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Towards model independent single-particle wave functions

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We report some results for light nuclei that strongly suggest that it is possible to construct good nuclear single-particle wave functions on the basis of recently available, shell related experimental information, by recourse to an information theory based inference approach.

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The density dependent Hartree-Fock (DDHF) approach (using zero-range interactions) provides us with a rather accurate description of the ground state (g.s.) properties of both spherical and deformed nuclei [1, 2].

Although several zero-range interactions are available, they yield rather similar results for the density [1] and the momentum distribution [3] of the g.s. In what respects to single-particle (sp) energies one may find significant differences, however, according to the value of the effective mass that characterizes the particular interaction one employs. This has thus far caused no undue worries, as the only experimental information available until recently, was that referring to a few sp energies and radii around the Fermi surface [4].

Using $(e,e'p)$ reactions it is possible to investigate properties of valence orbits and gain reliable information about deeper-lying orbits. By recourse to this technique, the experimental values corresponding to the expectation value of r^2, for each proton shell of some spherical nuclei, have become recently available [5]. In some cases these $\langle r^2\rangle$ values are adjusted by selecting a different Saxon-Woods well for each shell, a practical and convenient procedure [6]. It may be desirable, however, to have a unified theoretical description that encompasses all shells within the framework of a single theoretical construction. The aim of the present work is to present some preliminary results of an inference approach that may help one to achieve this goal.

To this end, we will try to *infer* single particle wave functions from those experimental $\langle r^2\rangle$ values, by recourse to a suitably modified (in order to describe pure states) version of the well-known maximum entropy principle (MEP) that has been recently advanced [7]. The method has been shown to provide a reasonable description of the properties of the g.s. (or of the excited states) of a quantum system on the basis of the knowledge of a few relevant expectation values. It has been successfully applied to exactly solvable models of the Lipkin type and to simple one-dimensional problems. One can use it to infer the radial part of the pertinent wave function (wf) either in the r or in the k space.

For closed-shell nuclei the sp levels are described by wf of the form $\phi_{nljm}(\mathbf{r}) = r^{-1}u_{nl}(r)\mathcal{J}_{lsjm}(\Omega,\sigma)$ with the constraints $\lim_{r\to\infty} u(r) = 0$ and $u(0) = 0$. The idea of the present effort is that of inferring the radial wf $u(r)$ on the basis of the knowledge of appropriate expectation values of suitable operators. For the sp levels with $n = 1$ according to MEP prescriptions, we can write the pertinent (to be inferred) wf in the fashion

$$u_{nl}(r) = r^{l+1} \exp\left[-\frac{1}{2}\left\{ \lambda_0 + \sum_{i=1}^{N} \lambda_i\, G_i(r) \right\}\right]. \tag{1}$$

The $(l+1)$ factor incorporates, according to Bayesian strictures [8], our knowledge concerning the behavior of the radial wf near the origin. The exponential form is the canonical MEP one of Jaynes [9], suitably modified to accommodate the description of quantum (pure) states as described in [7]. The λ's are Lagrange multipliers that guarantee both normalization and the fulfillment of the N constraints

$$\langle G_i(r)\rangle = g_i \tag{2}$$

that represent our *a priori* knowledge (see Ref. [7] for a detailed discussion), that is, one assumes that experi-

TABLE I. Overlaps between HF and inferred wave functions corresponding to all proton levels of ^{4}He, ^{16}O, and ^{40}Ca using $G_1(r) = r$ and $G_2(r) = r^2$.

	Shell	r space	p space
^{4}He	$1S_{1/2}$	0.9991	0.9991
^{16}O	$1S_{1/2}$	0.9998	0.9997
	$1P_{3/2}$	0.9993	0.9989
	$1P_{1/2}$	0.9991	0.9996
^{40}Ca	$1S_{1/2}$	0.9998	0.9986
	$1P_{3/2}$	0.9997	0.9987
	$1P_{1/2}$	0.9999	0.9994
	$1D_{5/2}$	0.9995	0.9981
	$2S_{1/2}$	0.9917	0.9887
	$1D_{3/2}$	0.9993	0.9995

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TABLE II. Comparison between HF and inferred values $\langle r^4 \rangle$ and $\langle k^4 \rangle$ for each single particle proton level of ^{4}He, ^{16}O and ^{40}Ca using $G_1(r) = r$ and $G_2(r) = r^2$.

	Shell	Quantal $\langle r^4 \rangle$	Inferred $\langle r^4 \rangle$	Quantal $\langle k^4 \rangle$	Inferred $\langle k^4 \rangle$
^{4}He	$1S_{1/2}$	21.65	20.82	0.739	0.720
^{16}O	$1S_{1/2}$	33.69	33.90	0.413	0.409
	$1P_{3/2}$	79.66	78.65	0.988	0.986
	$1P_{1/2}$	97.44	95.31	0.870	0.866
^{40}Ca	$1S_{1/2}$	67.30	67.93	0.198	0.197
	$1P_{3/2}$	131.62	132.23	0.556	0.558
	$1P_{1/2}$	126.81	126.84	0.583	0.586
	$1D_{5/2}$	215.70	214.86	1.138	1.140
	$2S_{1/2}$	293.47	284.13	1.245	1.247
	$1D_{3/2}$	235.18	232.52	1.085	1.091

mental information concerning the expectation values (2) is available.

For the sp levels with $n > 1$ the expression (1) must be multiplied by a factor r^n

$$u_{nl}(r) = r^{l+1+n} \exp\left[-\frac{1}{2}\left\{\lambda_0 + \sum_{i=1}^{N} \lambda_i \, G_i(r)\right\}\right] \quad (3)$$

and the set of functions with the factors r^{l+1}, r^{l+2}, r^{l+3}, ... is orthogonalized according to the Gramm-Schmidt procedure. In this way, approximate values of the nodes of the sp wf are obtained [10, 11] thus allowing for the posterior inference of the Lagrange multipliers corresponding to these sp states. If one performs the appropriate Fourier transformation, similar recipes hold (if spherical symmetry is assumed) in k space. This is an interesting facet of our approach, in view of the fact that the sp momentum distribution can also be obtained by analyzing the results of $(e, e'p)$ experiments [5].

As this is an introductory study undertaken with a view to test the possibilities that this MEP inference approach offers, we shall take the input values g_i of Eq. (2) to be those obtained in a DDHF calculation, performed with the SIII, Skyrme-like interaction [12]. We shall work with two operators ($N = 2$) and select $G_1(r) = r$ and $G_2(r) = r^2$ in r space, and a similar choice in k space. These are, obviously, the simplest possible functions $G(r)$ [or $G(k)$].

In the present work, we have applied this MEP-based inference approach in order to infer sp wf corresponding to all the (proton) levels of some light, doubly-closed shell nuclei: ^{4}He, ^{16}O, and ^{40}Ca. As previously stated, the corresponding input information is that of the appropriate expectation values $\langle r \rangle$ and $\langle r^2 \rangle$ (or $\langle k \rangle$ and $\langle k^2 \rangle$) evaluated with HF Slater determinants obtained with the SIII interaction [12]. The overlaps between our inferred wf and the pertinent HF ones are displayed in Table I. Our results can be regarded as fairly good ones, as these overlaps are all of the order of a 99%.

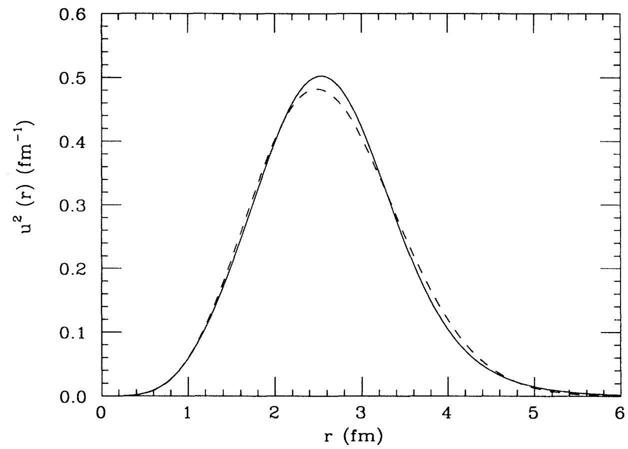

FIG. 1. Comparison between HF (continuous line) and inferred (dashed line) probability densities for the $1P_{3/2}$ proton level of ^{16}O in r space using $G_1(r) = r$ and $G_2(r) = r^2$.

Table II lists our *predicted* values for $\langle r^4 \rangle$ and $\langle k^4 \rangle$, which are compared to the pertinent HF figures. The agreement between the corresponding figures is rather good, the discrepancies being of the order of 3% at the most. Some typical quantum probability densities are depicted in Figs. 1–3. The corresponding MEP densities are compared to the HF ones. At first glance, the fact is appreciated that the agreement is also of a rather good quality.

Making the choice $G_1(r) = r$ and $G_2(r) = r^2$ the wave function described by Eq. (3) does not guarantee the correct asymptotic behavior in r space. This behavior can be introduced by replacing the second operator by a different one, namely, setting $G_2(r) = r\exp(-\alpha r^2)$. To show this we display in Table III the predicted values of $\langle r^2 \rangle$, $\langle r^4 \rangle$, and $\langle r^6 \rangle$ with $\alpha = 0.04$ and the HF results for ^{16}O. The discrepancies are lower than 0.1%, 2%, and 10%, respectively.

Our main conclusion is that experimental measure-

TABLE III. Comparison between HF and inferred values $\langle r^2 \rangle$, $\langle r^4 \rangle$, and $\langle r^6 \rangle$ for each single-particle proton level of ^{16}O using $G_1(r) = r$ and $G_2(r) = r\exp(-\alpha r^2)$ ($\alpha = 0.04$).

Shell	Quantal $\langle r^2 \rangle$	Inferred $\langle r^2 \rangle$	Quantal $\langle r^4 \rangle$	Inferred $\langle r^4 \rangle$	Quantal $\langle r^6 \rangle$	Inferred $\langle r^6 \rangle$
$1S_{1/2}$	4.553	4.552	33.69	33.84	345.31	349.68
$1P_{3/2}$	7.565	7.561	79.66	78.66	1120.0	1051.6
$1P_{1/2}$	8.164	8.155	97.44	95.37	1640.7	1483.9

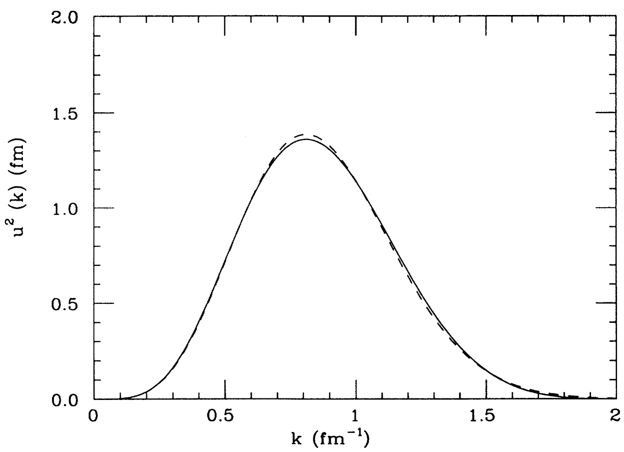

FIG. 2. Same as Fig. 1 in k space.

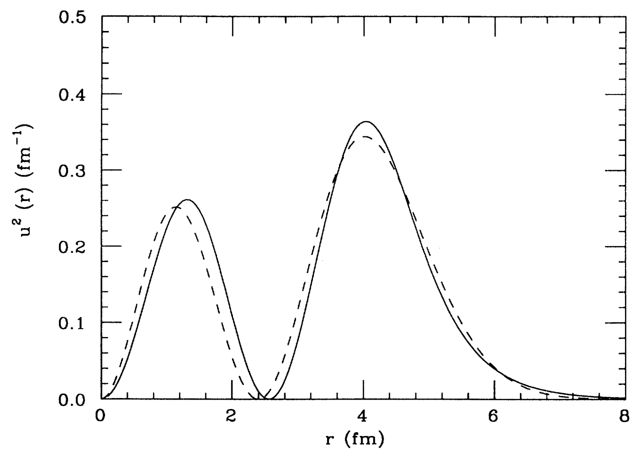

FIG. 3. Same as Fig. 1 for the $2S_{1/2}$ proton level of ^{40}Ca in r space.

ments of expectation values of a few selected nuclear observables for each shell may become of great significance, as these experimental values would allow for the possibility of inferring sp wave functions of good quality, independent in principle, of any theoretical many-body interaction, assuming, of course, that one employs a model-independent experimental input. If the experimental information about the deepest states is not of a good quality or not available in some cases, the results obtained using the experimental values of states around the Fermi sea can be used to choose the best mean field and one can apply this theoretical result to the deeper-lying orbits.

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