ure 2 shows the part of the absorption curve we are able to calculate for $\alpha = 6$. The dashed vertical line indicates the position of the zero-phonon peak, which has not been drawn. The dashed curve is the one-phonon contribution.

The general behavior predicted here is valid for $\alpha \gtrsim 5$ and is expected to remain qualitatively the same for $\alpha \gtrsim 3$ (except for some "threshold" values of α). The most important conclusion of this Letter is the appearance of a complex dependence of the optical absorption on Ω, entirely different from the peaks predicted by FHIP[4] which are just at the FC levels. In fact, we show that the concept of an FC state breaks down for continuum polarons certainly if $\alpha > 3$.

We finally wish to point out that the present results are of great importance for the possible experimental confirmation of the existence of internal excited polaron states and also of the whole polaron theory.

Unfortunately, no experimental result on the absorption spectra of free continuum polarons is available, and a comparison with experiment is not possible yet. The optical experiments by Mühlstroh and Reik[6] on $LaCO_3$ and those by Baer[7] on $SrTiO_3$ are not relevant for the present calculations, the former because small polarons are involved, the latter because one gets in a complex situation and, e.g., continuum polaron theory is not adequate to describe transport phenomena. We will discuss this situation in detail in a forthcoming publication.

However, some systems involving continuum polarons, such as color centers or excitons, have absorption spectra showing a structure similar to that described here.[8,9] We show in a subsequent paper that those systems, and especially the F center in AgBr, can be described by a continuum polaron approximation. This gives qualitative evidence of the validity of our conclusions.

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IS THE STRUCTURE OF O^{16} UNDERSTOOD?

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We argue that the structure of O^{16} cannot be completely understood unless the position of the first 0^+ state can be calculated without using adjustable parameters. We further demonstrate that this state cannot be calculated by Hartree-Fock or related methods using the present generation of nuclear forces.

Following the proposal that the low-lying positive-parity states in O^{16} might be rotational,[1] a great amount of effort has gone into an attempt at a unified description of the O^{16} energy spectrum. After the initial investigations based upon SU(3) symmetry,[2] increasingly more complex calculations, either variational[3] or shell model,[4] have been undertaken to gain understanding of the low-lying states and especially the 0^+ state at 6.06 MeV.

It became increasingly clear following the Hartree-Fock (HF) calculation of Bassichis and Ripka[3] that the four-particle, four-hole (4p-4h) state played an important role in the structure of these states. In fact because in the above calculation the 4p-4h state was well isolated, it was conjectured that it should give rise to a simple rotational band, such as that beginning at 6.06

MeV. Although this argument was convincingly made in the paper, quantitative agreement with experiment could only be obtained by using a two-body interaction which was somewhat too strong. In spite of the fact that succeeding shell-model calculations[4] produced wave functions for the first excited 0^+ state which were strongly dominated by the 4p-4h intrinsic state, no HF calculation without adjustable parameters has been able to bring the 4p-4h state down far enough to justify its interpretation as the head of the first rotational band. (By adjustable parameters we mean the use of an "effective" force whose parameters were not chosen in an independent calculation, and adjustable single-particle energies.)

Thus one has on the one hand the success of the shell model in fitting the energy of the first 0^+ state with a wave function whose major amplitude corresponds to a 4p-4h state, while, on the other hand, one has the inability of the HF calculations to provide the required 4p-4h state. Because the shell model must ultimately rely on "HF" for its theoretical justification [by "HF" we mean to include theories, e.g., Brueckner-Hartree-Fock (BHF), which treat "strong" potentials for which the ordinary perturbation series does not converge] we feel that no complete understanding of the O^{16} spectrum can be claimed until either a complete HF calculation is successful in lowering the 4p-4h state to the vicinity of 6 MeV, or the failure of HF is understood and one can otherwise derive the values of the necessary shell-model parameters. As we shall see the conclusions which we draw here are expected to remain valid for "HF" in the generalized sense we use here.

In this work we use a recently developed velocity-dependent potential which contains two-body spin-orbit and tensor terms, and which was especially derived for use in HF calculations. Full details concerning this potential are given in Nestor et al.[5] HF calculations of spherical nuclei using this potential[6] have given results in reasonable agreement with experiment for the light nuclei, although total binding energies have been too small. The results using this potential are, however, similar to, and in fact slightly better than, the results obtained in BHF calculations[7] using Kuo's G matrix.[8]

Because it is necessary in practice to truncate the basis in which the HF wave function is expanded, the choice of the basis is not arbitrary. Because it is expected that the determinant which we seek will not display axial symmetry, it will be advantageous to expand our orbitals in a Cartesian oscillator basis,

$$|\lambda\rangle = \sum_{n_x n_y n_z \sigma} a^{\lambda}_{n_x n_y n_z \sigma} |n_x\rangle |n_y\rangle |n_z\rangle \chi_\sigma^{\frac{1}{2}},$$

where

$$\langle x | n_x \rangle = [\pi^{\frac{1}{2}} 2^{n_x} n_x! b_x]^{-\frac{1}{2}} H_{n_x}(x/b_x) \exp(-x^2/2b_x^2),$$

and H_n is the Hermite polynomial given in terms of its generating function by

$$e^{-s^2+2s\xi} = \sum_{n=0}^{\infty} (s^n/n!) H_n(\xi).$$

The advantage of this choice of basis is that the nuclear deformation can be incorporated directly into the basis. That is, by proper choice of the harmonic oscillator parameters b_x, b_y, b_z, we can accelerate the convergence of the calculation with dimensionality. Stated differently we can produce deformations with a basis extending through the s-d shell, for example, that a calculation utilizing a basis of cylindrical or spherical oscillator functions could not produce even if it were to include perhaps the p-f and g shells.

We have allowed general ellipsoidal deformation subject to the following additional symmetries: (1) The orbitals are assumed to have good parity. (2) The HF wave function is assumed to be invariant under time reversal. (3) It is invariant under rotations in isospin space. [Assumptions (2) and (3) together require that each spatial state be four-fold occupied.] The validity of assumptions (1) and (2) has been tested for a number of spherical and deformed nuclei by the MIT group,[9] and in all cases, for reasonable interaction strengths, the symmetries have been found valid. Assumption (3) means that we are neglecting the Coulomb force, which is of small effect in light nuclei. Note that even with the above reduction we find that if we include in our calculation the orbitals through the p-f shell, then 72 010 (independent) matrix elements must be calculated.

The eigenfunctions and eigenvalues obtained upon solving the HF equations in the matrix representation using a basis which extends through the s-d shell are given in Table I. We have also performed the calculation including the orbitals of the p-f shell. However this increase in dimensionality results in a change of energy relative

Table I. Energies and wave functions of the occupied states of the deformed state of O^{16}. The oscillator parameters are $b_x=1.46$, $b_y=1.70$, and $b_z=2.07$.

$n_x n_y n_z \sigma$	Even-parity states ϵ −41.7	−9.99
000+	0.997	0.017
i110+	0.009	−0.003
200+	−0.068	0.018
020+	−0.024	−0.073
002+	−0.017	0.991
−101−	−0.012	0.076
i011−	0.003	−0.081
$n_x n_y n_z \sigma$	Odd-parity states ϵ −24.3	−15.7
001+	0.997	0.051
−100−	0.057	0.142
i010−	−0.059	0.989

to the ground state of less than 1 MeV. (Because of our choice of basis the necessary deformation of this state could be produced at very low dimensionality. Thus increasing the dimensionality lowers the energy of this state and the ground state by essentially the same amount, an amount due to further improvement of the shape of the tails of the single-particle wave functions.) The energy of the state is found to be 26.1 MeV. Allowing for an expected 6 MeV to be obtained upon projection of angular momentum, we obtain an excitation energy of approximately 20 MeV to be compared with the experimental value of 6 MeV.

Before discussing this result let us first reexamine the approximations which we have made. Of the symmetries which we have assumed it has been suggested only by Kelson[3,4] that one, parity, should be broken. Even if we were to relax this symmetry, however, we could certainly not gain enough energy to claim agreement with experiment. Further, as we have discussed, the effect of truncating the basis was examined and found to be negligible. We thus conclude that it is not possible using the present generation of nuclear forces to calculate the position of the first 0^+ state in a calculation without adjustable parameters. We feel confident, for example, from the work of Refs. 6 and 7, that we would obtain similar results were we to do a complete BHF calculation using Kuo's G matrix.[8]

Possibly the resolution of this problem will come only through an improved treatment of higher order diagrams, in particular the (momentum-nonconserving) diagrams associated with the nuclear surface. (Such diagrams would be of more importance in the calculation of the excited state with its greater surface; one may further speculate that the omission of such diagrams is responsible for the fact that finite nuclei tend to be underbound relative to the value one expects on the basis of nuclear matter calculations using the same force.) But the conclusion of this Letter, the one note on which we wish to close, is the fact that we do not completely understand the low-lying states in O^{16} and cannot claim that we do, until a complete calculation as defined here is successful.

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