VALIDITY OF NUCLEAR DEFORMATION ENERGIES OBTAINED FROM SINGLE-PARTICLE LEVELS*†

W. H. Bassichis
Laboratory for Nuclear Science and Physics Department,
Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

and

L. Wilets
Department of Physics, University of Washington, Seattle, Washington 98105
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Several prescriptions have been pursued for approximating the nuclear deformation-energy surface employing single-particle energies and wave functions. Theoretical arguments are presented to demonstrate that such a program cannot be valid without utilization of further information about the two-body potential. A numerical test is performed on various approximative schemes; all were found to be substantially in error.

The problem of nuclear deformation-energy surfaces has been of great interest, since it enters directly into the description of nuclear collective properties such as quadrupole moments, vibrational force constants, and the entire fission process. Various techniques and prescriptions are currently being utilized in attempts to extract deformation energy from single-particle models of the Nilsson type.[1-4] Such approaches have been subject to practical ambiguities with respect to the handling of saturation, the detailed shape of the independent-particle model (IPM) potential, etc. A partial resolution of these difficulties has been effected through the incorporation of various kinds of empirical data, averaging procedures, etc., in order to normalize or determine model parameters.

Beyond practical difficulties, however, there remain fundamental difficulties which appear to severely limit, if not negate, the utility of such programs. We proffer theoretical arguments and numerical calculations in support of this assertion. We emphasize, however, that this in no way should be construed as casting any doubt on the utility of Nilsson-type wave functions and energy levels in any context other than mapping out the deformation-energy surface. When the nuclear deformation is known, the Nilsson wave functions and energies appear to describe the system very satisfactorily.

We present first an interpretation of the Nilsson IPM.[5,6] We consider that there exists some effective Hamiltonian

$$H=\sum_i P_i^2/2m+\tfrac{1}{2}\sum_{i\neq j} v(x_i,x_j)\equiv T+V \tag{1}$$

that is amenable to Hartree-Fock (HF) calculations. Minimization of the expectation value of H with respect to a determinental wave function leads to the HF equations

$$h\psi_n(x)=\epsilon_n\psi_n(x), \tag{2}$$

where

$$h\psi_n(x)=(P^2/2m)\psi_n(x)+\sum_{n'}\int dx'\,\psi_{n'}^*(x')v(x,x')[\psi_{n'}(x')\psi_n(x)-\psi_n(x')\psi_{n'}(x)]\equiv(t+u)\psi_n(x). \tag{3}$$

The energy can be written

$$E=\langle H\rangle=\langle T\rangle+\langle V\rangle=\tfrac{1}{2}\sum_n(\epsilon_n+\langle n|t|n\rangle) \tag{4a}$$

$$=\sum_n\langle n|t+\tfrac{1}{2}u|n\rangle. \tag{4b}$$

In general, the single-particle, HF, self-consistent potential u will not be spherically symmetric but will contain multipole terms which we denote symbolically by

$$u=u_0-\xi q. \tag{5}$$

For quadrupole deformations, in particular, $q=r^2Y_{20}$ and the ξ is then proportional to Nilsson's β. (We will ignore the proportionality constant in subsequent discussions.)

In order to study the energy of the system at other than the minimum (equilibrium), it is necessary to impose a constraint, say that certain multipole moments $Q=\sum_i q_i(x_i)$ have some prescribed value

$$\langle Q\rangle=\bar{Q}. \tag{6}$$

This is equivalent to solving the problem described by the Hamiltonian

$$\mathcal{H} = H + \lambda Q, \tag{7}$$

where λ is a Lagrange multiplier and λQ acts like an external independent-particle potential. Now the HF minimization procedure leads to the equations

$$h\psi_n = \epsilon_n \psi_n, \tag{8}$$

with

$$h = t + u_0 + (\lambda - \xi)q. \tag{9}$$

u_0 and $-\xi q$ are generated by the nucleon wave functions but λq is the Lagrange potential. The energy is given in terms of the original Hamiltonian H, not $\mathcal{H}$, and can be expressed variously as

$$E = \langle H \rangle = \langle \mathcal{H} \rangle - \lambda \langle Q \rangle \tag{10a}$$

$$= \tfrac{1}{2}\sum_n (\epsilon_n + \langle n | t | n \rangle) - \tfrac{1}{2}\lambda \langle Q \rangle \tag{10b}$$

$$= \tfrac{1}{2}\sum_n \langle n | t + \tfrac{1}{2}u_0 - \tfrac{1}{2}\xi q | n \rangle. \tag{10c}$$

We identify $\xi - \lambda$ with Nilsson's β. It is $-\beta q$ which describes the potential deformation and generates deformation of the wave functions, but only $-\xi q$ is regenerated by the wave functions. In order to calculate the energy, it is necessary to know λ and ξ separately, not just β. This requires a knowledge of the two-body potential. In the hopes of circumventing assumptions about the two-body potential, various prescriptions have been advanced.

Equilibrium is attained for $\lambda = 0$ (no constraint), and at those points

$$(\partial E/\partial \lambda)_{\lambda = 0} = 0. \tag{11}$$

One prescription[1] assumes that E is given by analogy with (4a), namely

$$\langle \mathcal{G} \rangle \equiv \tfrac{1}{2}\sum_n (\epsilon_n + \langle n | t | n \rangle) = E + \tfrac{1}{2}\lambda \langle Q \rangle. \tag{12}$$

Although $\langle \mathcal{G} \rangle = E$ at $\lambda = 0$, $\langle \mathcal{G} \rangle$ does not achieve a minimum at $\lambda = 0$. In fact

$$\left.\frac{\partial \langle \mathcal{G} \rangle}{\partial \lambda}\right|_{\lambda = 0} = \left(\frac{\partial E}{\partial \lambda} + \tfrac{1}{2}\langle Q \rangle + \tfrac{1}{2}\lambda \frac{\partial \langle Q \rangle}{\partial \lambda}\right)_{\lambda = 0} = \tfrac{1}{2}\langle Q \rangle \Big|_{\lambda = 0}, \tag{13}$$

which is not zero unless the equilibrium deformation happens to vanish.

In order to test the degree of validity or failure of various summation schemes, numerical calculations were performed using an effective interaction for which HF calculations had proved quite successful in reproducing a variety of nuclear properties. Our conclusions here do not depend upon detailed comparison with experiment, however, but only require that the interaction be reasonable—and especially that it produce saturation. What is described below is a numerical experiment: a comparison of an internally consistent model with various approximations to that model.

The HF calculations were carried out for Ne^{20} using the Tabakin[7] interaction, treating all 20 particles self-consistently, and using a space consisting of six complete harmonic oscillator shells plus the $i_{13/2}$ shell. This space is sufficiently large so that truncation effects are negligible.[8] Of the many possible configurations only the lowest three were considered, namely those in which the last four particles are placed in a positive-parity orbit with $m = \frac{1}{2}$, $\frac{3}{2}$, or $\frac{5}{2}$. The results of starting with these configurations and applying various Lagrange multipliers λ are shown in Fig. 1, where the energy $\langle H \rangle$ is plotted as a function of $\langle Q \rangle$. The $m = \frac{1}{2}$ solutions are seen to fall on two branches, with the positive deformation being lower in energy. One notes, from Fig. 2, that the quadrupole moment is a multivalued function of λ and that there is a region of $\langle Q \rangle$ which is inaccessible without changing the single-particle level filling. The solid portions of the curves indicate the configuration which yields the minimal energy in that region of $\langle Q \rangle$.

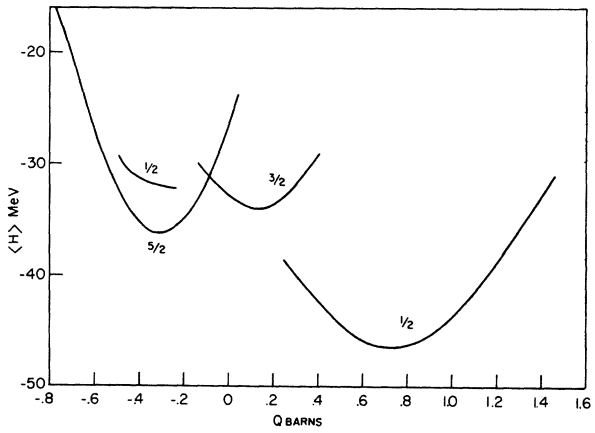

FIG. 1. The energy as a function of quadrupole moment for various single-particle level fillings.

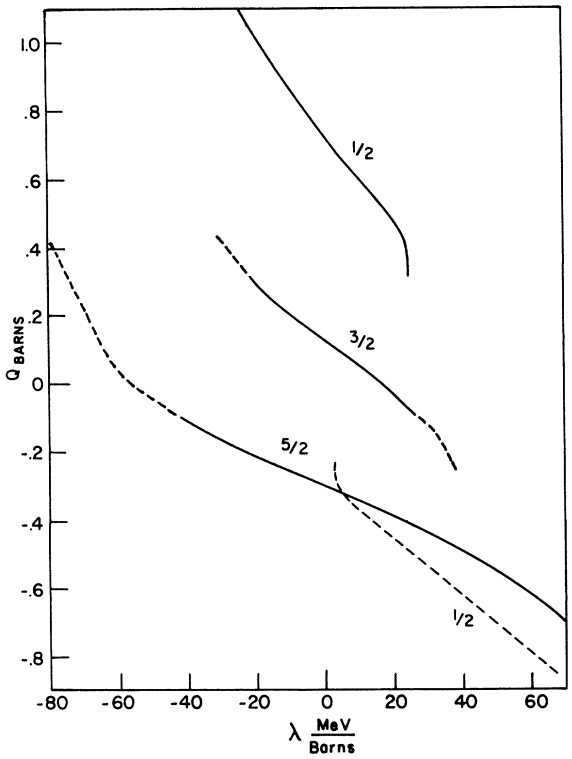

FIG. 2. The quadrupole moment as a function of the Lagrange multiplier for various configurations.

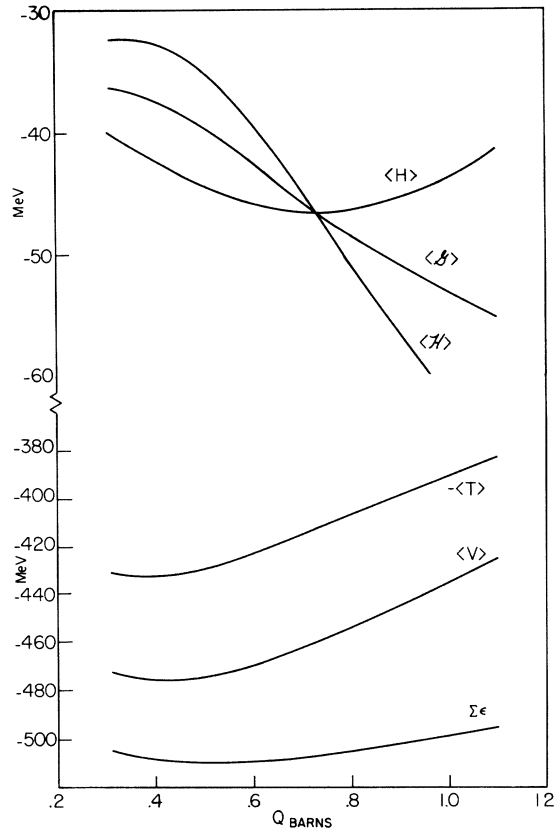

FIG. 3. Various energy-type quantities as a function of $\langle Q\rangle$. $\langle H\rangle$ is the energy, $\langle\mathcal{H}\rangle = \langle H+\lambda Q\rangle$, $\langle\mathcal{G}\rangle = \langle H+\frac{1}{2}\lambda Q\rangle$, $\langle T\rangle$ and $\langle V\rangle$ are the kinetic and potential energies, and $\sum\epsilon$ is the sum of the single-particle energies.

The comparison of the various schemes for obtaining the equilibrium deformation, Q_0, and the shape of the deformation-energy surface is found in Fig. 3. The correct procedure is, of course, to plot the energy $\langle H\rangle$ as a function of $\langle Q\rangle$. The true minimum is found to be $Q_0 = 0.73$ b. $\langle\mathcal{G}\rangle$, which is $\langle\mathcal{H}+\frac{1}{2}\lambda Q\rangle$, does not exhibit an extremum as a function of $\langle Q\rangle$ in the neighborhood of Q_0, and $\langle\mathcal{H}\rangle$, which is $\langle H+\lambda Q\rangle$, is seen to have only a maximum, occuring at $\langle Q\rangle = 0.34$ b. It has been suggested[4] that Q_0 is characterized by a minimum in the kinetic energy. There is a minimum of the potential energy which occurs at $\langle Q\rangle = 0.45$ b, but the kinetic energy has only a maximum in the neighborhood of Q_0, namely at $\langle Q\rangle = 0.38$ b. The most popular assumption[2,3] is that the variation in E is given by the variation of the summation of the single-particle energies ($\sum\epsilon$ in the figure). [This assumption is exact for the very special two-body interaction involved in the P_2 (quadrupole) model,[9] where the potential is quadratic in each particle coordinate. The P_2 model cannot be used for large deformation nor does the P_2 interaction approximate the two-body interaction generally employed in HF calculations.] Indeed, $\sum\epsilon$ does exhibit a minimum but at $\langle Q\rangle = 0.53$ b. Thus, quantitatively, none of the suggested schemes lead to the actual Q_0.

Another test of the various procedures is the deformability, i.e., the curvature of the various functions near their minima. The $\sum\epsilon$ scheme, which is the closest to being correct, has a curvature which is 1.6 times that of the true energy surface.

These calculations were performed on a light nucleus in order that the basis states employed be essentially a complete set. The failures of the various prescriptions noted here probably become more severe for a heavy nucleus at the large deformations involved in the fission process. The discrepancies there will be manifested in such crucial quantities as the position, energy, and curvature of the fission barrier and even in qualitative questions regarding existence of secondary minima.

We conclude that a quantitative calculation of the deformation surface requires a model which

incorporates detailed information about the two-body interaction.

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A_1-NUCLEON CROSS SECTION FROM COHERENT PRODUCTION IN NUCLEI

Alfred S. Goldhaber
Institute for Theoretical Physics, State University of New York, Stony Brook, New York 11790

and

Charles J. Joachain
Service de Physique Théorique et Mathématique,
Université Libre de Bruxelles, Faculté des Sciences, Bruxelles, Belgium

and

H. J. Lubatti
Department of Physics and Laboratory for Nuclear Science,
Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

and

J. J. Veillet
Faculté des Sciences, Ecole Normale Supérieure, Laboratoire de l'Accélérateur Linéaire, 91 Orsay, France
(Received 26 December 1968)

Comparison of A_1 coherent production in Freon with production in H_2 implies a total A_1-nucleon cross section $\sigma(A_1N) \leq (0.5^{+0.3}_{0.2})\sigma(\pi N)$ with a further theoretical uncertainty of about 10%. The result appears to preclude the possibility, suggested by the Deck model, that the ρ and π in the A_1 are produced close together without appreciable interaction between them.

Controversy surrounds the "A_1" bump[1] in the $(\rho\pi)$ mass spectrum observed in the reaction

$$\pi + N \to (\rho\pi) + N. \quad (1)$$

It is difficult to establish that this bump is a particle, or resonance, for the following reasons:

(1) With the usually accepted quantum numbers $J^{PG} = 1^{+-}$, $\rho\pi$ is the only available decay mode for the A_1. Thus a resonance cannot be confirmed by observing alternative decay modes.[2]

(2) A_1 has not been observed with convincing statistics in other reactions (e.g., $\pi + p \to A_1 + \pi + N$)[3].

(3) There is a theoretical model, the Deck or "diffraction dissociation" model, which predicts a low-mass enhancement in Reaction (1). In this model the outgoing ρ and π may be thought of as close to one another in position and velocity because of the production mechanism and not because of any strong interaction between them.[4]

If we are given two alternatives: (i) The A_1 is a resonance, or (ii) it is a kinematic enhancement with no strong $\rho\pi$ interaction, then we might settle the question by a measurement of