8)$$

where $Z_F(\rho)$ is the QP normalization in infinite liquid at density ρ . Thus, even though the NO and QP orbitals in finite systems are not equal to the MF orbitals, at least in helium liquid drops, good and simple approximations (4.7) and (4.8) relate them.

All the QP orbitals are more surface peaked than the MF orbitals. They should be used instead of MF orbitals to calculate the matrix elements of the effective interaction²⁶, the energies and transition densities of vibrational states²⁷, etc. In fact, some of the difficulties in the quantitative understanding of these matrix elements and transition densities may be due to the differences between MF and QP orbitals.

This work was supported by the US National Science Foundation under Grant PHY84-15064, and by the US Department of Energy (Nuclear Physics Division) under contract No. W-31-109-ENG-38.

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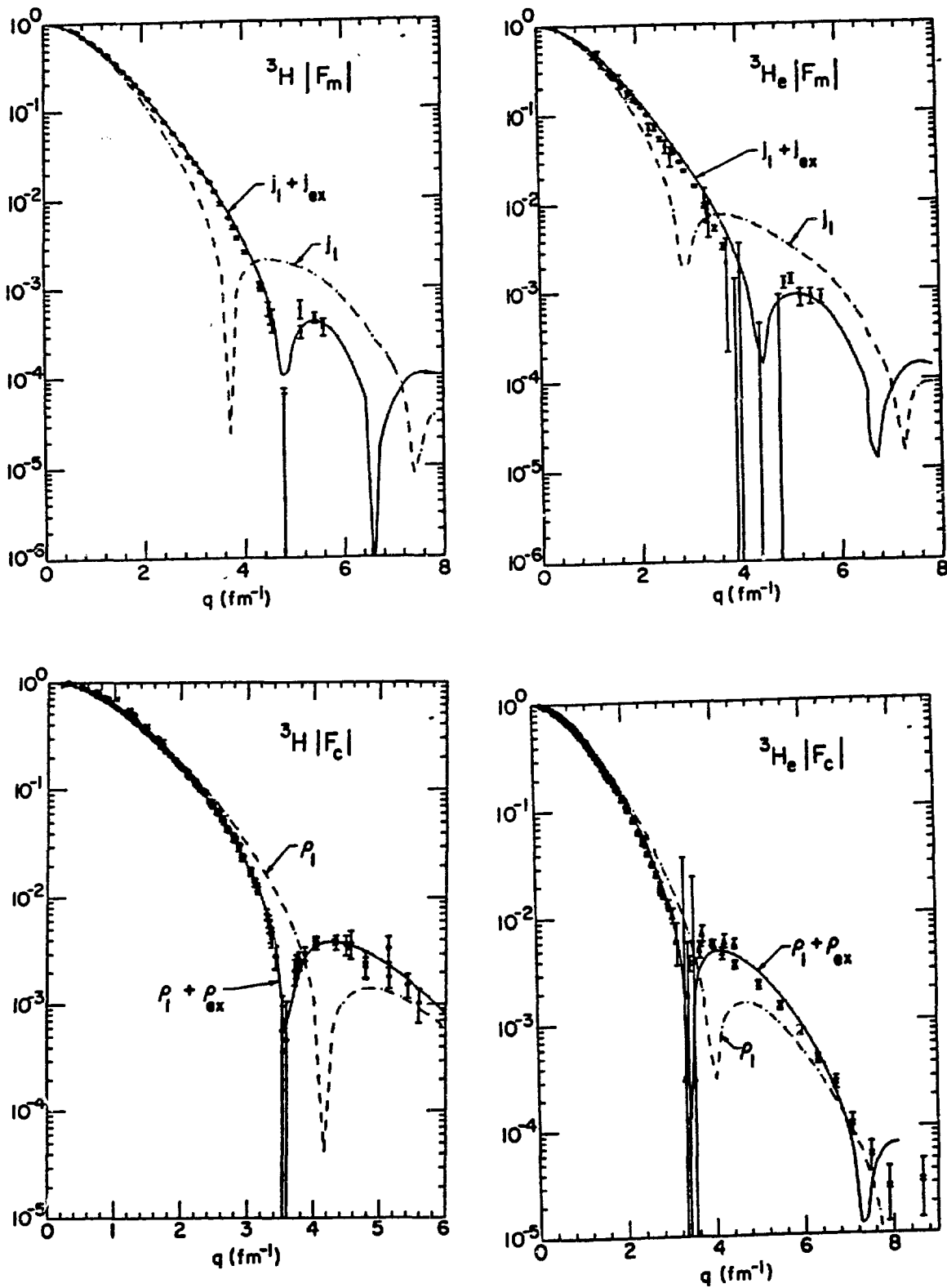


FIGURE 1

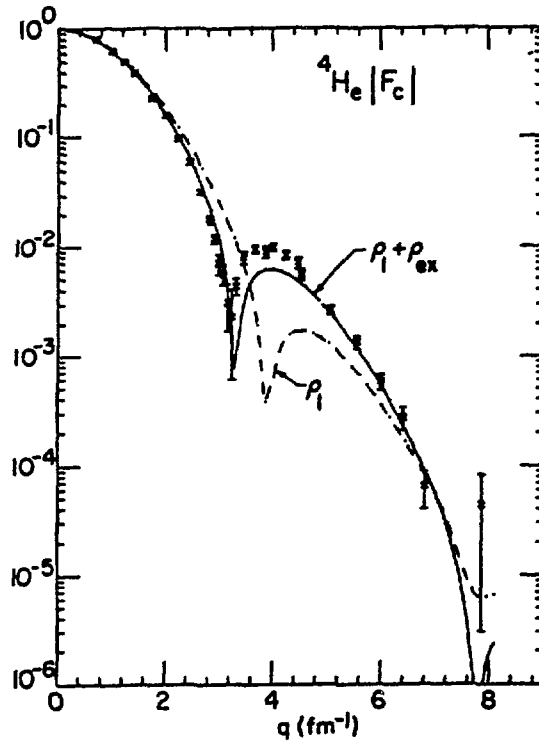


FIGURE 2

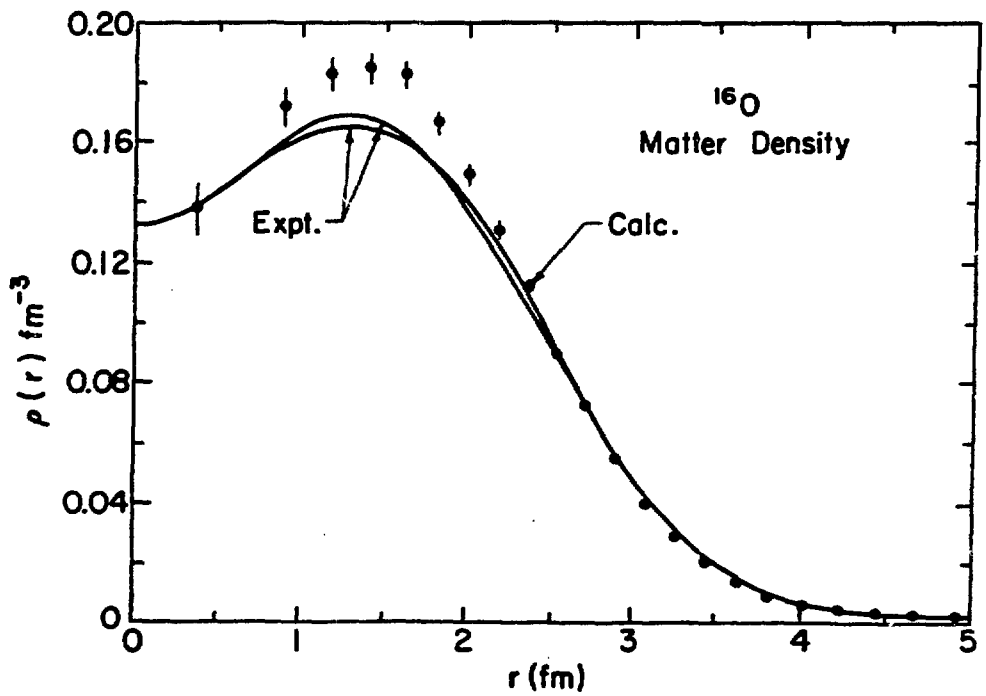


FIGURE 3

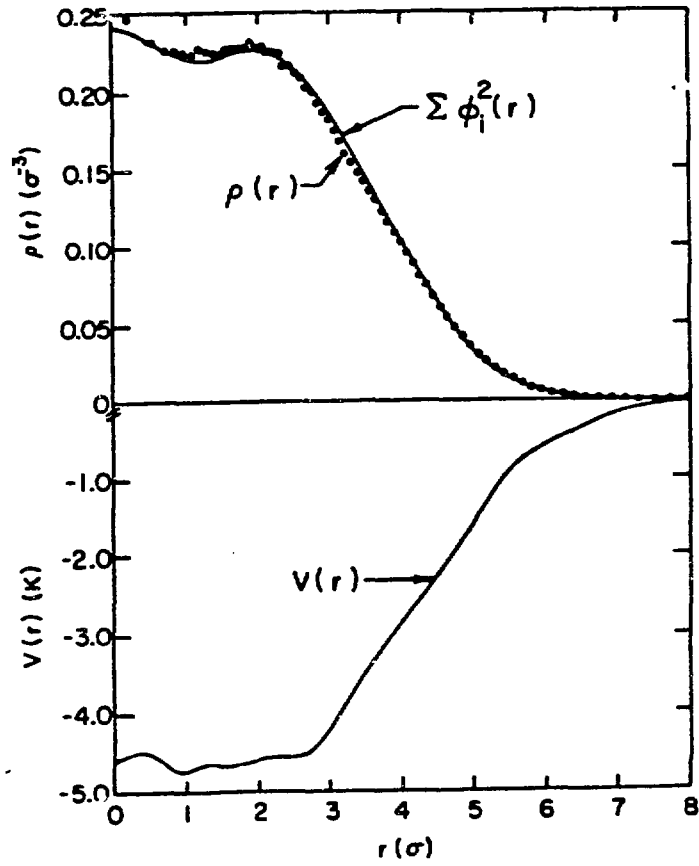


FIGURE 4

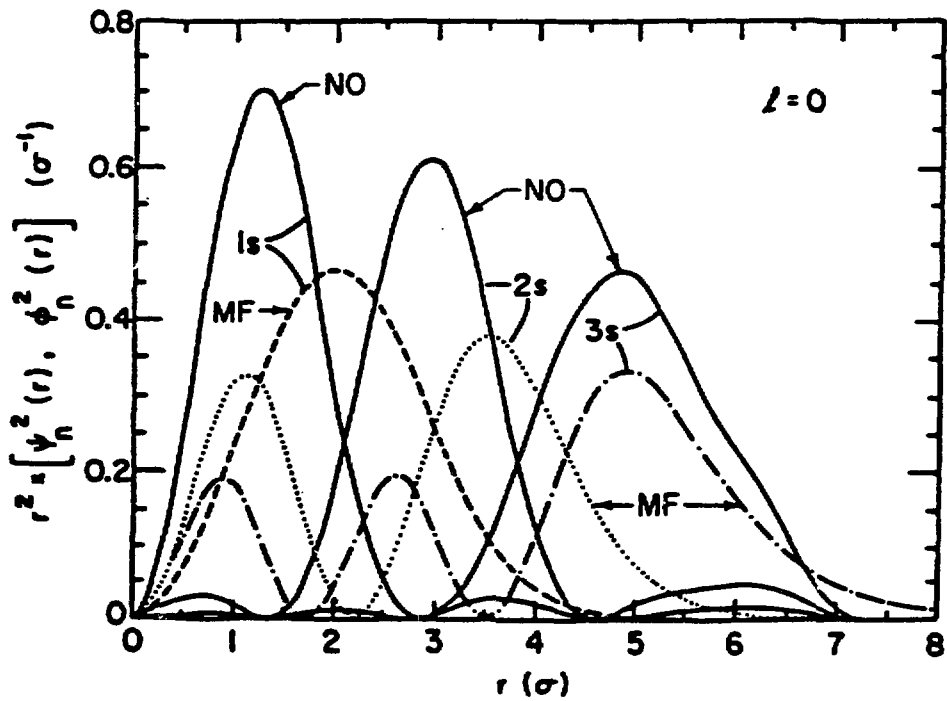


FIGURE 5

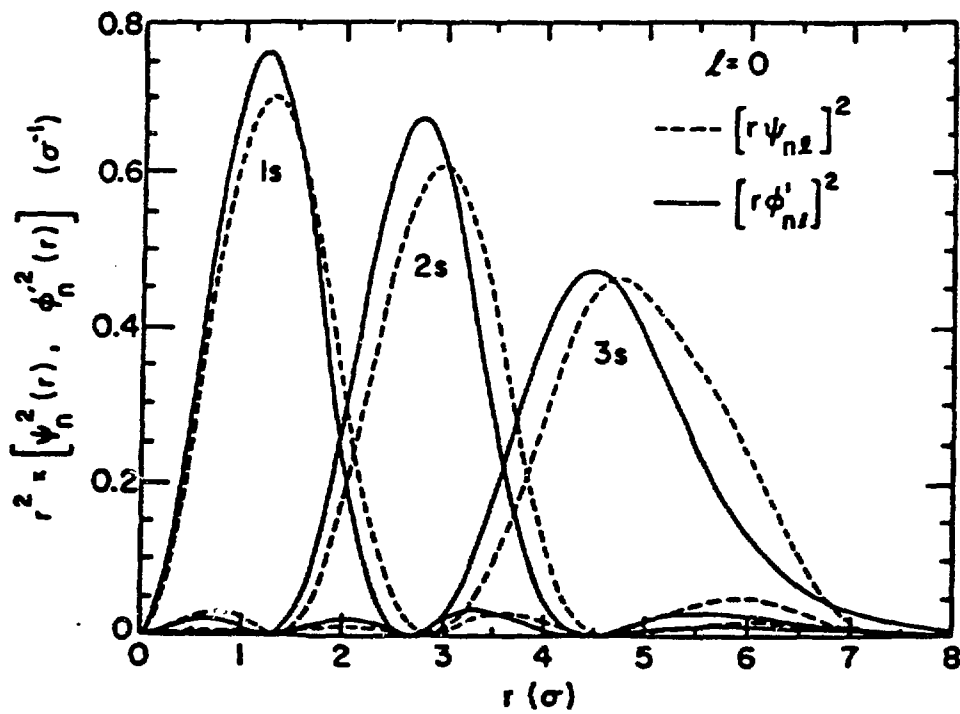


FIGURE 6

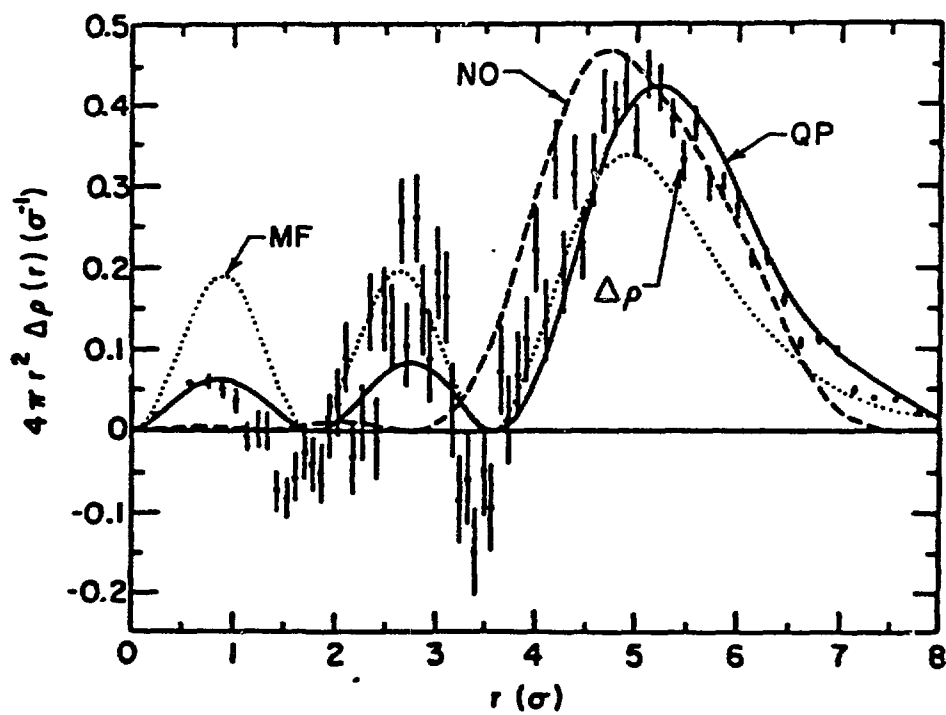


FIGURE 7