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LINEAR NUCLEI WITHOUT ALPHA-PARTICLES

J. Kolehmainen[1] M. Koskinen[2] M. Manninen[1]

[1]Department of Physics, University of Jyväskylä, P.O. Box 35, FIN-40351 Jyväskylä, Finland.

[2]Nordita, Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark.

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NORDITA · Nordisk Institut for Teoretisk Fysik

Blegdamsvej 17 DK-2100 København Ø Danmark

Linear nuclei without alpha-particles

J. Kolehmainen[1], M. Koskinen[2] and M. Manninen[1]

[1] *Department of Physics, University of Jyväskylä, P.O. Box 35, FIN-40351 Jyväskylä, Finland*

[2] *NORDITA, Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark*

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Abstract

We show that linear shape isomers of small even-even nuclei exist with nearly any internuclear interactions. The shapes of the linear isomers *look* like chains of alpha-particles, but single-particle spectrum reveals that alpha-particle interpretation is not needed. Indeed, the same shapes are obtained even with noninteracting particles in a rectangular cavity.

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Several scattering experiments of small nuclei have been interpreted with help of an intermediate excited nucleon which consists of alpha-particles bound in a linear chain [1–4]. Theoretical investigations have also suggested that such unstable isomers can exist at least for the following nuclei: ^{8}Be, ^{12}C, ^{16}O, ^{20}Ne, and ^{24}Mg, i.e. up to 6 alpha-particles [3,5–9]. Although the experimental evidence of such isomers might not be conclusive, the possibility of such isomers has met with great enthusiasm and also properties of other isomers of the above nuclei, e.g. ^{12}C and ^{16}O, have been interpreted with help of the alpha-particle model.

The purpose of this letter is to show that the existence of linear isomers of even-even nuclei is very general and independent of the model for the internucleon interactions. The shape of the isomers look like a chain of alpha-particles. Nevertheless, the binding properties and the single particle spectrum suggest that the interpretation that the chain is a molecule of alpha-particles is not needed and might even be wrong.

We use the density functional theory of Hohenberg, Kohn, and Sham [10,11], where the total particle density is written as a sum of (auxiliary) single-particle states

$$n(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2 \tag{1}$$

which are solutions of the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi_i + V_{\text{eff}}\psi_i = \epsilon_i\psi_i. \tag{2}$$

Above, the density and mass are those of protons or those of neutrons. The whole many-body problem is buried in the effective potential V_{eff}, which is slightly different for protons and neutrons. Apart from neglecting the spin-orbit interaction and other relativistic effects, the formalism is exact, i.e. there is a mean field that gives the exact particle density. In practise, however, there is no systematic way to calculate the exact effective potential although approximative formulas have been derived for nuclear matter [12] and for electron systems [13]

Fortunately, however, in the case of the smallest nuclei [14], or fermion clusters in general [15], the existence of shape isomers is not sensitive to the effective potential. Moreover, any model for the effective potential gives nearly similar results. We use the local density approximation which is the simplest self-consistent model which can result Jahn-Teller effect and shape isomers. Moreover, we neglect the difference between protons and neutrons. The Coulomb interaction is included only implicitly in the effective mean field. We approximate the potential energy of the system with a simple local function

$$V[n] = \int d^3r\,(bn(\mathbf{r}) + cn(\mathbf{r})^p)\,. \tag{3}$$

For the parameters b, c, and p we use values $b = 30.91$, $c = 4714$, and $p = 2.00$ (the unit of the length is 0.361 fm and the unit of energy is 318 MeV [14]). It shoud be stressed that the qualitative results of this work are completely insensitive to the parameters of the energy functional [14,15].

The Kohn-Sham equations were solved self-consistently using plane-wave technique [16]. A cylinder-shape finite potential well was used as an initial potential. Random perturbations were added in the effective potential during first 50 iterations to guarantee that the obtained shape isomer is stable and not a saddle point. No restrictions for the shape were included.

Linear isomers were searched for nuclei consisting up to six 'alpha-particles' In all cases a linear shape isomer was obtained. In the local density approximation the linear isomers are weakly stable, i.e. it costs energy to brake them into shorter linear nuclei. This stability would be removed with a proper treatment of the Coulomb interaction.

The calculated shape of the linear ^{20}Ne nucleus is shown in Fig. 1. Indeed the particle density has five maxima as if it would consist of five alpha-particles. All linear nuclei look very much alike, only the number of maxima depends on length of the chain. Now, we wish to show that the linear isomers are *not* chains of weakly bound alpha-particles. Rather, they are shape isomers of nearly free fermions (protons and neutrons).

First, we will compare the particle density inside a linear nucleus to that of free fermions confined in a cavity. We take the simplest possible model: Free fermions in a rectangular cavity with a square bottom and a length determined by the number of fermions. Assuming that the particles are in the lowest energy state perpendicular to the long side, the energy

eigenvalues are

$$\epsilon_i = \frac{\pi^2\hbar^2}{md^2} + \frac{i^2\pi^2\hbar^2}{2ml^2}, \tag{4}$$

where d is the side of the bottom and l the length of the box. The optimum shape (ratio l/d) of the cavity can be determined by minimizing the total energy (sum of eigenvalues) with a fixed volume. The single particle density is simply

$$n(\mathbf{r}) = \sum_{i=1}^{n} \sin^2(\pi x/d)\sin^2(\pi y/d)\sin^2(i\pi z/l). \tag{5}$$

Figure 1 shows the density contour for 10 free fermions (spin=1/2) in a rectangular box. There is a striking similarity between the density contour of free particles in a rectangular box and that obtained with self-consistent Kohn-Sham method for ^{20}Ne nucleus. This example shows that the maxima in the density are a natural result for linear and finite fermion systems and their existence does not require clustering of fermions to alpha-particles.

Secondly, we will show that the single particle eigenvalue spectrum of the density functional Kohn-Sham theory is very similar to that of free fermions, but differs drastically from that expected for linear 'molecules' of tightly bound alpha-particles. Figure 2 shows the single-particle eigenvalues of linear isomers with 2 to 12 protons. For comparison, we show the eigenvalues for 12 particles in a rectangular cavity. The spectrum of the cavity nearly coincides with that obtained with the Kohn-Sham method for the linear nucleus with 12 protons. Similar agreement is obtained for all sizes of linear nuclei.

For comparison we also assumed an extreme tight-binding model, i.e. the alpha-particles are closed systems which interact only weakly. In that case we can solve the single particle spectrum from a tight-binding Hamiltonian

$$H_{ij} = \begin{cases} \epsilon_0, & \text{if } i = j \\ \beta, & \text{if } i \text{ and } j \text{ neighbours} \end{cases} \tag{6}$$

where ϵ_0 corresponds to the single-particle state in an alpha-particle and β is the strength of the interaction between alpha particles. Figure 2 shows also the single-particle spectrum of the tight-binding model. The parameters ϵ_0 and β were chosen so that the bottom of the band and the band width correspond to the results of the self-consistent Kohn-Sham method. Clearly, the spectrum of the tight-binding model is very different from that of the self-consistent model.

It is interesting to compare linear nuclei to molecules of divalent atoms. Magnesium, which is a nearly free electron metal in bulk, has two isomers for trimer, a triangle and a linear chain [17]. The same is true for beryllium [18] and barium [19]. However, a linear chain would be a saddle point if the atoms were bonded only via polarization forces, like in the case of rare gases.

In conclusion, both the particle density and the single-particle spectrum of linear shape isomers of small nuclei are consistent of a model where the fermions (protons and neutrons) behave like free particles and do not group to alpha-particles. The insensitivity of the results to the model means that any mean field model gives this same result. Moreover, since the Kohn-Sham method allows the description of the exact ground state with help of a mean field (apart of the spin-orbit interaction), the exact shapes for linear isomers should also look alike. These conclusions are supported also by the fact that the Nilsson-Strutinsky model gives similar shape isomers [20].

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FIGURES

FIG. 1. Constant density contour for linear ^{20}Ne nucleus calculated using the self-consistent Kohn-Sham method (left) compared to the constant density contour of free fermions in a rectangular box (right).

FIG. 2. Single particle (Kohn-Sham) energy levels for linear nuclei with 2 to 12 protons. The dashed lines show first unoccupied levels. For comparison, the energy levels of free particles in a box (BOX) and for the tight-binding model (TB) are also shown.

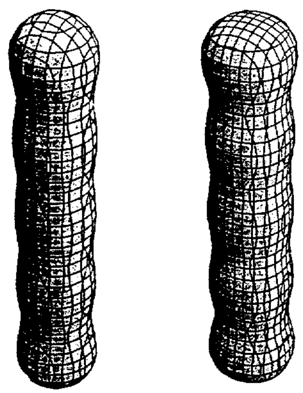
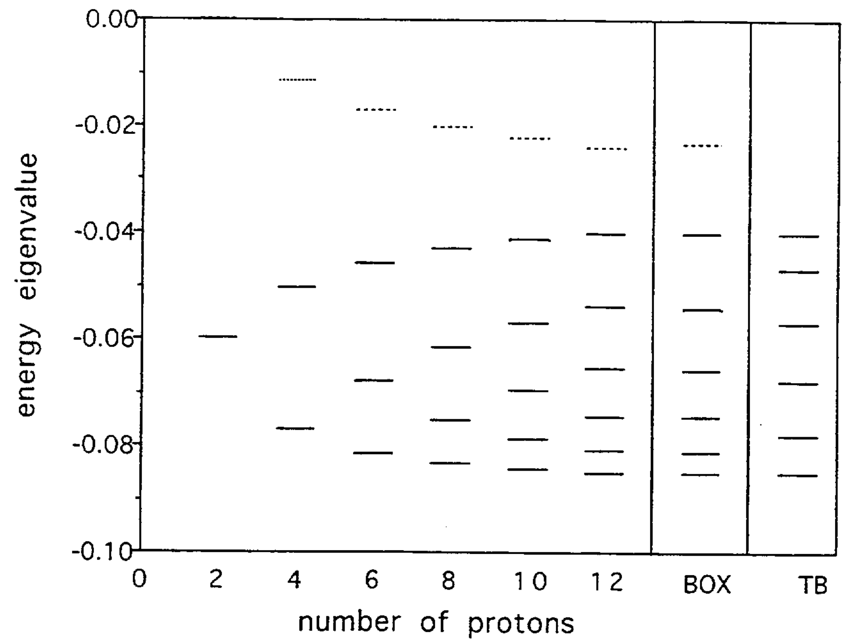


Fig. 1



0.00
-0.02
-0.04
-0.06
-0.08
-0.10
energy eigenvalue
0
2
4
6
8
10
12
BOX
TB
number of protons

Fig. 2