

Describing the clustering phenomena via DFT

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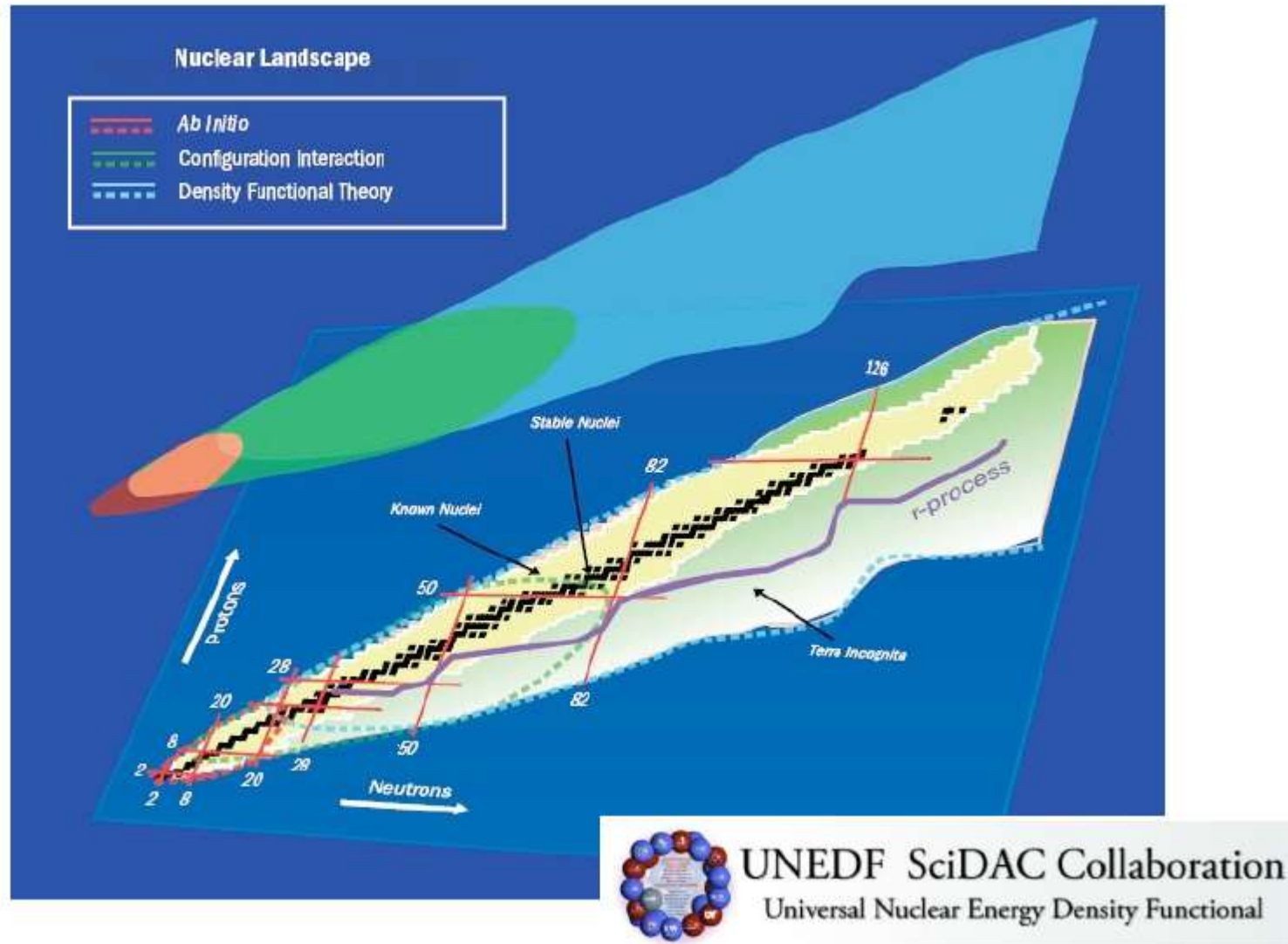
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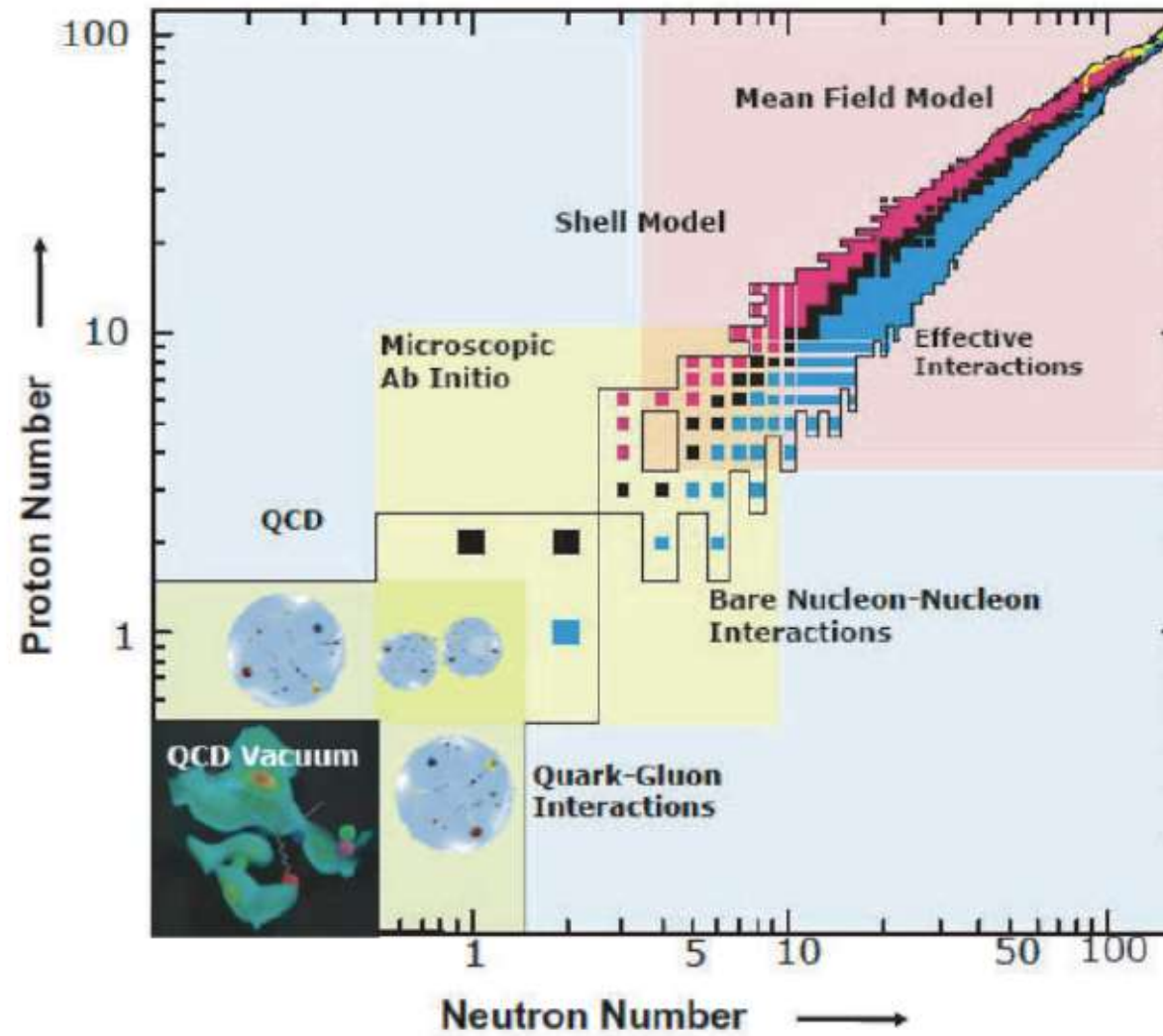
The method:

Density functional theory

Nuclear landscape vs. methods



Physics and degrees of freedom



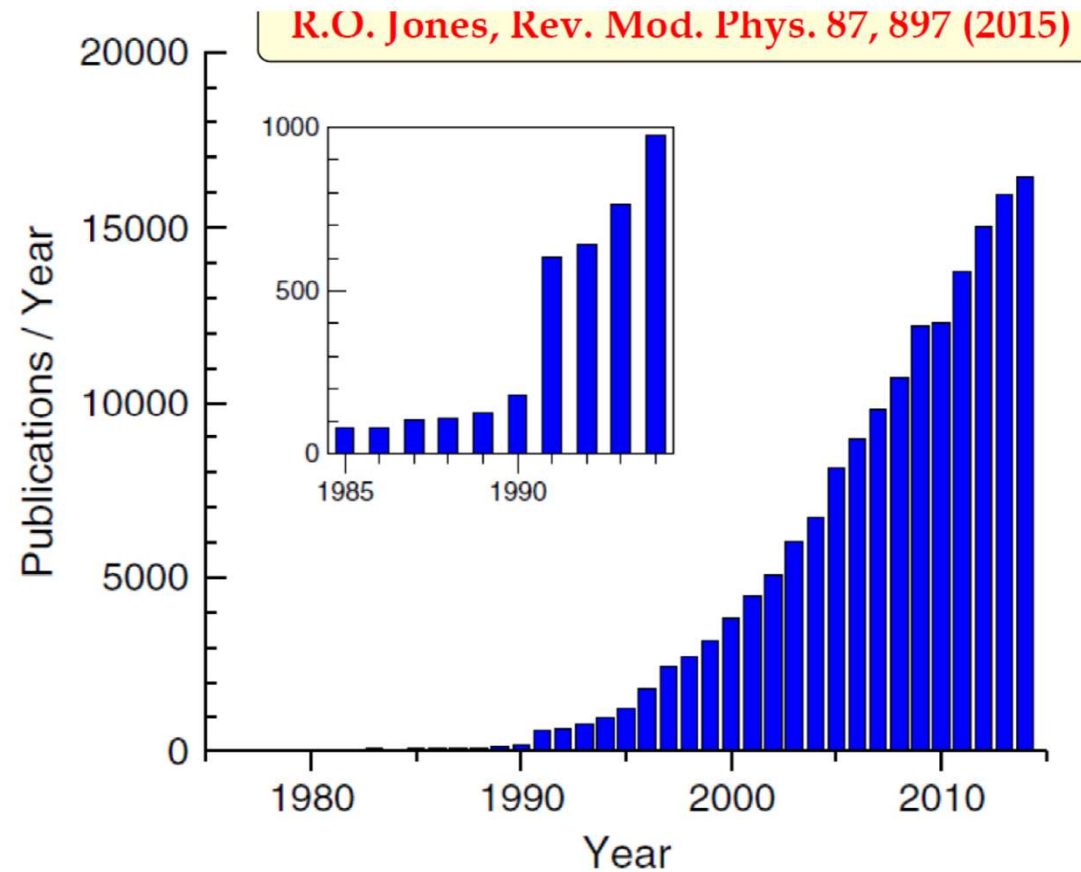


FIG. 1 (color online). Number of publications per year (1975–2014) on topics (“density functional” or “DFT”), according to the Web of Science Core Collection (February 2015). The inset shows data near 1990 on an expanded scale. The number of publications depends on the precise search criteria, but the overall picture is unchanged. From Mavropoulos, 2015.

Density functional theory is based on a constraint variational approach that uses observables as variational parameters.

We now solve the constraint variational equation for the routhian \hat{R} :

$$\hat{R} = \hat{H} - \lambda\hat{Q},$$

that is,

$$\delta\langle\hat{H} - \lambda\hat{Q}\rangle \equiv \nabla\langle\hat{H} - \lambda\hat{Q}\rangle \equiv \nabla E - \lambda\nabla Q \equiv \frac{\partial}{\partial p_i} [E(\mathbf{p}) - \lambda Q(\mathbf{p})] \equiv \frac{\partial E(\mathbf{p})}{\partial p_i} - \lambda \frac{\partial Q(\mathbf{p})}{\partial p_i} = 0,$$

where λ is called Lagrange multiplier.

After solving variational equation (2.3) for all λ we obtain the "path" $\mathbf{p}(\lambda)$, and

$$\begin{aligned} E(\lambda) &\equiv E(\mathbf{p}(\lambda)), \\ Q(\lambda) &\equiv Q(\mathbf{p}(\lambda)). \\ R(\lambda) &\equiv R(\mathbf{p}(\lambda)) = E(\lambda) - \lambda Q(\lambda). \end{aligned}$$

Assuming that function $Q(\lambda)$ can be inverted into $\lambda(Q)$ we obtain

$$E(Q) = \min_{\mathbf{p}} E(\mathbf{p}) \Big|_{Q(\mathbf{p})=Q} \equiv E(\lambda(Q)) \equiv E(\mathbf{p}(\lambda(Q))).$$

Energy E is now a function of observable Q . By minimizing $E(Q)$, $E_0 = \min_Q E(Q)$ that is, by solving

$$\frac{d}{dQ} E(Q) = 0, \quad (2.6)$$

we obtain E_0 and Q_0

Density functional theory is based on replacing the exact variational method with a two-stage variational method:

- 1: Minimization of energy E under constraint on value Q of observable \hat{Q} , which gives energy $E(Q)$ as function of Q .
- 2: Minimization of energy $E(Q)$ with respect to Q .

In this way the minimization of energy $E(Q)$ gives the exact ground-state energy E_0 and exact value of observable Q_0 .

Depending on which observable we pick, we can have very different DFTs:

$$\delta \left\langle \hat{H} - \lambda \hat{Q} \right\rangle = 0 \implies E = E(Q),$$

$$\delta \left\langle \hat{H} - \sum_{k=1}^K \lambda_k \hat{Q}_k \right\rangle = 0 \implies E = E(Q_k),$$

$$\delta \left\langle \hat{H} - \int dq \lambda(q) \hat{Q}(q) \right\rangle = 0 \implies E = E[Q(q)],$$

$$\delta \left\langle \hat{H} + \int d\mathbf{r} U(\mathbf{r}) \hat{\rho}(\mathbf{r}) \right\rangle = 0 \implies E = E[\rho(\mathbf{r})],$$

$$\delta \left\langle \hat{H} + \sum_{\sigma} \int d\mathbf{r} U(\mathbf{r}; \sigma) \hat{\rho}(\mathbf{r}; \sigma) \right\rangle = 0 \implies E = E[\rho(\mathbf{r}; \sigma)],$$

$$\delta \left\langle \hat{H} + \sum_{\sigma\sigma'} \int d\mathbf{r} U(\mathbf{r}; \sigma'\sigma) \hat{\rho}(\mathbf{r}; \sigma\sigma') \right\rangle = 0 \implies E = E[\rho(\mathbf{r}; \sigma\sigma')],$$

$$\delta \left\langle \hat{H} + \sum_{\sigma\tau, \sigma'\tau'} \int d\mathbf{r} U(\mathbf{r}; \sigma'\tau', \sigma\tau) \hat{\rho}(\mathbf{r}; \sigma\tau, \sigma'\tau') \right\rangle = 0 \implies E = E[\rho(\mathbf{r}; \sigma\tau, \sigma'\tau')],$$

$$\delta \left\langle \hat{H} + \int d\mathbf{r} \left(U(\mathbf{r}) \hat{\rho}(\mathbf{r}) + M(\mathbf{r}) \hat{\tau}(\mathbf{r}) \right) \right\rangle = 0 \implies E = E[\rho(\mathbf{r}), \tau(\mathbf{r})],$$

$$\delta \left\langle \hat{H} + \int d\mathbf{r} \int d\mathbf{r}' U(\mathbf{r}', \mathbf{r}) \hat{\rho}(\mathbf{r}, \mathbf{r}') \right\rangle = 0 \implies E = E[\rho(\mathbf{r}, \mathbf{r}')],$$

$$\delta \left\langle \hat{H} + \int dx \int dx' U(x', x) \hat{\rho}(x, x') \right\rangle = 0 \implies E = E[\rho(x, x')].$$

$$\delta \left\langle \hat{H} + \int d\mathbf{r} \left(U(\mathbf{r})\hat{\rho}(\mathbf{r}) + M(\mathbf{r})\hat{\tau}(\mathbf{r}) \right) \right\rangle = 0 \quad \Longrightarrow \quad E = E[\rho(\mathbf{r}), \tau(\mathbf{r})]$$

One-body density operator is the DFT observable:

$$\hat{\rho}(\mathbf{r}) = \sum_{i=1}^A \delta(\mathbf{r} - \mathbf{r}_i) \equiv a_{\mathbf{r}}^+ a_{\mathbf{r}}.$$

$$a_{\mathbf{r}} := \sum_{\mu} \phi_{\mu}(\mathbf{r}) a_{\mu},$$

$$a_{\mathbf{r}}^+ := \sum_{\mu} \phi_{\mu}^*(\mathbf{r}) a_{\mu}^+.$$

The position-dependent Lagrange multipliers are identical to one-body (mean-field) potentials $U(\mathbf{r})$:

$$\langle \hat{U} \rangle = \left\langle \int d\mathbf{r} U(\mathbf{r})\hat{\rho}(\mathbf{r}) \right\rangle = \int d\mathbf{r} U(\mathbf{r})\rho(\mathbf{r}),$$

for

$$\langle \hat{\rho}(\mathbf{r}) \rangle = \rho(\mathbf{r}).$$

$$\delta \left\langle \hat{H} + \int d\mathbf{r} \left(U(\mathbf{r}) \hat{\rho}(\mathbf{r}) + M(\mathbf{r}) \hat{\tau}(\mathbf{r}) \right) \right\rangle = 0 \implies E = E[\rho(\mathbf{r}), \tau(\mathbf{r})]$$

$$\hat{\tau}(\mathbf{r}) = - \sum_{i=1}^A \nabla_i \cdot \delta(\mathbf{r} - \mathbf{r}_i) \nabla_i \equiv \nabla(a_{\mathbf{r}}^+) \cdot \nabla(a_{\mathbf{r}}),$$

for

$$\nabla(a_{\mathbf{r}}) := \sum_{\mu} \nabla(\phi_{\mu}(\mathbf{r})) a_{\mu},$$

$$\nabla(a_{\mathbf{r}}^+) := \sum_{\mu} \nabla(\phi_{\mu}^*(\mathbf{r})) a_{\mu}^+,$$

$$\tau(\mathbf{r}) = \langle \hat{\tau}(\mathbf{r}) \rangle = \nabla \cdot \nabla' \rho(\mathbf{r}, \mathbf{r}') \Big|_{\mathbf{r}'=\mathbf{r}}.$$

This gives

$$\frac{\hbar^2}{2m} \int d\mathbf{r} \hat{\tau}(\mathbf{r}) = -\frac{\hbar^2}{2m} \sum_{i=1}^A \Delta_i = \hat{T}.$$

$$\delta \left\langle \hat{H} + \int d\mathbf{r} \left(U(\mathbf{r}) \hat{\rho}(\mathbf{r}) + M(\mathbf{r}) \hat{\tau}(\mathbf{r}) \right) \right\rangle = 0 \implies E = E[\rho(\mathbf{r}), \tau(\mathbf{r})]$$

$$\begin{aligned} & \delta \left\langle \hat{V} + \int d\mathbf{r} \left[U(\mathbf{r}) \hat{\rho}(\mathbf{r}) + \left(\frac{\hbar^2}{2m} + M(\mathbf{r}) \right) \hat{\tau}(\mathbf{r}) \right] \right\rangle \\ &= \delta \langle \hat{V} \rangle + \delta \int d\mathbf{r} \left[U(\mathbf{r}) \rho(\mathbf{r}) + \left(\frac{\hbar^2}{2m} + M(\mathbf{r}) \right) \tau(\mathbf{r}) \right] = 0, \end{aligned}$$

which gives the functional:

$$E[\rho, \tau] = \frac{\hbar^2}{2m} \int d\mathbf{r} \tau(\mathbf{r}) + V[\rho, \tau],$$

with the kinetic energy explicitly and exactly singled out.

We now minimize this functional with respect to density and kinetic density under the condition that the number of particles is A . For that we again minimize the Routhian:

$$R[\rho, \tau] = E[\rho, \tau] - \lambda \int d\mathbf{r} \rho(\mathbf{r}) = \frac{\hbar^2}{2m} \int d\mathbf{r} \tau(\mathbf{r}) + V[\rho, \tau] - \lambda \int d\mathbf{r} \rho(\mathbf{r}).$$

This gives variational equations:

$$\begin{aligned} \frac{\delta R[\rho, \tau]}{\delta \rho(\mathbf{r})} &= \frac{\delta V[\rho, \tau]}{\delta \rho(\mathbf{r})} - \lambda = U(\mathbf{r}) - \lambda = 0, \\ \frac{\delta R[\rho, \tau]}{\delta \tau(\mathbf{r})} &= \frac{\delta V[\rho, \tau]}{\delta \tau(\mathbf{r})} + \frac{\hbar^2}{2m} = M(\mathbf{r}) = 0. \end{aligned}$$

Steepest-descent minimization of the functional $E[\rho, \tau]$ can proceed as follows.

1° Begin with reasonable initial guesses for the densities $\rho^{(0)}(\mathbf{r})$ and $\tau^{(0)}(\mathbf{r})$. Set the iteration number $k = 0$.

2° Calculate the derivatives:

$$U_{(k)}(\mathbf{r}) = \frac{\delta V[\rho^{(k)}, \tau^{(k)}]}{\delta \rho^{(k)}(\mathbf{r})}, \quad M_{(k)}(\mathbf{r}) = \frac{\delta V[\rho^{(k)}, \tau^{(k)}]}{\delta \tau^{(k)}(\mathbf{r})} + \frac{\hbar^2}{2m}, \quad (2.31)$$

3° Calculate new approximations to densities:

$$\rho^{(k+1)}(\mathbf{r}) = \rho^{(k)}(\mathbf{r}) - \epsilon(U_{(k)}(\mathbf{r}) - \lambda), \quad (2.32a)$$

$$\tau^{(k+1)}(\mathbf{r}) = \tau^{(k)}(\mathbf{r}) - \epsilon M_{(k)}(\mathbf{r}). \quad (2.32b)$$

4° Iterate the loop 2°–3° until convergence is reached.

Hohenberg-Kohn theorem (1964)

The exact energy of a quantum mechanical many body system is a functional of the local density $\rho(\mathbf{r})$

$$E[\rho] = \langle \Psi | H | \Psi \rangle$$

This functional is universal. It does not depend on the system, only on the interaction.

One obtains the exact density $\rho(\mathbf{r})$ by a variation of the functional with respect to the density

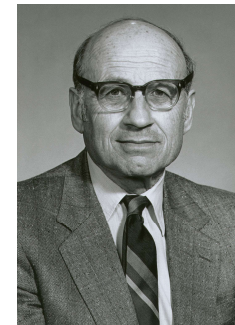
note:

$\rho(\mathbf{r})$ is a function of 3 variables.

$\Psi(\mathbf{r}_1 \dots \mathbf{r}_N)$ is a function of $3N$ variables.



Hohenberg



Kohn

The Kohn-Sham Approach (1965)

Reference

W. Kohn and L.J. Sham, Phys. Rev. (1965) 140, A1133
http://prola.aps.org/abstract/PR/v140/i4A/pA1133_1



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Self-Consistent Equations Including Exchange and Correlation Effects*

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From a theory of Hohenberg and Kohn, approximation methods for treating an inhomogeneous system of interacting electrons are developed. These methods are exact for systems of slowly varying or high density. For the ground state, they lead to self-consistent equations analogous to the Hartree and Hartree-Fock equations, respectively. In these equations the exchange and correlation portions of the chemical potential of a uniform electron gas appear as additional effective potentials. (The exchange portion of our effective potential differs from that due to Slater by a factor of $\frac{2}{3}$.) Electronic systems at finite temperatures and in magnetic fields are also treated by similar methods. An appendix deals with a further correction for systems with short-wavelength density oscillations.

Kohn and Sham made a key assumption:

For a real (interacting) system, for which the ground state density is $\rho(\mathbf{r})$, there exists a reference system (non-interacting) that has exactly the same ground-state density.

The densities for which there exists such reference system are called *pure-state non-interacting v -representable* or just *Kohn-Sham representable*.

A larger class of densities are the densities which are representable by some wavefunction of the Slater determinant form (not necessarily ground-states).

For any interacting system, there exists a **local single-particle potential $v_s(\mathbf{r})$** , such that the **exact** ground-state density of the interacting system equals the ground-state density of the auxiliary non-interacting system:

$$\rho(\mathbf{r}) = \rho_s(\mathbf{r}) \equiv \sum_i^{\text{occ}} |\phi_i(\mathbf{r})|^2$$

... there exists a unique energy functional:

$$E_s[\rho] = T_s[\rho] + \int d^3r v_s(\mathbf{r})\rho(\mathbf{r})$$

for which the variational equation yields the **exact ground-state density n_s** .

$T_s[n]$ - universal kinetic energy functional of non-interacting particles.

$$v_s[\rho(\mathbf{r})] = v(\mathbf{r}) + U[\rho(\mathbf{r})] + v_{xc}[\rho(\mathbf{r})]$$

external potential

exchange-correlation

Hartree term

Density functional theory in nuclei:

In nuclei DFT has been introduced by **effective Hamiltonians**:

$$E = \langle \Psi | H | \Psi \rangle \approx \langle \Phi | \hat{H}_{eff}(\hat{\rho}) | \Phi \rangle = E[\hat{\rho}]$$

Skyrme Gogny Rel. MF

More degrees of freedom: **spin, isospin, “pairing”**

Nuclei are **self-bound systems**.

The exact density is a constant. $\rho(r) = \text{const}$

Hohenberg-Kohn theorem is true, but *useless*...

$\rho(r)$ has to be replaced by the **intrinsic density**:

$$\rho_I(\vec{r}) = \rho(\vec{r} + \vec{R}_{CM}) \quad \text{with} \quad \vec{R}_{CM} = \frac{1}{A} \sum_i \vec{r}_i$$

Density functional theory in nuclei is probably **not exact**,
but a very good approximation.

How do we proceed?

$$E(\rho)$$

$|\Phi\rangle$ Slater determinant $\Leftrightarrow \hat{\rho}$ density matrix ($\hat{\rho}^2 = \hat{\rho}$)

$$|\Phi\rangle = \mathcal{A}(\varphi_1(\mathbf{r}_1) \cdots \varphi_A(\mathbf{r}_A)) \quad \hat{\rho}(\mathbf{r}, \mathbf{r}') = \sum_{i=1}^A |\varphi_i(\mathbf{r})\rangle \langle \varphi_i(\mathbf{r}')|$$

Mean field:

$$\hat{h} = \frac{\delta E}{\delta \hat{\rho}}$$

Eigenfunctions:

$$\hat{h}|\varphi_i\rangle = \varepsilon_i|\varphi_i\rangle$$

Interaction:

$$\hat{V} = \frac{\delta^2 E}{\delta \hat{\rho} \delta \hat{\rho}}$$

Extensions: Pairing correlations

The general nuclear Hamiltonian reads

$$H = \frac{-\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{i \leq j} v_{ij} + \sum_{i \leq j \leq k} V_{ijk} + \dots + \text{n-body terms}$$

where v_{ij} is the 2-body Nucleon-Nucleon interaction (NN) and V_{ijk} is the 3-body one.

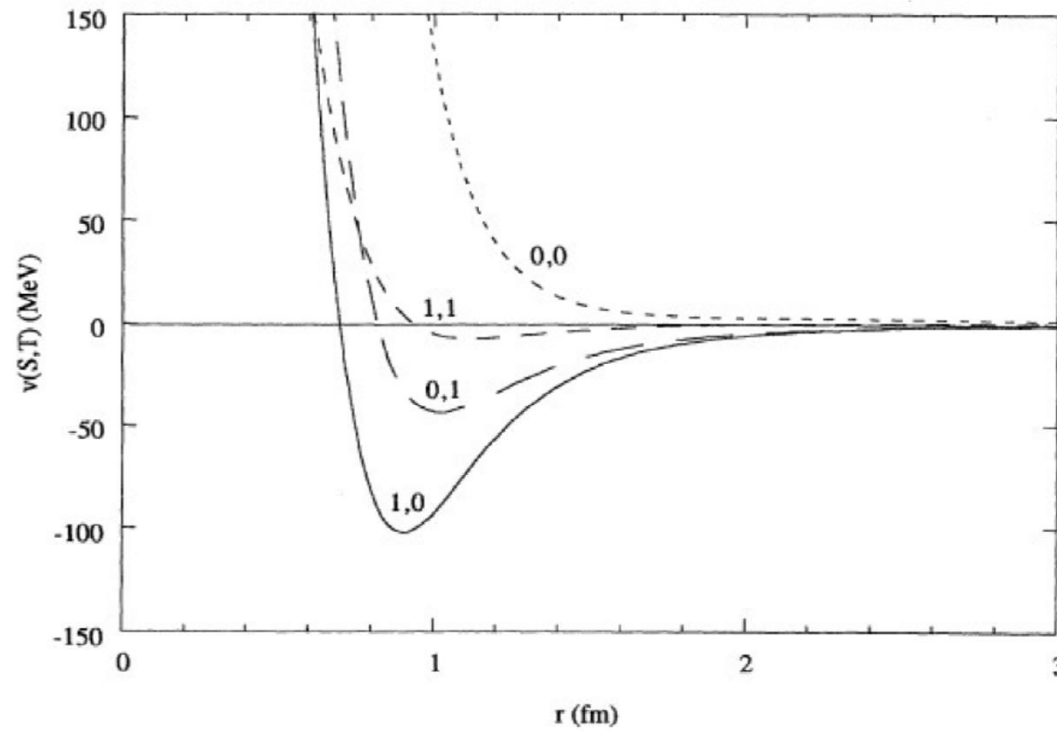
A possible representation of the 2-body interaction looks like

$$v_{ij} = \sum_{p=1,n} v_p(\mathbf{r}_{ij}) O_{ij}^p$$

which is a form factor (typically a sum of Yukawa potential $\sum_a \exp^{-k_a r} / r$) times an operator. To reproduce scattering data a minimum of 8 operators is required

$$O_{ij}^{p=1,8} = 1, \tau_i \tau_j, \sigma_i \sigma_j, (\tau_i \tau_j)(\sigma_i \sigma_j), S_{ij}, S_{ij}(\tau_i \tau_j), \mathbf{L} \cdot \mathbf{S}, \mathbf{L} \cdot \mathbf{S} \tau_i \tau_j$$

To reproduce with more accuracy data, extra operators are needed, typically 14 or 18.



the shape of the NN potential for the different channels of spin and isospin.

Hartree-Fock method

replacing the nuclear potential

$$\sum_{i \leq j} v_{ij} \approx \sum_i v_i$$

The total Hamiltonian of the system reads

$$H^{HF} = \sum_i^A h(i)$$

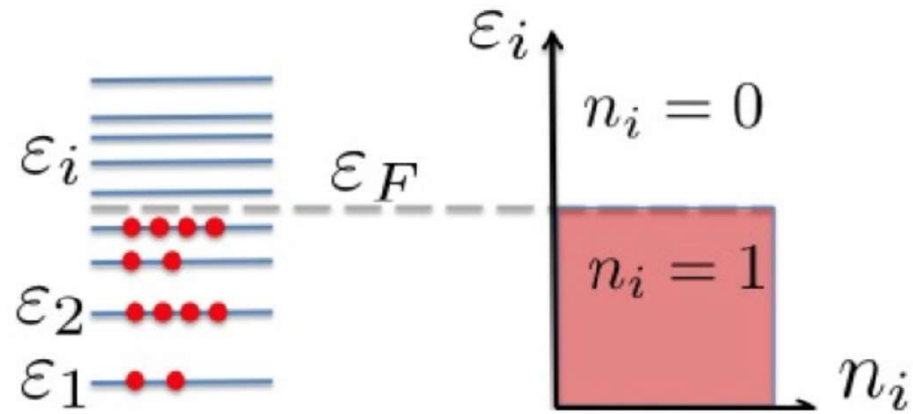
The corresponding energy of the system E_0^{HF} can be seen as an approximation to the exact ground state energy of the system. The total wave-function of the system is a *Slater determinant* $\Phi(1, \dots, A)$

$$|HF\rangle = |\Phi(1, \dots, A)\rangle = \Pi_i^A a_i^\dagger |-\rangle$$

where a_i^\dagger is the single particle creator operator. To calculate the single particle wave functions $\phi_k(i)$ we need to solve a system of coupled equations of the form

$$h(i)\phi_k(i) = \varepsilon_k\phi_k(i) \text{ with } i = (\mathbf{r}, \sigma, \tau)$$

Hartree-Fock method



Single particle levels: occupy and empty; Fermi energy is between the last occupied and the first empty orbital.

Hartree-Fock method

$$|\tilde{Z}\rangle = \exp\left(\sum_{ph} Z_{ph}^* a_p^\dagger a_h\right) a_1^\dagger \dots a_A^\dagger |0\rangle \quad (\text{ Thouless theorem, } p \text{ for particle, } h \text{ for hole})$$

We define the HF energy as

$$E_{HF} = \frac{\langle \tilde{Z} | H | \tilde{Z} \rangle}{\langle \tilde{Z} | \tilde{Z} \rangle}$$

The variational principle $\delta E_{HF} = 0$ means

$$\delta E_{HF} = \frac{\langle \tilde{Z} | H | \delta_\perp \tilde{Z} \rangle}{\langle \tilde{Z} | \tilde{Z} \rangle}$$

a orthogonal variation of $|\tilde{Z}\rangle \Rightarrow |\delta_\perp \tilde{Z}\rangle = |\delta \tilde{Z}\rangle - \frac{\langle \tilde{Z} | \delta \tilde{Z} \rangle}{\langle \tilde{Z} | \tilde{Z} \rangle} |\tilde{Z}\rangle$

$$\delta := \sum_{ph} \delta Z_{ph}^* \frac{\partial}{\partial Z_{ph}^*} \quad \Rightarrow \quad \begin{aligned} |\delta \tilde{Z}\rangle &= \sum_{ph} \delta Z_{ph}^* a_p^\dagger a_h |\tilde{Z}\rangle \\ |\delta_\perp \tilde{Z}\rangle &= \sum_{ph} \delta Z_{ph}^* (a_p^\dagger a_h - \rho_{hp}) |\tilde{Z}\rangle \end{aligned} \quad \Rightarrow \quad \begin{aligned} \delta E_{HF} &= \frac{\langle \tilde{Z} | H | \delta_\perp \tilde{Z} \rangle}{\langle \tilde{Z} | \tilde{Z} \rangle} \\ &= \frac{1}{\langle \tilde{Z} | \tilde{Z} \rangle} \langle \tilde{Z} | H | \sum_{ph} \delta Z_{ph}^* (a_p^\dagger a_h - \rho_{hp}) |\tilde{Z}\rangle \end{aligned}$$

Set Zero! $\Rightarrow \langle \tilde{Z}_0 | H | (a_p^\dagger a_h - \rho_{hp}) | \tilde{Z}_0 \rangle = 0$

"0" means a product state that obeys this variational principle.

Apply Wick on the Hamiltonian

$$H = T + V = \sum_{\mu\nu} T_{\mu\nu} a_{\mu}^{\dagger} a_{\nu} + \frac{1}{4} \sum_{\mu\lambda\nu\pi} V_{\mu\lambda\nu\pi} a_{\mu}^{\dagger} a_{\lambda}^{\dagger} a_{\pi} a_{\nu}$$

by doing that we get

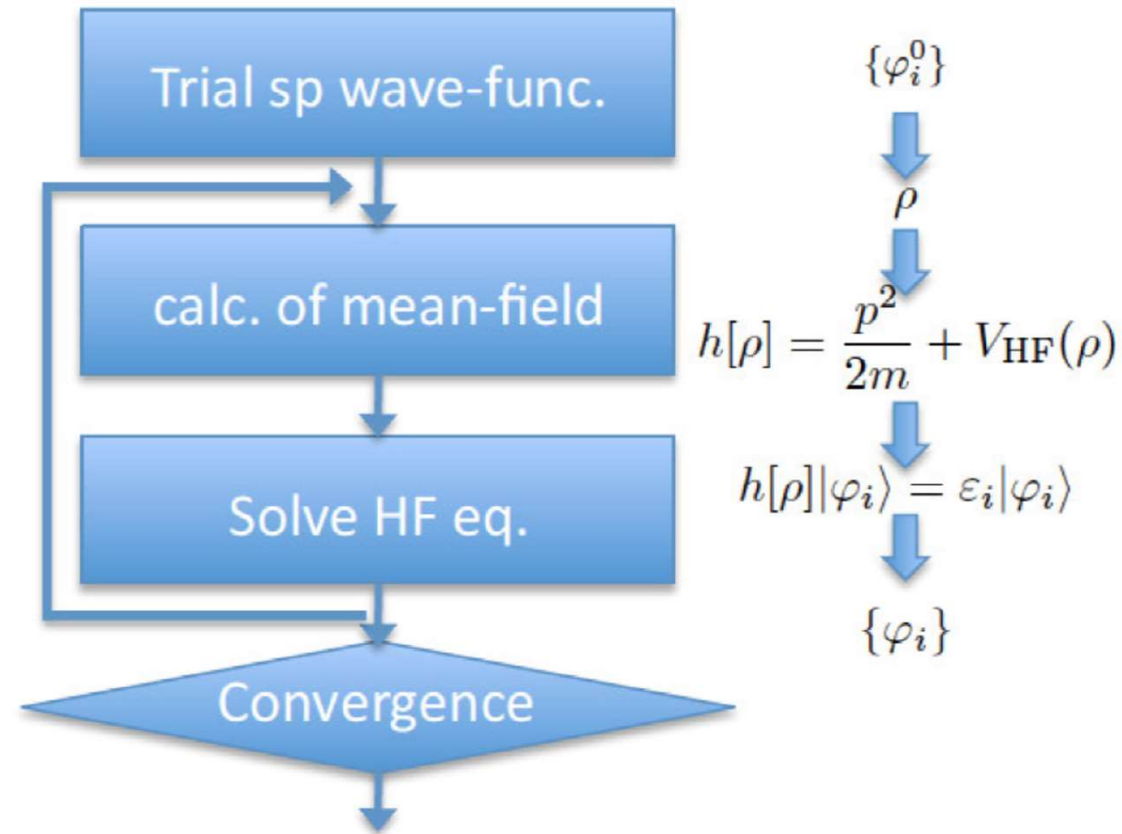
$$\begin{aligned} \langle \tilde{Z} | H | (a_{\mu}^{\dagger} a_{\nu} - \rho_{\nu\mu}) | \tilde{Z} \rangle &= \langle \tilde{Z} | H | a_{\mu}^{\dagger} a_{\nu} | \tilde{Z} \rangle - \rho_{\nu\mu} \langle \tilde{Z} | H | \tilde{Z} \rangle \\ &= (\rho h (1 - \rho))_{\mu\nu} \end{aligned}$$

$$\begin{aligned} \text{where } h_{\mu\nu} &= T_{\mu\nu} + \Gamma_{\mu\nu}. \\ \Gamma_{\mu\nu} &= \sum_{\lambda\pi} V_{\mu\lambda\nu\pi} \rho_{\pi\lambda} \end{aligned}$$

We can summarise the result by showing that the product state $|\tilde{Z}_0\rangle$ obeys the variational Hartree-Fock condition if its density matrix ρ_0 obeys

$$[h_0, \rho_0] = 0$$

To solve this equation we have to set up a self-consistent procedure as illustrated in



We can now calculate the HF energy

$$\begin{aligned} E^{HF} &= \text{Tr}T\rho + \frac{1}{2}\text{TrTr}(\rho\bar{v}\rho) \\ &= \text{Tr}T\rho + \frac{1}{2}\text{Tr}(\rho\Gamma) \\ &= \text{Tr}T\rho + \frac{1}{2}\text{Tr}(\rho h - \rho T) \\ &= \frac{1}{2}\text{Tr}T\rho + \frac{1}{2}\text{Tr}h\rho \end{aligned}$$

in canonical basis

$$E^{HF} = \frac{1}{2} \sum_{h=1}^A (T_{hh} + \varepsilon_h)$$

T_{hh} are the diagonal matrix element of the kinetic energy operator

The HFB Theory

Bogoliubov transformation

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix}, \quad \mathcal{W} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}$$

Unitarity of the Bogoliubov transformation

$$\mathcal{W}\mathcal{W}^\dagger = \mathcal{W}^\dagger\mathcal{W} = 1.$$



Nikolay Bogolyubov (1909-1992)

The HFB Theory

From particles to quasiparticles (and back)

$$\begin{aligned}\mathcal{W} & : \{\beta, \beta^\dagger\} \rightarrow \{a, a^\dagger\} \equiv \langle a|\beta\rangle, \\ \mathcal{W}^\dagger & : \{a, a^\dagger\} \rightarrow \{\beta, \beta^\dagger\} \equiv \langle \beta|a\rangle.\end{aligned}$$

Quasiparticle (Bogoliubov, HFB) vacuum

$$|\Phi\rangle = \prod_{\mu=1}^{N_p} \beta_\mu |0\rangle, \quad \forall \mu, \beta_\mu |\Phi\rangle = 0$$

with $N_p \leq M$

Quasiparticles represent excitations of the system: the vacuum is the state with no excitation (ground-state). Contrary to HF, HFB gives a recipe for both the g.s. and the excited states.

Quasiparticle operators $\{\beta, \beta^\dagger\}$ are fermionic operators and the HFB vacuum is a product state: general conditions for the Wick theorem apply.

If the reference state $|\Phi\rangle$ is a HFB vacuum (product state of quasiparticle operators), then

$$\rho = V^*V^T, \quad \kappa = V^*U^T. \quad (6.18)$$

Therefore, there is a one-to-one mapping between the set of densities, the reference state and the matrices of the Bogoliubov transformation

$$|\Phi\rangle \Leftrightarrow (U, V) \Leftrightarrow (\rho, \kappa) \quad (6.19)$$

Generalized density

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix}, \quad \mathcal{R}^2 = \mathcal{R}, \quad \mathcal{R}^\dagger = \mathcal{R}$$

The HFB Theory

For the HFB ansatz and a two-body Hamiltonian,

$$E = \sum_{ij} t_{ij} \rho_{ji} + \frac{1}{2} \sum_{ijkl} \bar{v}_{ijkl} \rho_{lj} \rho_{ki} + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} \kappa_{ij}^* \kappa_{kl}.$$

Variational principle for E as a functional of \mathcal{R} (or equivalently of ρ , ρ^* , κ , κ^*) is expressed as

$$\delta E = 0 \Rightarrow \sum_{kl} \frac{\partial E}{\partial \mathcal{R}_{kl}} \delta \mathcal{R}_{kl} = 0$$

Notations

$$\frac{\partial E}{\partial \rho_{kl}} = \frac{1}{2} h_{lk}, \quad \text{and} \quad \frac{\partial E}{\partial \rho_{kl}^*} = \frac{1}{2} h_{lk}^*.$$

and

$$\frac{\partial E}{\partial \kappa_{kl}} = \frac{1}{2} \Delta_{kl}^*, \quad \text{and} \quad \frac{\partial E}{\partial \kappa_{kl}^*} = \frac{1}{2} \Delta_{kl}.$$

HFB matrix

$$\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix},$$

where the HFB matrix

- is defined by $\frac{1}{2} \mathcal{H}_{kl} = \partial E / \partial \mathcal{R}_{kl}$
- obeys the HFB equation $[\mathcal{H}, \mathcal{R}] = 0$
- is such that $\delta E = \frac{1}{2} \text{Tr}(\mathcal{H} \delta \mathcal{R})$

Effective Interaction: Skyrme force

$$\begin{aligned}
 \tilde{v}^{\text{Skyrme}}(r_{12}) = & t_0(1 + x_0 P^\sigma) \delta(\mathbf{r}_1 - \mathbf{r}_2) \\
 & + \frac{1}{2} t_1 (1 + x_1 P^\sigma) [\delta(\mathbf{r}_1 - \mathbf{r}_2) k'^2 + k^2 \delta(\mathbf{r}_1 - \mathbf{r}_2)] && \text{Momentum Dependent} \\
 & + t_2 (1 + x_2 P^\sigma) \mathbf{k}'^* \delta(\mathbf{r}_1 - \mathbf{r}_2) \cdot \mathbf{k} && \text{Momentum Dependent} \\
 & + \frac{1}{6} t_3 (1 + x_3 P^\sigma) \rho^\alpha(\mathbf{R}) \delta(\mathbf{r}_1 - \mathbf{r}_2) && \text{Density Dependent} \\
 & + i W_0 (\sigma_1 + \sigma_2) \mathbf{k}'^* \delta(\mathbf{r}_1 - \mathbf{r}_2) \times \mathbf{k} && \text{Spin-Orbit}
 \end{aligned}$$

with \mathbf{k} the relative momentum operator

$$\mathbf{k} = \frac{1}{2i} (\nabla_1 - \nabla_2).$$

Skyrme potential is local, zero-range

$$\hat{V}_{\text{Skyrme}}(\mathbf{r}_1, \mathbf{r}_2) \propto \delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_1 - \mathbf{r}'_1)\delta(\mathbf{r}_2 - \mathbf{r}'_2)$$

which leads to a functional of the local density $\rho(\mathbf{r})$ and derivatives $\tau(\mathbf{r})$, etc.,

$$E[\rho] = \int d^3\mathbf{r} \mathcal{H}(\mathbf{r}), \quad \mathcal{H}(\mathbf{r}) = C^{\rho\rho}\rho^2 + C^{\rho\tau}\rho\tau + \dots$$

Time even fields

$$\rho_t(\mathbf{r}, \mathbf{r}') = \sum_{i, \sigma} \psi_i^*(\mathbf{r}, \sigma, \tau) \psi_i(\mathbf{r}', \sigma, \tau),$$
 particle density,

$$\tau_t(\mathbf{r}) = \nabla \cdot \nabla' \rho(\mathbf{r}, \mathbf{r}')|_{\mathbf{r}=\mathbf{r}'},$$
 kinetic energy density,

$$\mathbf{j}_t(\mathbf{r}) = \mathbf{k} \rho_t(\mathbf{r}, \mathbf{r}')|_{\mathbf{r}=\mathbf{r}'},$$
 current density,

Time odd fields

$$\mathbf{s}_t(\mathbf{r}) = \sum_{\sigma, \sigma'} \rho_t(\mathbf{r}\sigma, \mathbf{r}\sigma') \langle \sigma' | \hat{\boldsymbol{\sigma}} | \sigma \rangle,$$
 spin density,

$$\mathbf{T}_t(\mathbf{r}) = \nabla \cdot \nabla' \mathbf{s}_t(\mathbf{r}, \mathbf{r}')|_{\mathbf{r}=\mathbf{r}'},$$
 spin kinetic energy density,

$$\mathbb{J}_t(\mathbf{r}) = \mathbf{k} \otimes \mathbf{s}_t(\mathbf{r}, \mathbf{r}')|_{\mathbf{r}=\mathbf{r}'},$$
 spin current density,

where ψ_i are the Kohn-Sham wavefunctions that determine the Kohn-Sham densities.

It determines the following energy densities for the odd and even fields,

$$\mathcal{E}_t^e(\mathbf{r}) = C_t^\rho \rho_t^2 + C_t^{\Delta\rho} \rho_t \Delta\rho + C_t^\tau \rho_t \tau_t + C_t^j \mathbf{j}_t^2 + C_t^{\nabla j} \rho_t \nabla \cdot \mathbf{j}_t,$$

$$\mathcal{E}_t^o(\mathbf{r}) = C_t^s \mathbf{s}_t^2 + C_t^{\Delta s} \mathbf{s}_t \cdot \Delta \mathbf{s} + C_t^T \mathbf{s}_t \cdot \mathbf{T}_t + C_t^J \mathbb{J}_t^2 + C_t^{\nabla J} \mathbf{s}_t \nabla \times \mathbb{J}_t,$$

giving the total energy density as

$$\mathcal{E}(\mathbf{r}) = \sum_t \mathcal{E}_t^e + \mathcal{E}_t^o.$$

Where C are constants combinations of the coupling constants of the functional generator (t_i , x_i and W_0 ; cf. [24] for a complete and definitive list) which depends on the symmetries assumed, in particular the density dependent term is reabsorbed in

$$C_t^\rho = C_t^\rho + C_t^{\rho DD} \rho_0^\alpha.$$

Effective Interaction: Pairing force

Surface-Volume pairing force

$$\hat{V}_{\text{pair}}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{t=n,p} V_t \left(1 - \alpha \frac{\rho(\mathbf{R})}{\rho_0} \right) \delta(\mathbf{r}_1 - \mathbf{r}_2),$$

with $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, $\rho_0 = 0.16 \text{ fm}^{-3}$ is the saturation density. If $\alpha = 1$, we have a *surface* pairing force, if $\alpha = 0$ we have a *volume* pairing force; often, $\alpha = 1/2$.

Effective Interaction: Gogny force

$$\tilde{v}^{\text{Gogny}}(r_{12}) = \sum_j^{2(3)} = 1 \quad e^{-(\mathbf{r}_1 - \mathbf{r}_2)^2 / \mu_j^2} (W_j + B_j P^\sigma - H_j P^\tau - M_j P^\sigma P^\tau) \quad \text{sum of Gaussians,}$$

$$+ t_3 (1 + x_3 P^\sigma) \rho^\alpha(\mathbf{R}) \delta(\mathbf{r}_1 - \mathbf{r}_2) \quad \text{Density Dependent,}$$

$$+ i W_0 (\sigma_1 + \sigma_2) \mathbf{k}^* \delta(\mathbf{r}_1 - \mathbf{r}_2) \times \mathbf{k} \quad \text{Spin-Orbit.}$$

Gogny potential is local, finite range

$$\hat{V}_{\text{Gogny}}(\mathbf{r}_1, \mathbf{r}_2) \propto e^{-(\mathbf{r}_1 - \mathbf{r}_2)^2 / \mu^2} \delta(\mathbf{r}_1 - \mathbf{r}'_1) \delta(\mathbf{r}_2 - \mathbf{r}'_2)$$

which leads to a functional of the non-local density $\rho(\mathbf{r}, \mathbf{r}')$,

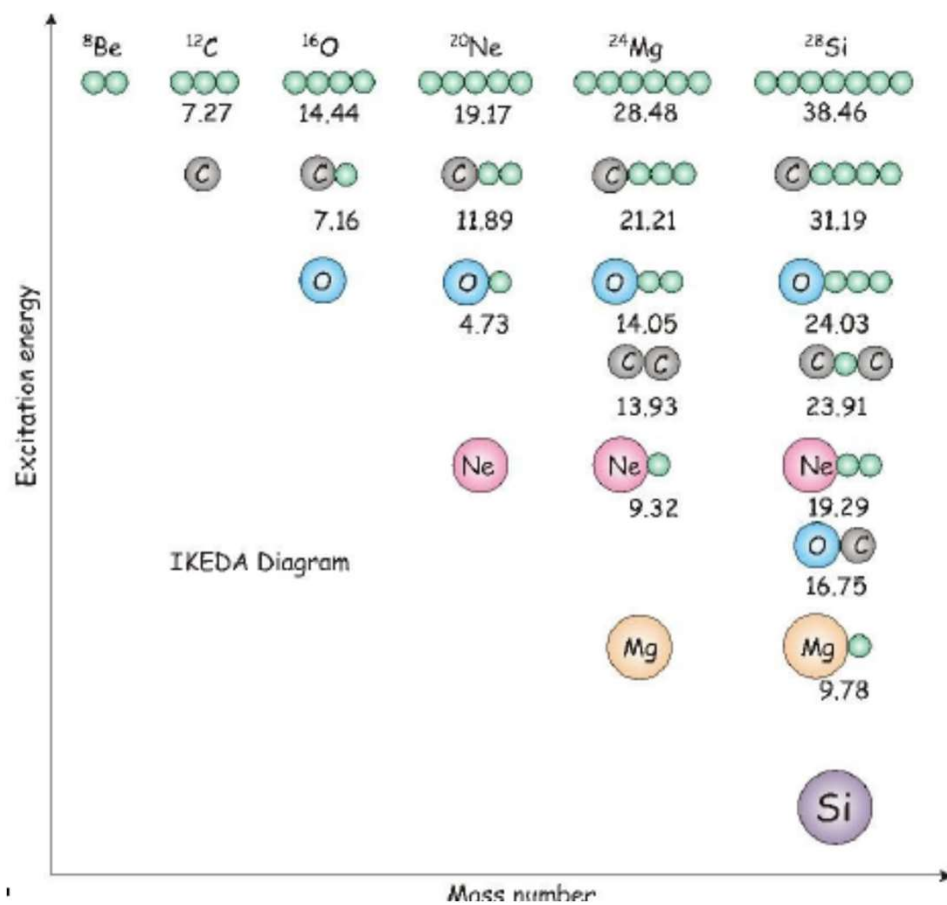
$$E[\rho] = \int d^3\mathbf{r} \int d^3\mathbf{r}' \mathcal{H}(\mathbf{r}, \mathbf{r}'), \quad \mathcal{H}(\mathbf{r}, \mathbf{r}') = C^{\rho\rho} \rho^2(\mathbf{r}, \mathbf{r}') e^{-(\mathbf{r} - \mathbf{r}')^2 / \mu^2} + \dots$$

The physics:

Clustering in nuclei

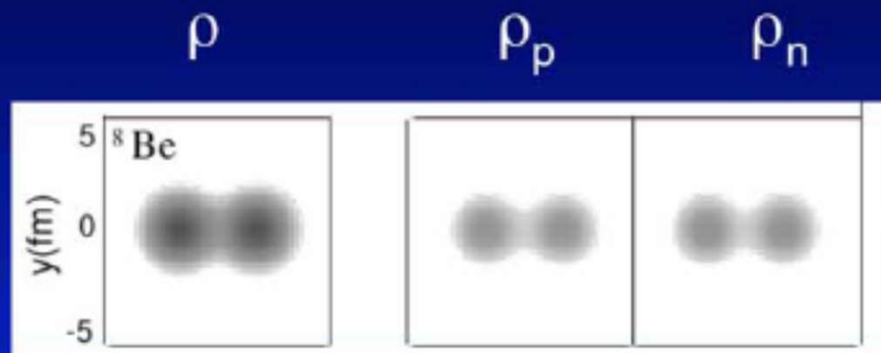
α - cluster states in N=Z light nuclei

Introduction: Ikeda diagram



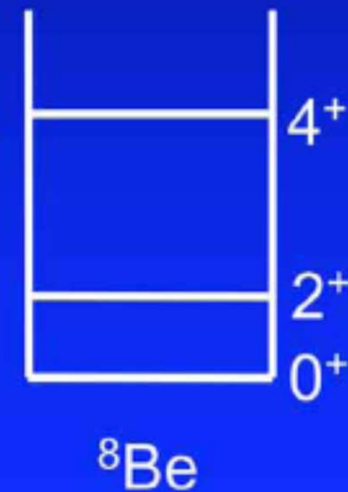
Clustering appears close to the cluster-decay thresholds, quoted here in MeV. For heavy nuclei, the α -cluster thresholds lie at very high energies.

α – Clusterization in ${}^8\text{Be}$

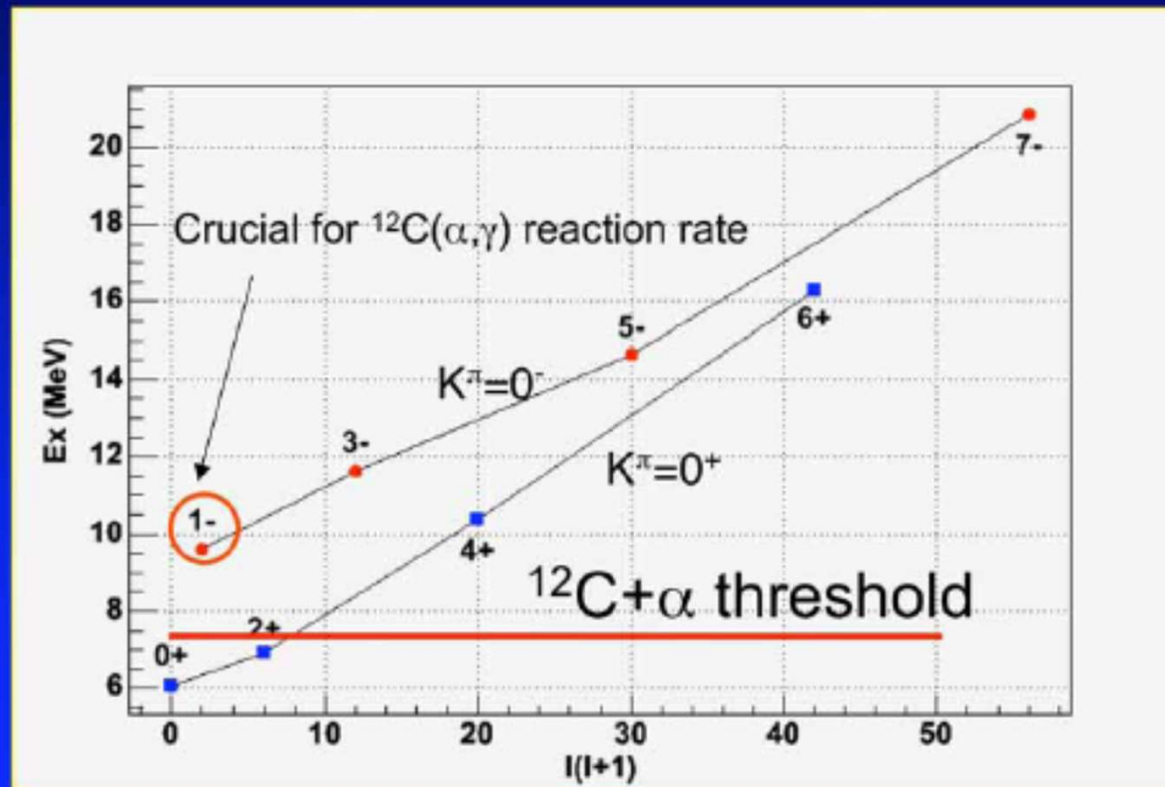


Prog. Theor. Phys. Suppl.
No. 142, 2001
Y. Kanada-En'yo and H. Horiuchi

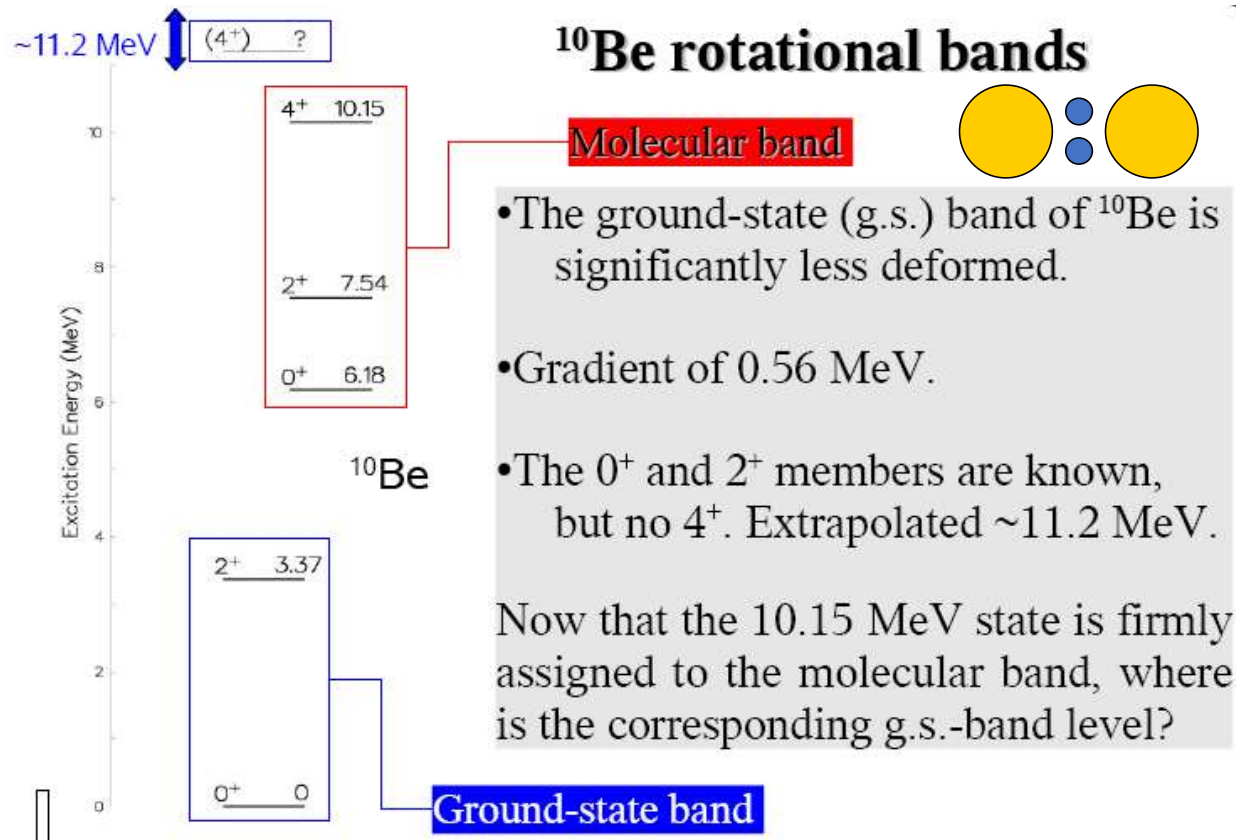
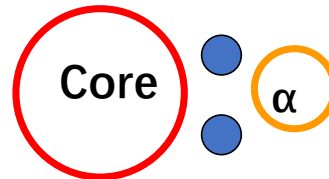
- Density distribution shows developed cluster structure.
- Spectrum of low lying states corresponds to the α - α rotational band.



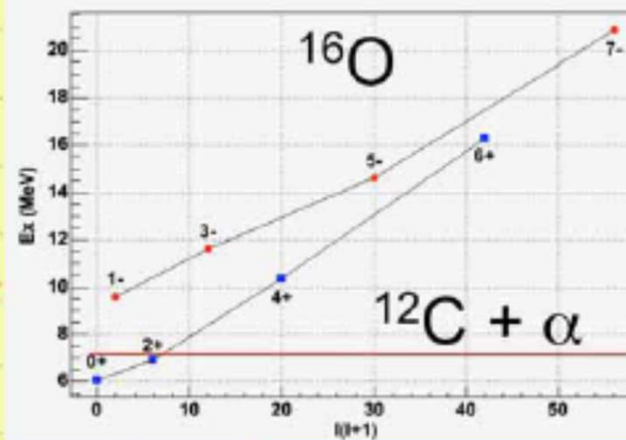
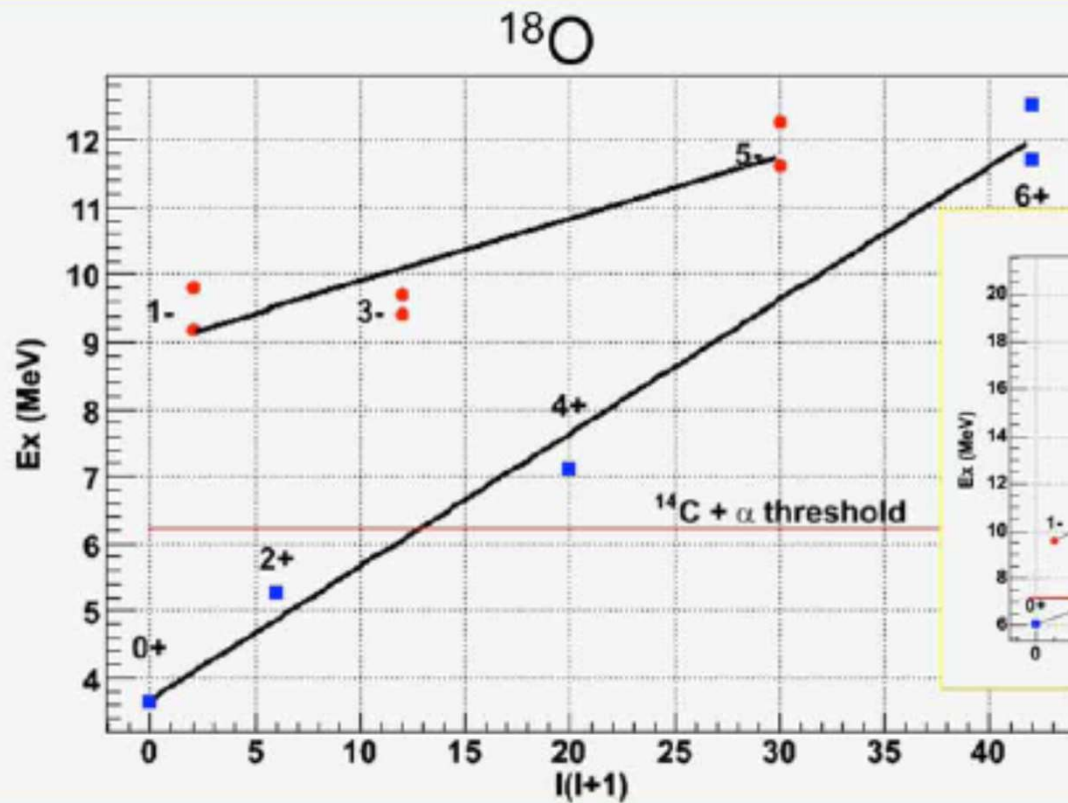
α -cluster rotational bands in ^{16}O



Molecular structures in T=1 nuclei



α – cluster bands in ^{18}O



TOPICAL REVIEW

Developments in the study of nuclear clustering in light even–even nuclei

M Freer† and A C Merchant‡§

† School of Physics and Space Research, University of Birmingham, Birmingham B15 2TT, UK

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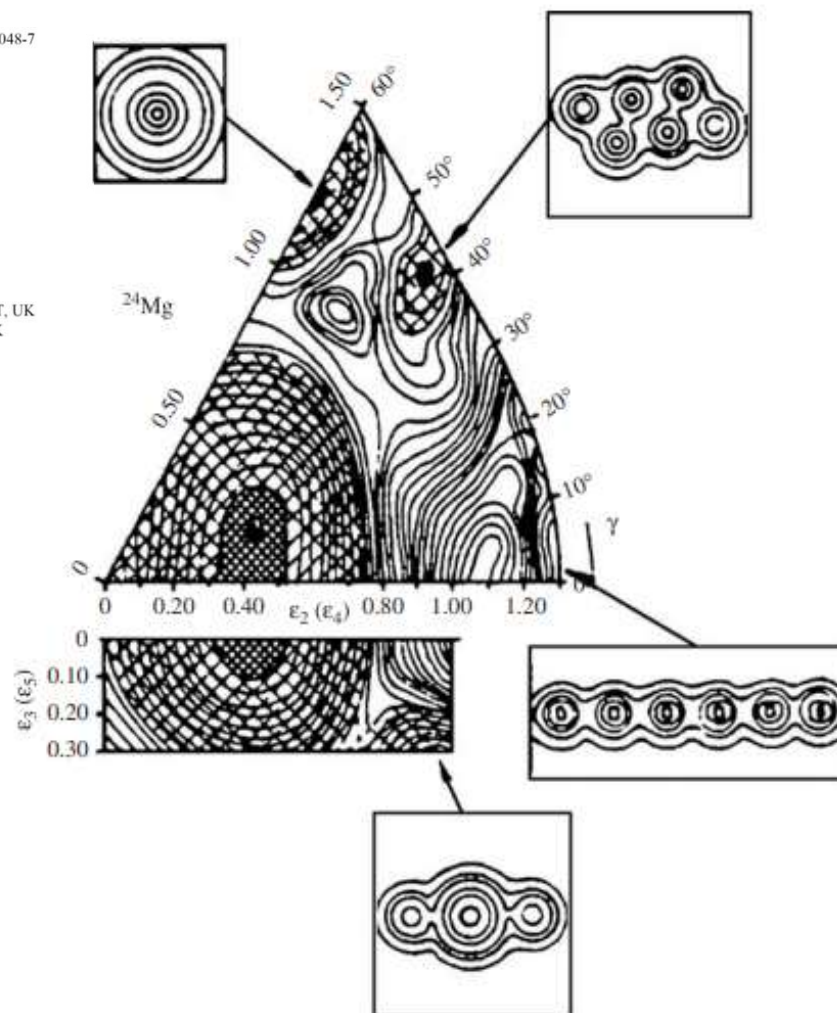
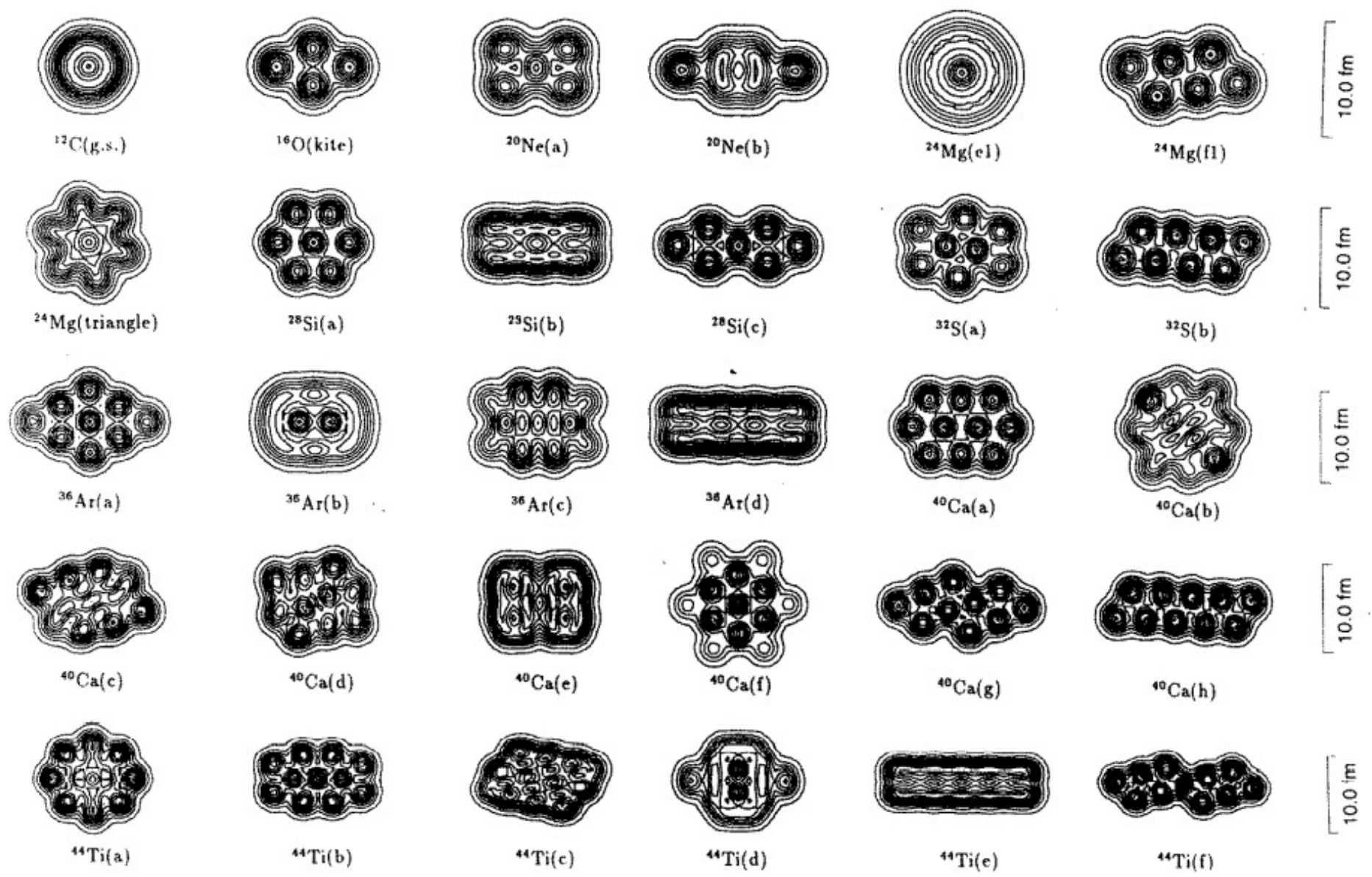
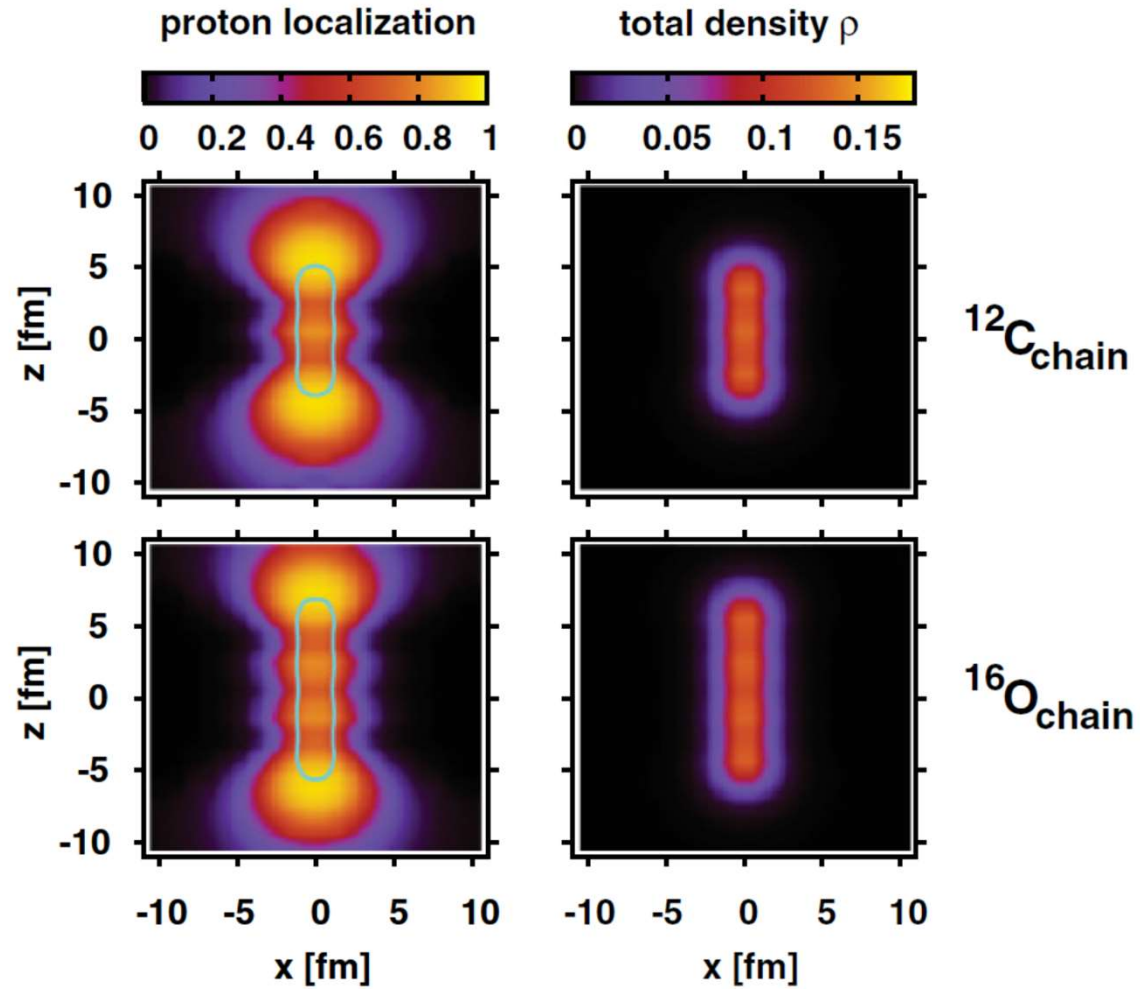


Fig. 6. Nilsson–Strutinsky and α -cluster model calculations for ^{24}Mg [191,113]. The potential energy is shown as a contour plot for the deformation parameters ϵ_2 and γ . Minima are found at particular deformations. For some of the potential minima the shapes obtained with the α -cluster model are indicated. The lower part shows the potential energy for the extension to octupole shapes with the parameter ϵ_3 .



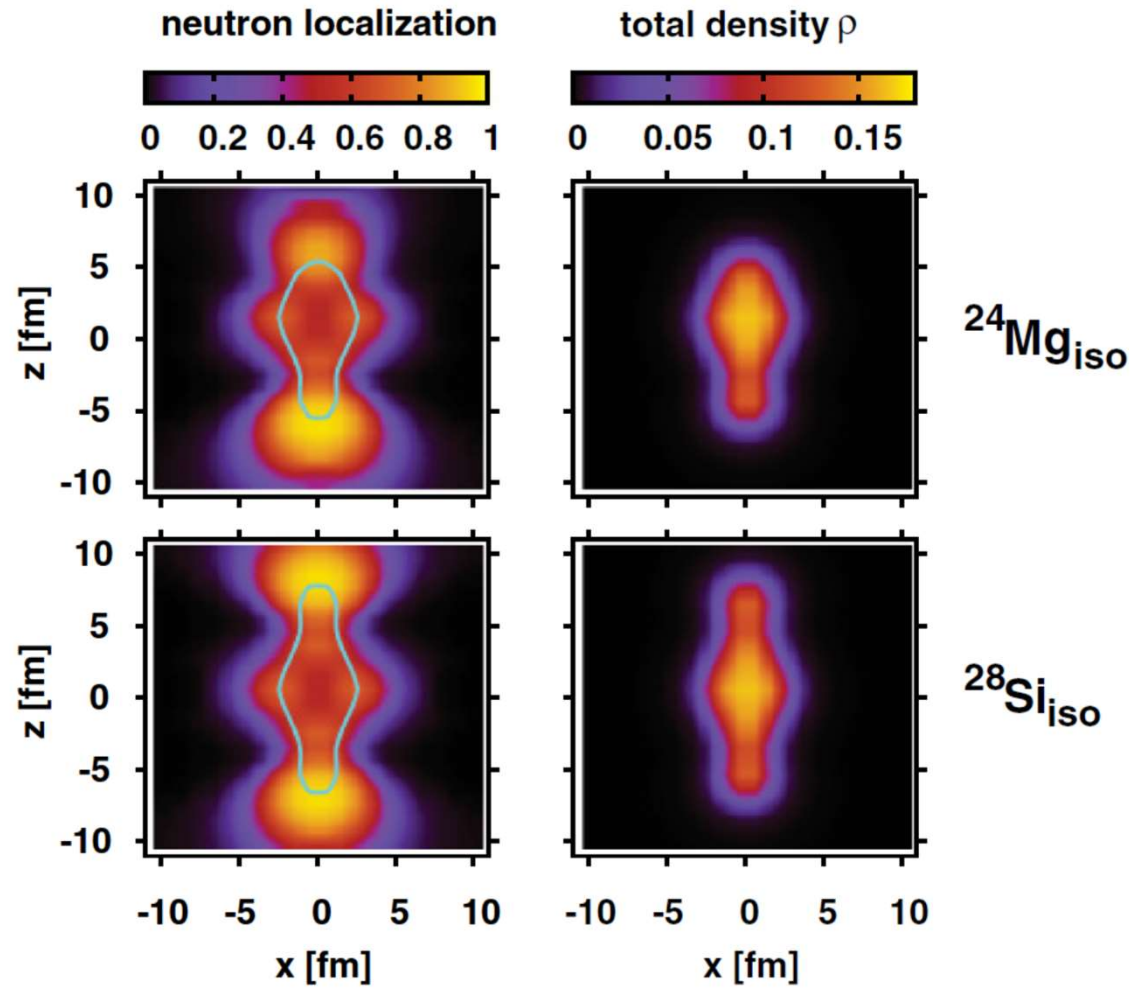
Localization in light nuclei

P.-G. Reinhard,¹ J. A. Maruhn,² A. S. Umar,^{3,*} and V. E. Oberacker³



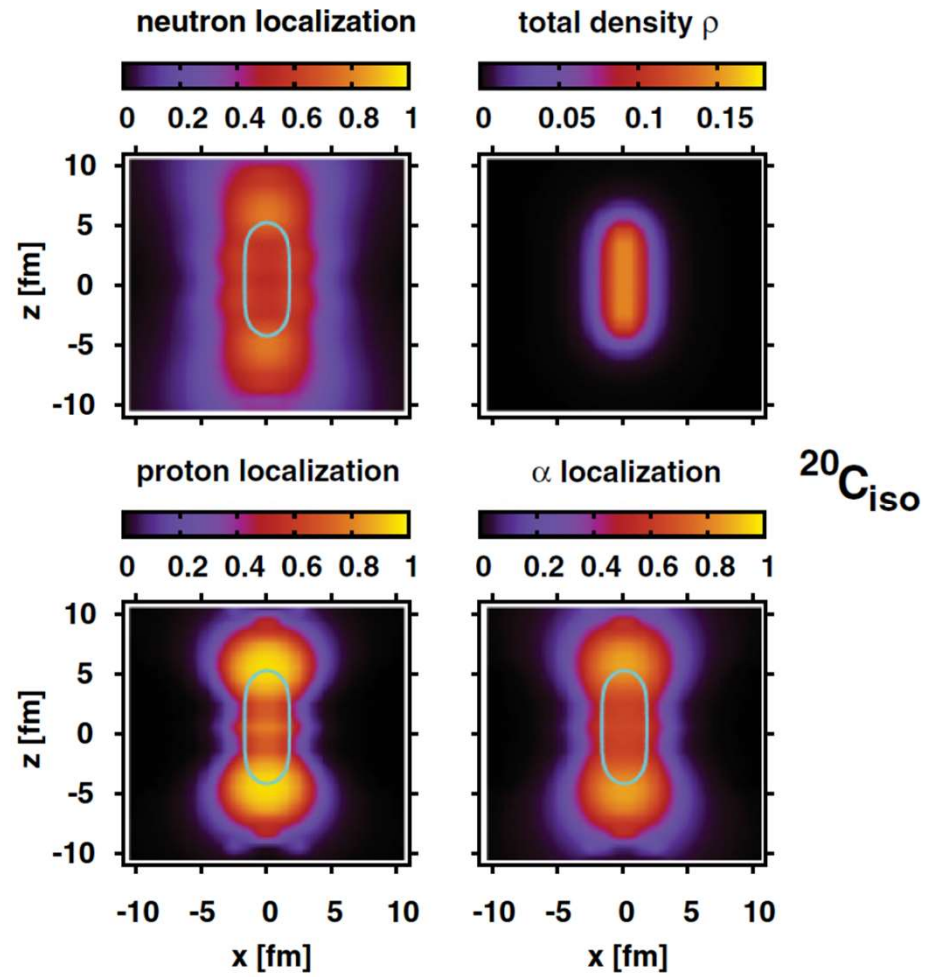
Localization in light nuclei

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Localization in light nuclei

P.-G. Reinhard,¹ J. A. Maruhn,² A. S. Umar,^{3,*} and V. E. Oberacker³



Rod-shaped Nuclei at Extreme Spin and Isospin

P. W. Zhao (赵鹏巍),^{1,2,3} N. Itagaki (板垣直之),¹ and J. Meng (孟杰)^{3,4,5,*}

For light nuclei, there have been indications that even more exotic states above 1:3 might exist in light $N = Z$ nuclei due to the α cluster structure. However, there is still no firm

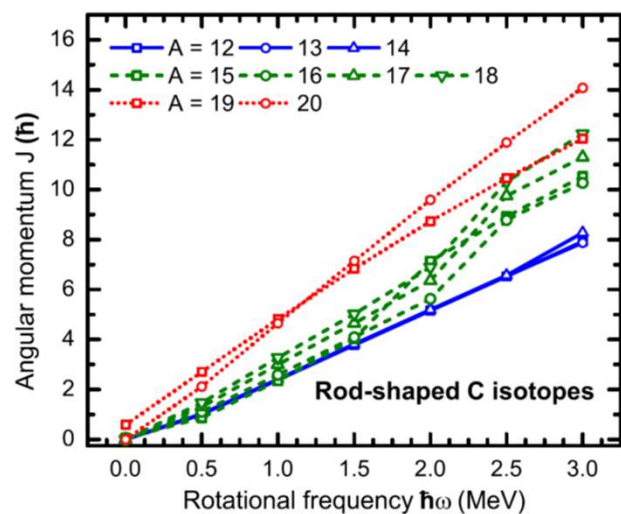


FIG. 1 (color online). Angular momenta as functions of the rotational frequency for C isotopes from $A = 12$ to $A = 20$.

- 12~14: Rigid rotor;
- 15~18: Back-bending;
- 19~20: Rigid rotor again.

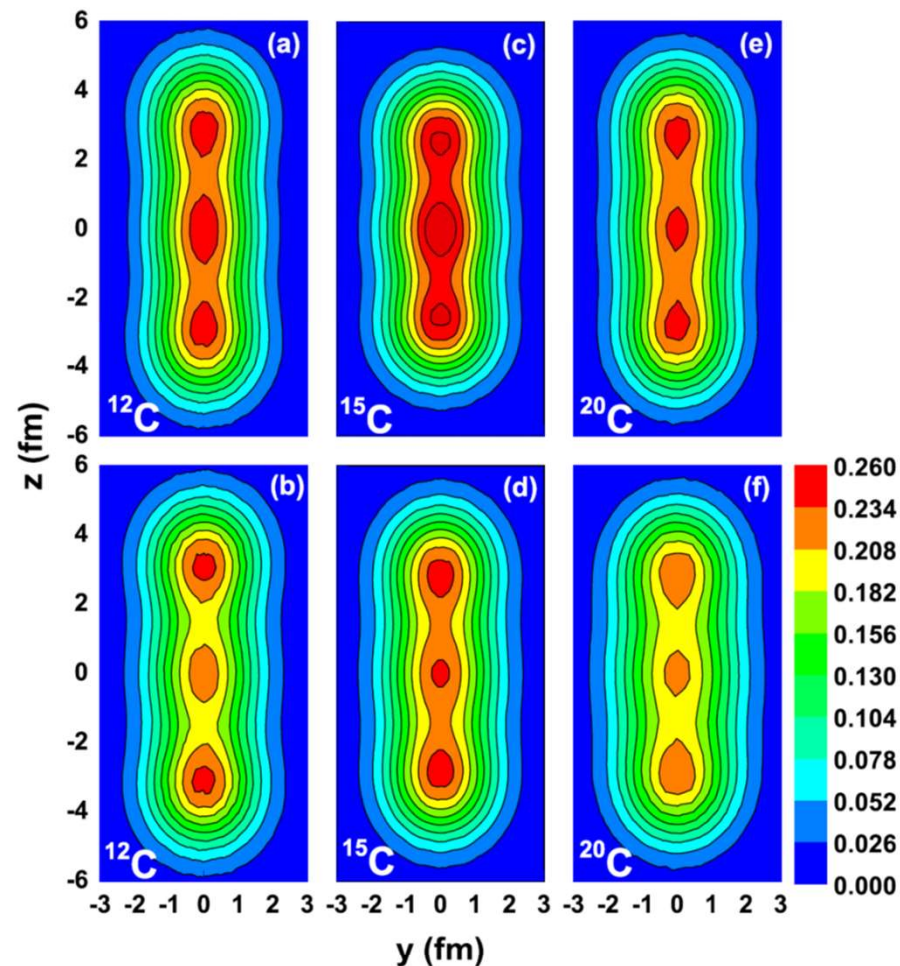


FIG. 2 (color online). Proton density distributions in the y - z plane (x direction is integrated) calculated by using the cranking covariant density functional theory for ^{12}C , ^{15}C , and ^{20}C at the rotational frequencies $\hbar\omega = 0.0$ MeV (a),(c),(e) and $\hbar\omega = 3.0$ MeV (b),(d),(f).

The valence neutron densities outside the core ^{12}C

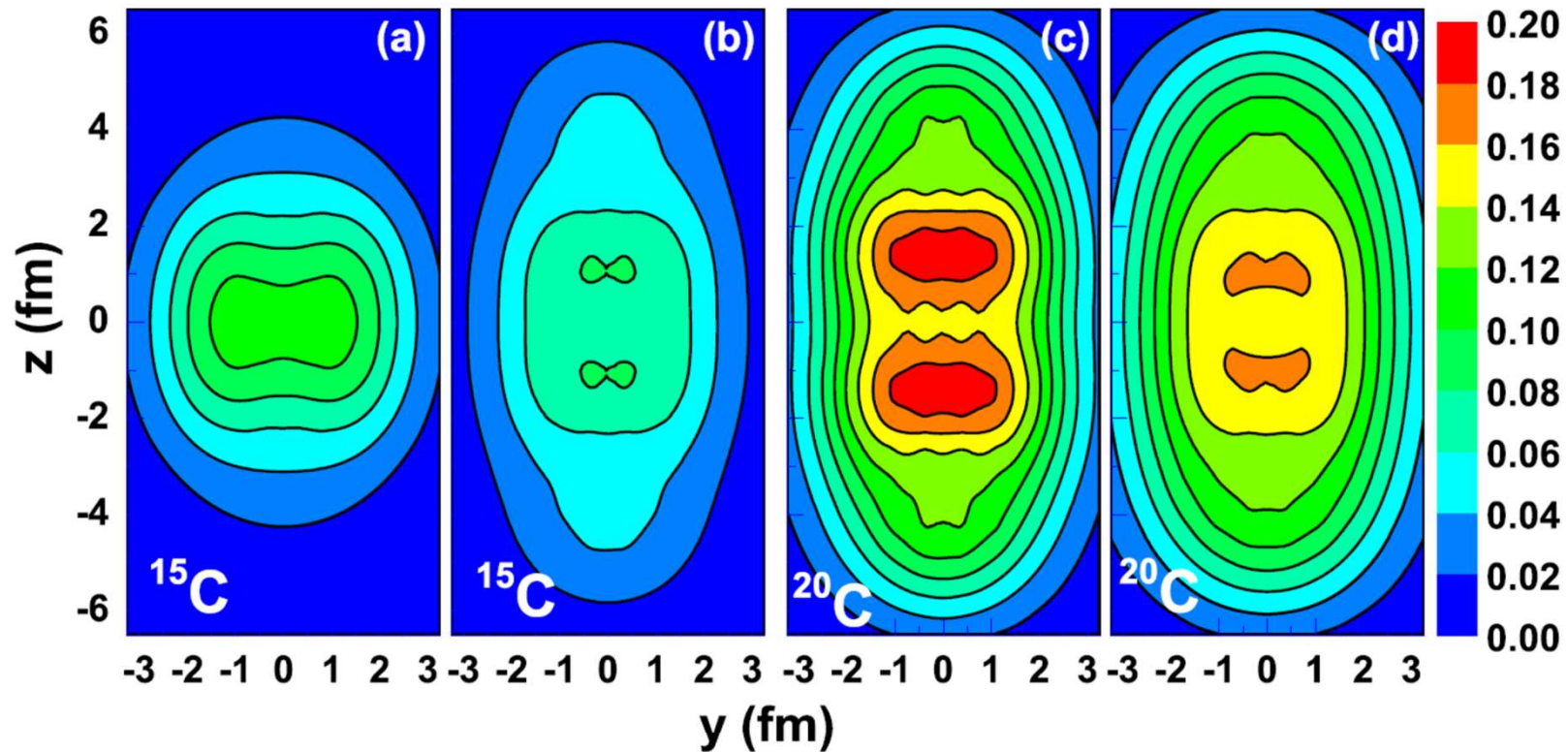
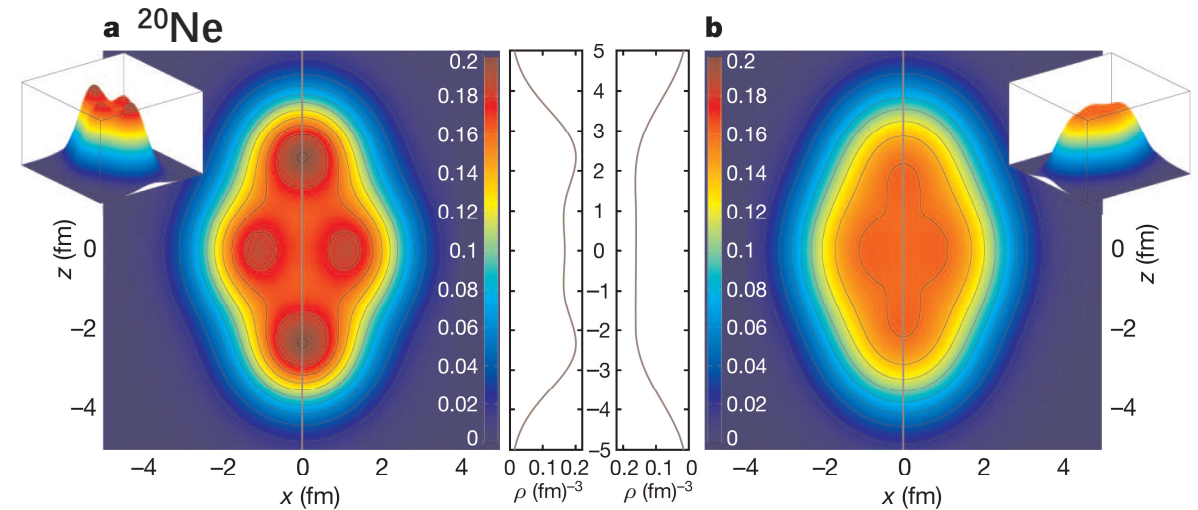


FIG. 4 (color online). Valence neutron distributions in the y - z plane (x direction is integrated) defined as the difference between the neutron and proton densities for ^{15}C and ^{20}C at the rotational frequencies $\hbar\omega = 0.0$ MeV (a),(c) and $\hbar\omega = 3.0$ MeV (b),(d).

How atomic nuclei cluster

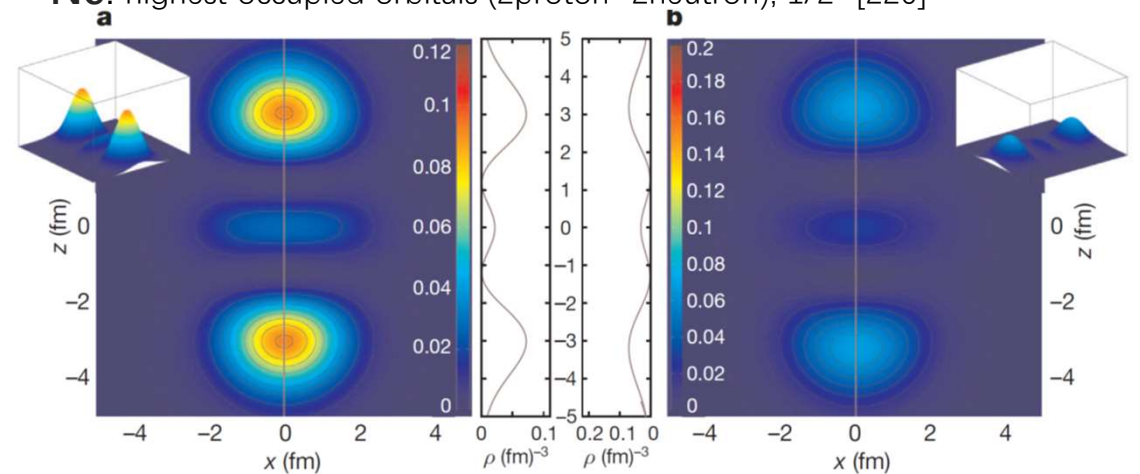
J.-P. Ebran¹, E. Khan², T. Nikšić³ & D. Vretenar³

Nucleonic matter displays a quantum-liquid structure, but in some cases finite nuclei behave like molecules composed of clusters of protons and neutrons. Clustering is a recurrent feature in light nuclei, from beryllium to nickel^{1–3}. Cluster structures are typically observed as excited states close to the corresponding decay threshold; the origin of this phenomenon lies in the effective nuclear interaction, but the detailed mechanism of clustering in nuclei has not yet been fully understood. Here we use the theoretical framework of energy-density functionals^{4,5}, encompassing both cluster and quantum liquid-drop aspects of nuclei, to show that conditions for cluster formation can in part be traced back to the depth of the confining nuclear potential. For the illustrative example of neon-20, we show that the depth of the potential determines the energy spacings between single-nucleon orbitals in deformed nuclei, the localization of the corresponding wavefunctions and, therefore, the degree of nucleonic density clustering. Relativistic functionals, in particular, are characterized by deep single-nucleon potentials. When compared to non-relativistic functionals that yield similar ground-state properties (binding energy, deformation, radii), they predict the occurrence of much more pronounced cluster structures. More generally, clustering is considered as a transitional phenomenon between crystalline and quantum-liquid phases of fermionic systems.



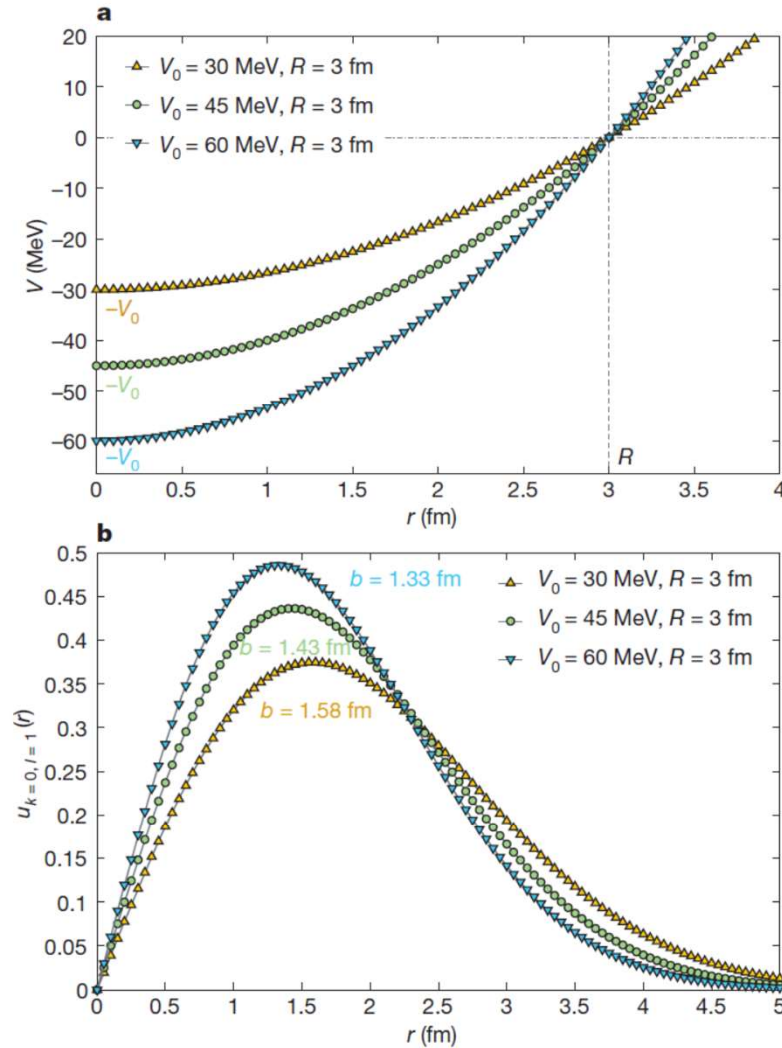
a, DD-ME2 (ref. 22), and **b**, Skyrme SLy4

²⁰Ne: highest occupied orbitals (2proton+2neutron), 1/2+[220]



How atomic nuclei

J.-P. Ebran¹, E. Khan², T. Nikšić³ & D. Vreteno¹



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Figure 3 | Harmonic oscillators of different depths. **a**, Potentials plotted against the radial coordinate r for harmonic oscillators with the same radius, $R = 3$ fm, and depths (V_0) of 30, 45 and 60 MeV. **b**, The radial wavefunctions $U_{k,l}$ of the corresponding first p -state, where k is the radial quantum number and l the azimuthal one. The position of the maximum is determined by the oscillator length b .

How atomic nuclei cluster

J.-P. Ebran¹, E. Khan², T. Nikšić³ & D. Vretenar³

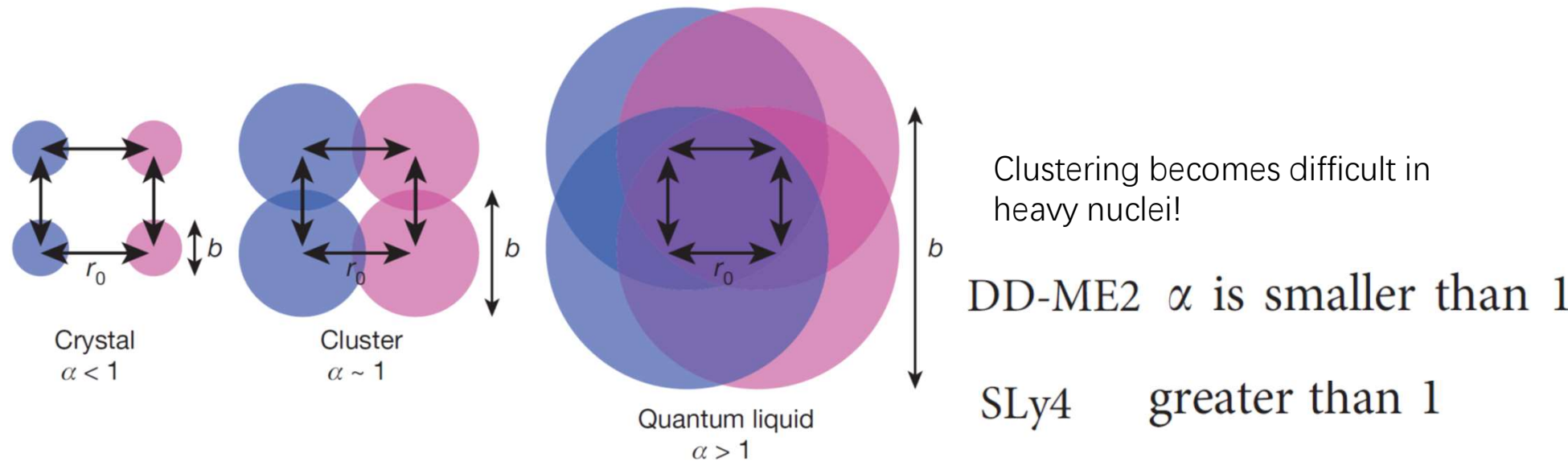


Figure 4 | Schematic illustration of the transition from a crystalline to a quantum liquid phase, including the cluster phase. The dimensionless parameter $\alpha = b/r_0$, where b is the dispersion of the fermion wavefunction and r_0 the typical inter-fermion distance, quantifies nuclear clustering. For a harmonic oscillator $\alpha = (\hbar R)^{1/2} (2mV_0)^{-1/4} r_0^{-1}$, where V_0 is the depth of the potential, R the radius of the system, m the mass of the nucleon and \hbar Planck's constant/ 2π .

α -Particle Clustering from Expanding Self-Conjugate Nuclei within the Hartree-Fock-Bogoliubov Approach

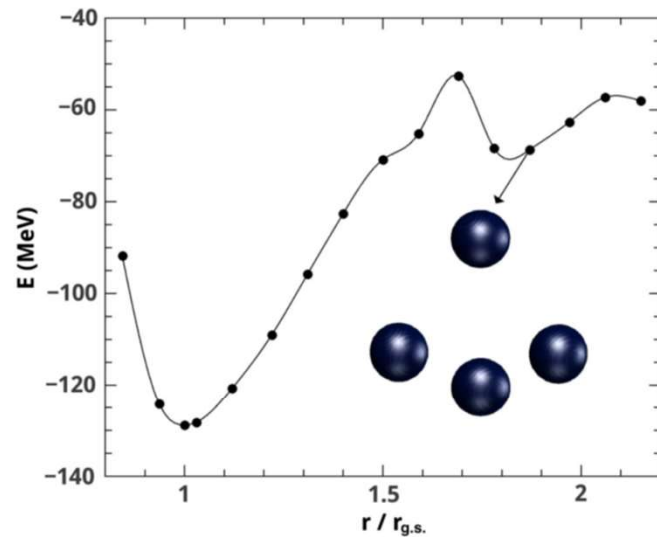
M. Girod¹ and P. Schuck^{2,3}

FIG. 1 (color online). Total energy of ^{16}O as a function of the radius scaled with respect to the one of the ground state $r_{\text{g.s.}}$. At $r/r_{\text{g.s.}} = \sim 1.8$, we see that a tetrahedron of four α particles is formed. No c.m. correction for individual α 's is applied here. The arrow indicates to which $r/r_{\text{g.s.}}$ value the α configuration corresponds.

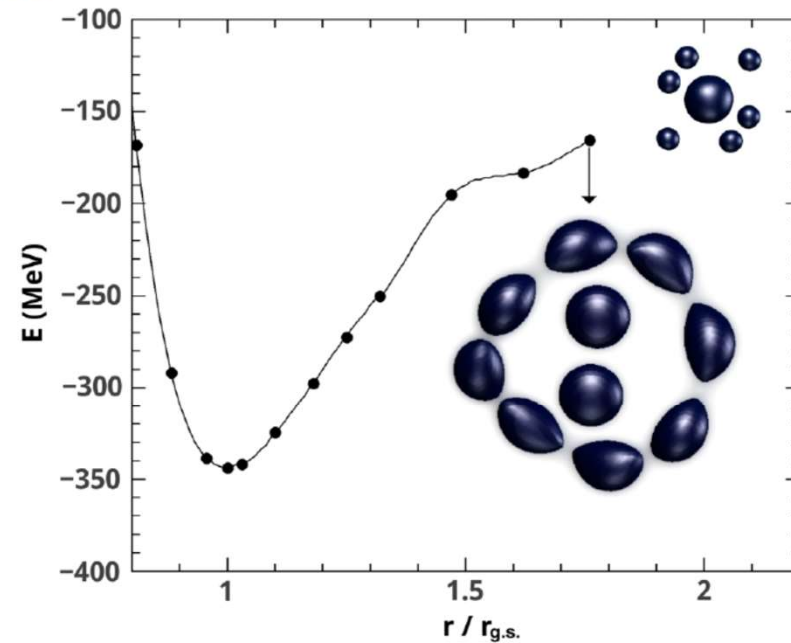


FIG. 4 (color online). Same as Fig. 1 but for ^{40}Ca with ten α 's. Also, configurations with a ^{16}O surrounded by six α 's are shown.

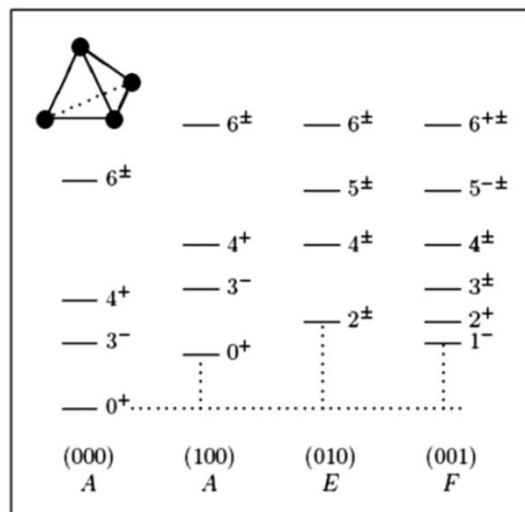
Evidence for Tetrahedral Symmetry in ^{16}O R. Bijker¹ and F. Iachello²

FIG. 1. Schematic spectrum of a spherical top with tetrahedral symmetry and $\omega_1 = \omega_2 = \omega_3$. The rotational bands are labeled by (v_1, v_2, v_3) (bottom). All states are symmetric under S_4 .

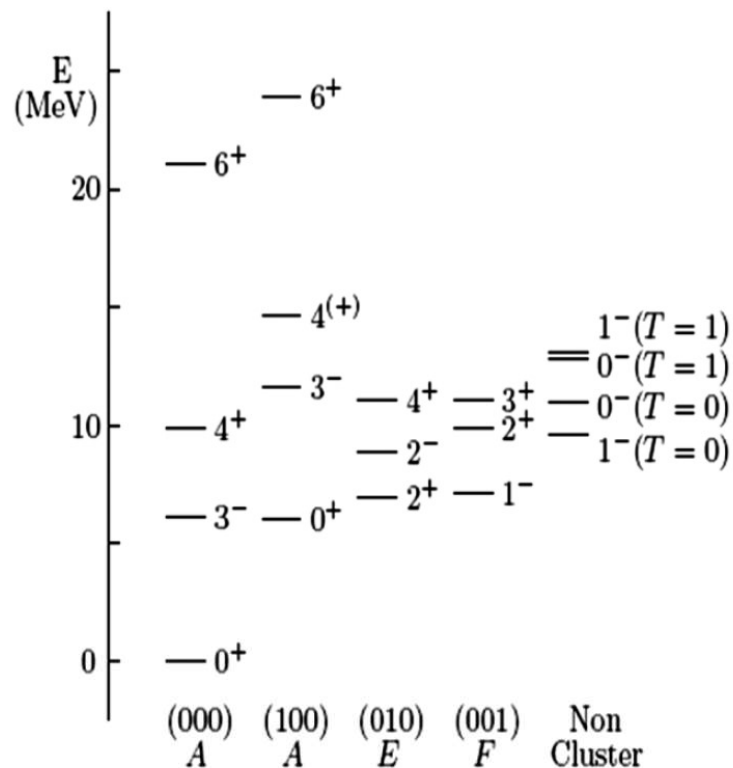


FIG. 2. The observed spectrum of ^{16}O [17]. The levels are organized in columns corresponding to the ground-state band and the three vibrational bands with A , E , and F symmetry of a spherical top with tetrahedral symmetry. The last column shows the lowest noncluster levels.

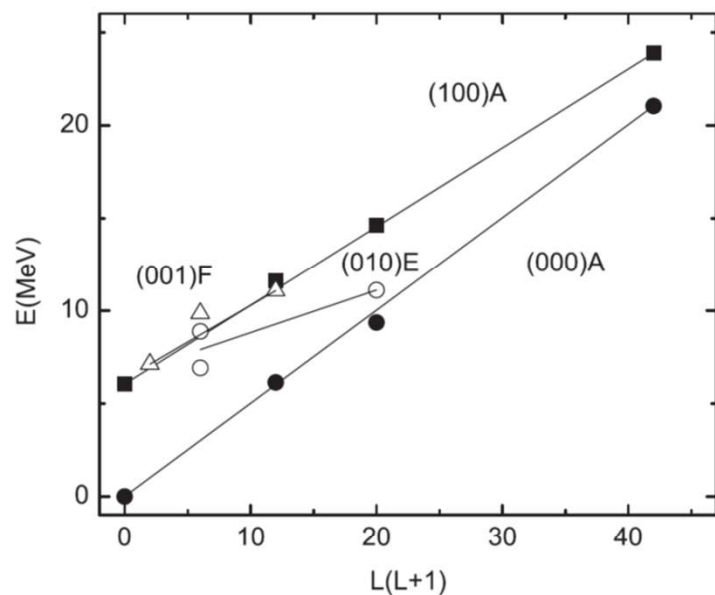
Evidence for Tetrahedral Symmetry in ^{16}O R. Bijker¹ and F. Iachello²

FIG. 3. The excitation energies of cluster states in ^{16}O plotted as a function of $L(L+1)$: closed circles for the ground-state band, closed squares for the A vibration, open circles for the E vibration, and open triangles for the F vibration.

TABLE I. Comparison of theoretical and experimental $B(EL)$ values in $e^2 \text{fm}^{2L}$ and E_γ values in keV, along the ground-state band. The theoretical $B(EL)$ values are obtained from Eq. (6), and the E_γ values are obtained from $E = 0.511L(L+1)$ MeV. The experimental values are taken from Ref. [17].

$B(EL; L^P \rightarrow 0^+)$	Theoretical	Experimental	$E_\gamma(L^P)$	Theoretical	Experimental
$B(E3; 3_1^- \rightarrow 0_1^+)$	181	205 ± 10	$E_\gamma(3_1^-)$	6132	6130
$B(E4; 4_1^+ \rightarrow 0_1^+)$	338	378 ± 133	$E_\gamma(4_1^+)$	10220	10356
$B(E6; 6_1^+ \rightarrow 0_1^+)$	8245		$E_\gamma(6_1^+)$	21 462	21 052

Evidence for the Tetrahedral Nature of ^{16}O

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(Received 9 January 1979)

Evidence is given to show that ^{16}O behaves like a tetrahedral rotor with a level sequence $0^+, 3^-, 4^+, 6^+, 7^-, 8^+, \dots$. The charge form factors for excited states can be predicted from the ground-state form factor and excellent agreement with experiment is obtained for the 3^- and 4^+ states at 6.13 and 10.35 MeV, respectively. The elastic-scattering data are fitted using deformed rather than spherical α clusters.

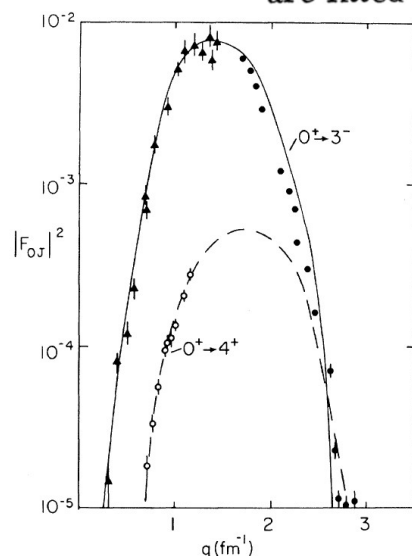


FIG. 1. Theoretical predictions for the inelastic charge form factors for the $0^+ \rightarrow 3^-$ transition (solid line) and the $0^+ \rightarrow 4^+$ transition (broken line). Experimental points for the 3^- state are from Ref. 7 and for the 4^+ state from Ref. 8. Note that the high- q data and some of the points around the maximum of the 3^- data involve a weak contribution from the unresolved 0^+ state at 6.05 MeV.

The form factor for the 3^- state (also completely predicted by the model from the 0^+ form factor) is a remarkably good fit to the data. Although

$BE(3)$ value is easily calculated from the $|F_{03}|^2$ curve and is found to be $1200 e^2 \cdot \text{fm}^6$ which is in close agreement with experimental values¹⁰ (1150 – $1500 e^2 \cdot \text{fm}^6$). The result for $|F_{03}|^2$ in Fig. 1 is the major result of this work and represents strong evidence for the rotational character of the 3^- (6.13) level in ^{16}O .

Relationships proposed here between the $3^-, 4^+$ form factors and the elastic form factor for ^{16}O depend only upon the assumption of a tetrahedral rotor and not on the details of the clusters themselves.

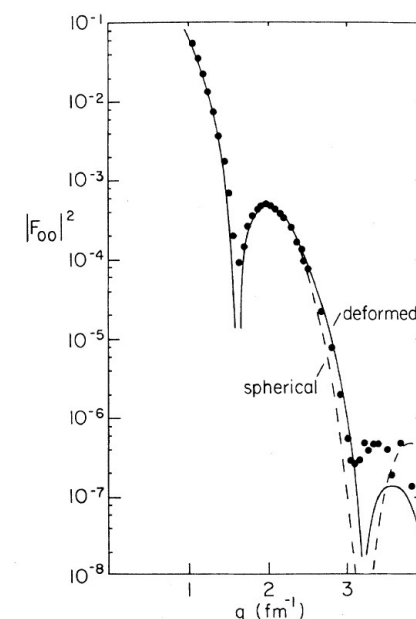


FIG. 2. Theoretical calculations for the elastic charge form factor squared for deformed clusters (full line) with $\alpha = 0.23 \text{ fm}^2$ and spherical clusters (broken line) with $\alpha = 0.06 \text{ fm}^2$. The value of $R = 1.96 \text{ fm}$ is taken from the close-packing arguments of Ref. 12. The experimental points are from Ref. 13.

Giant Dipole Resonance as a Fingerprint of α Clustering Configurations in ^{12}C and ^{16}O

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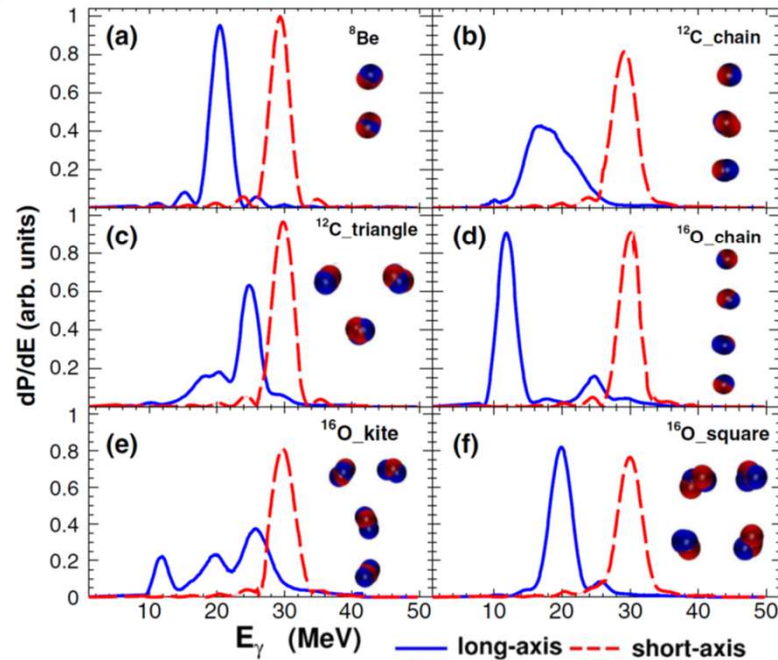
¹Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 201800, China

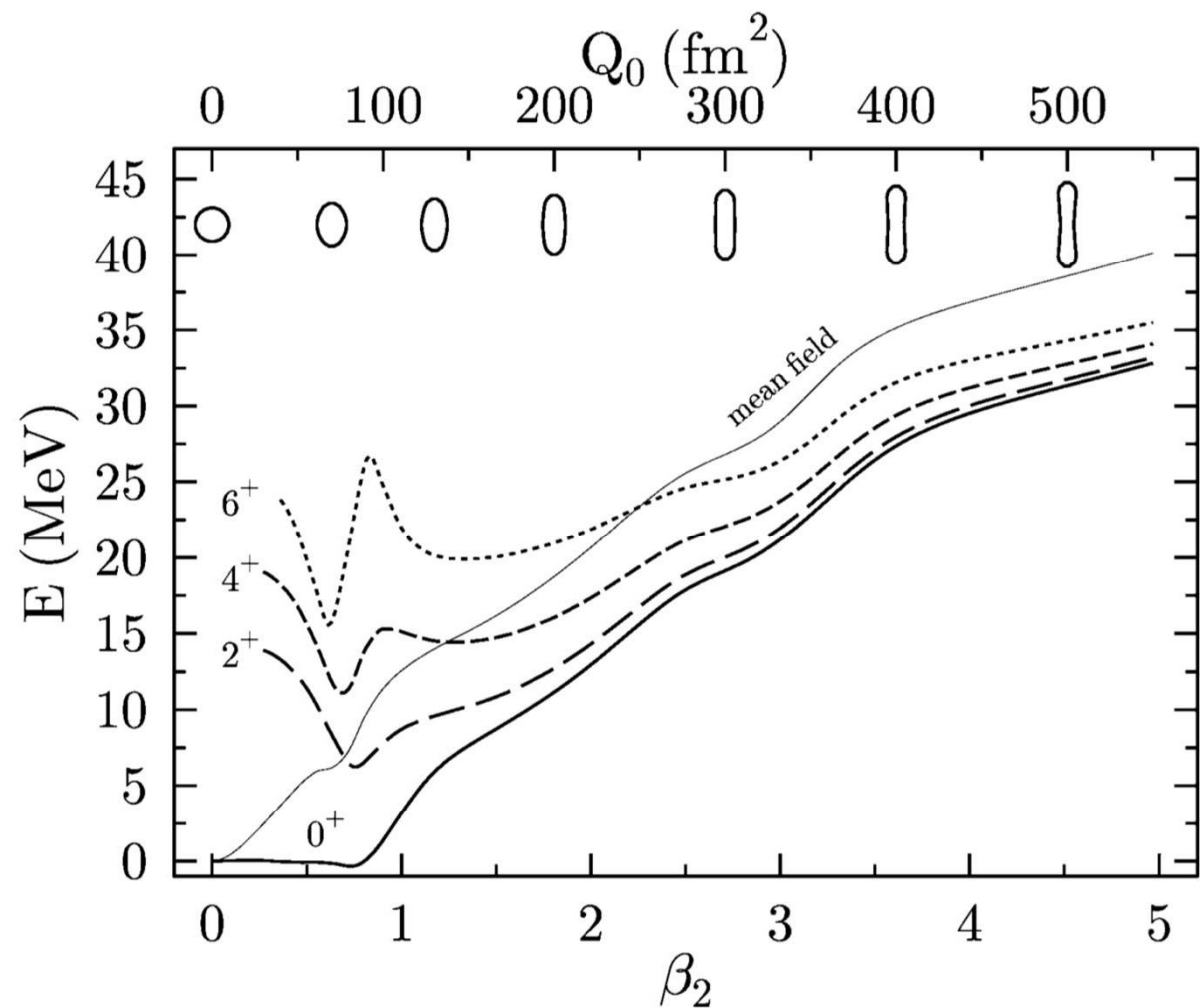
²University of the Chinese Academy of Sciences, Beijing 100080, China

³Shanghai Tech University, Shanghai 200031, China

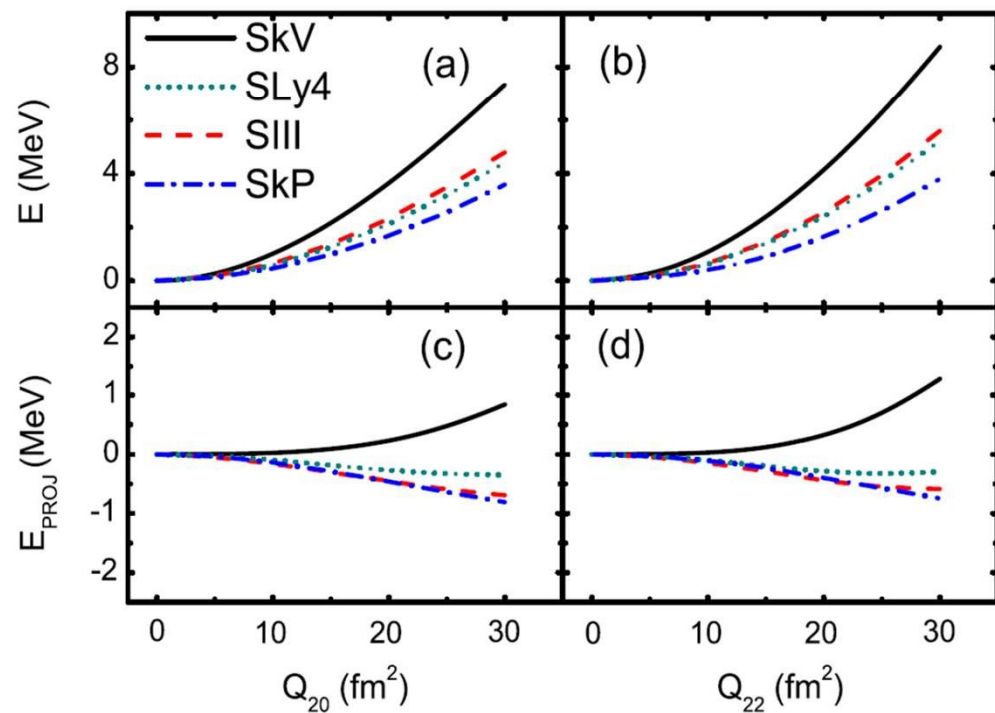
(Received 6 May 2014; published 17 July 2014)

It is studied how the α cluster degrees of freedom, such as α clustering configurations close to the α decay threshold in ^{12}C and ^{16}O , including the linear chain, triangle, square, kite, and tetrahedron, affect nuclear collective vibrations with a microscopic dynamical approach, which can describe properties of nuclear ground states well across the nuclide chart and reproduce the standard giant dipole resonance (GDR) of ^{16}O quite nicely. It is found that the GDR spectrum is highly fragmented into several apparent peaks due to the α structure. The different α cluster configurations in ^{12}C and ^{16}O have corresponding characteristic spectra of GDR. The number and centroid energies of peaks in the GDR spectra can be reasonably explained by the geometrical and dynamical symmetries of α clustering configurations. Therefore, the GDR can be regarded as a very effective probe to diagnose the different α cluster configurations in light nuclei.



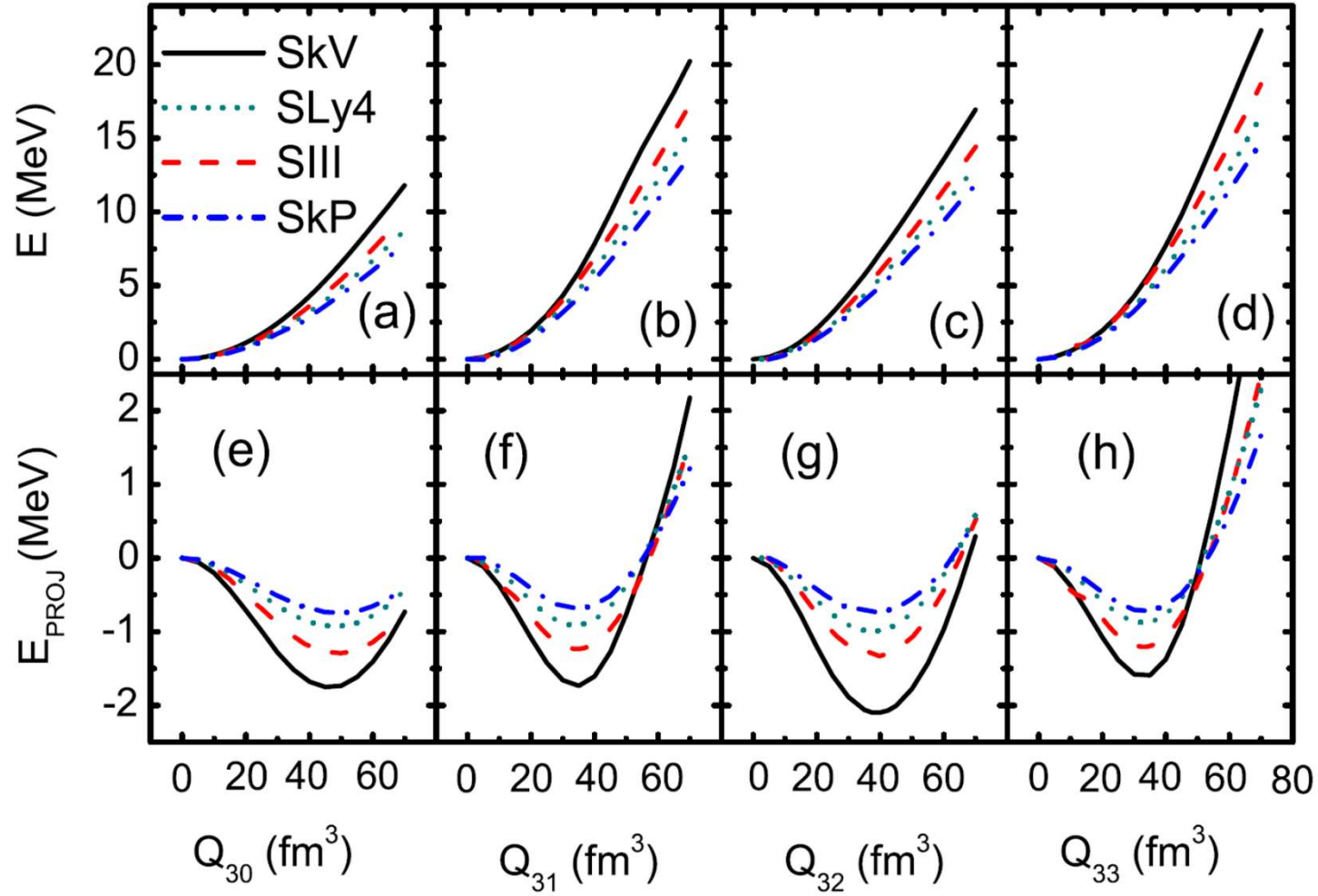


M. Bender, P.-H. Heenen / Nuclear Physics A 713 (2003) 390–401

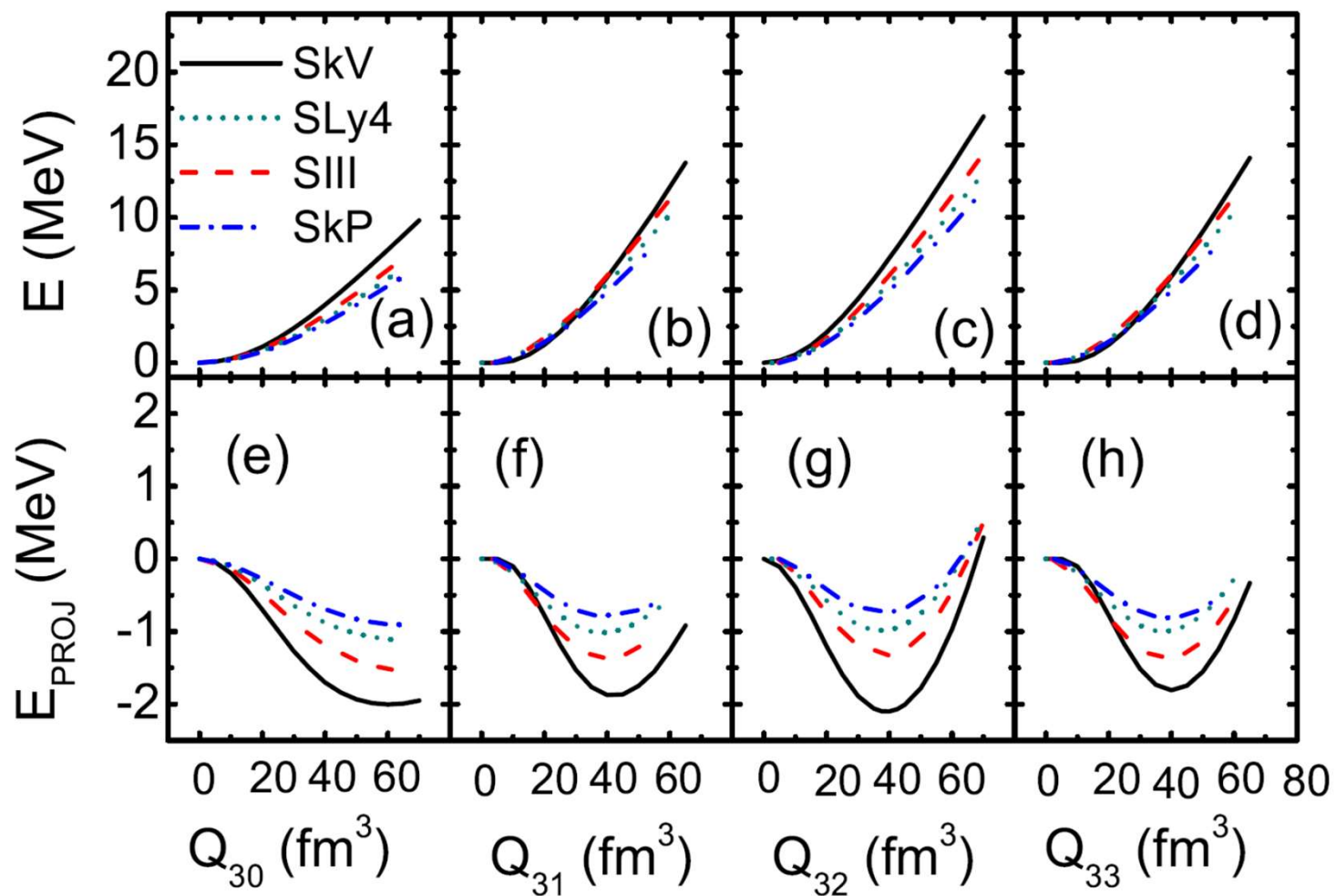


Q3形状自由度冻结

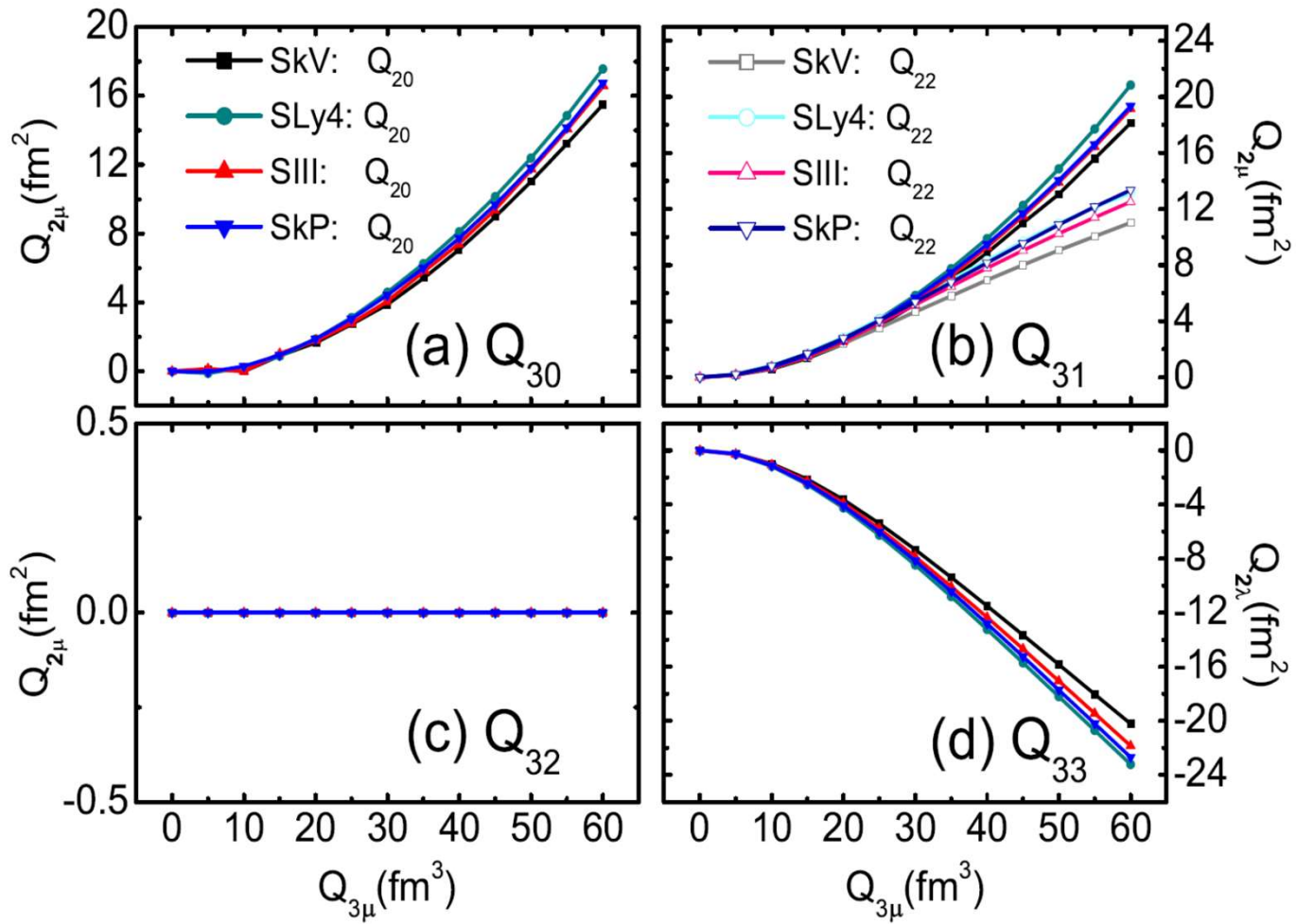
X.B.Wang, G.X.Dong, Z.C.Gao, Y.S.Chen, C.W.Shen,
Physics Letters B 790(2019)498–501



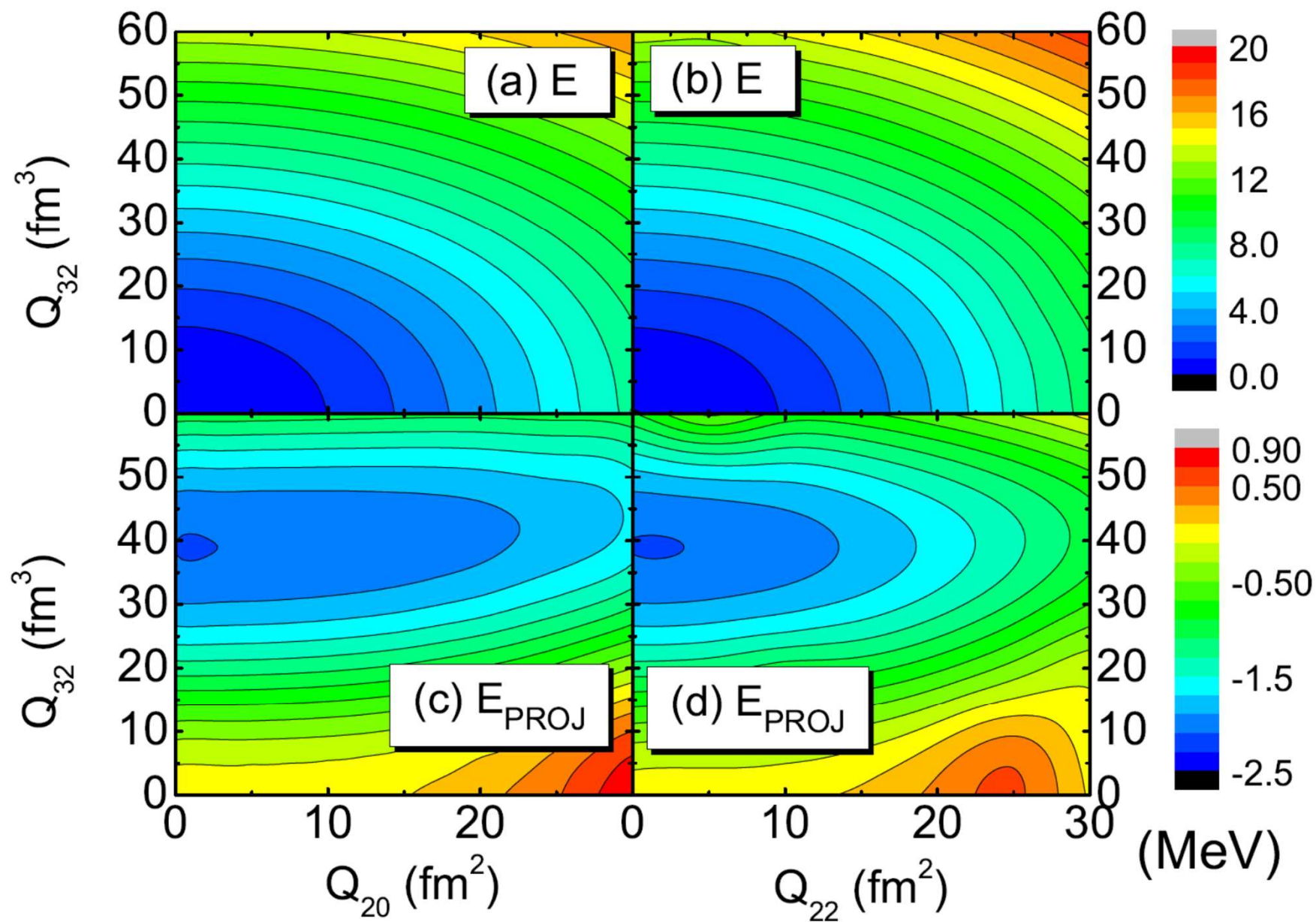
Q2形状自由度冻结

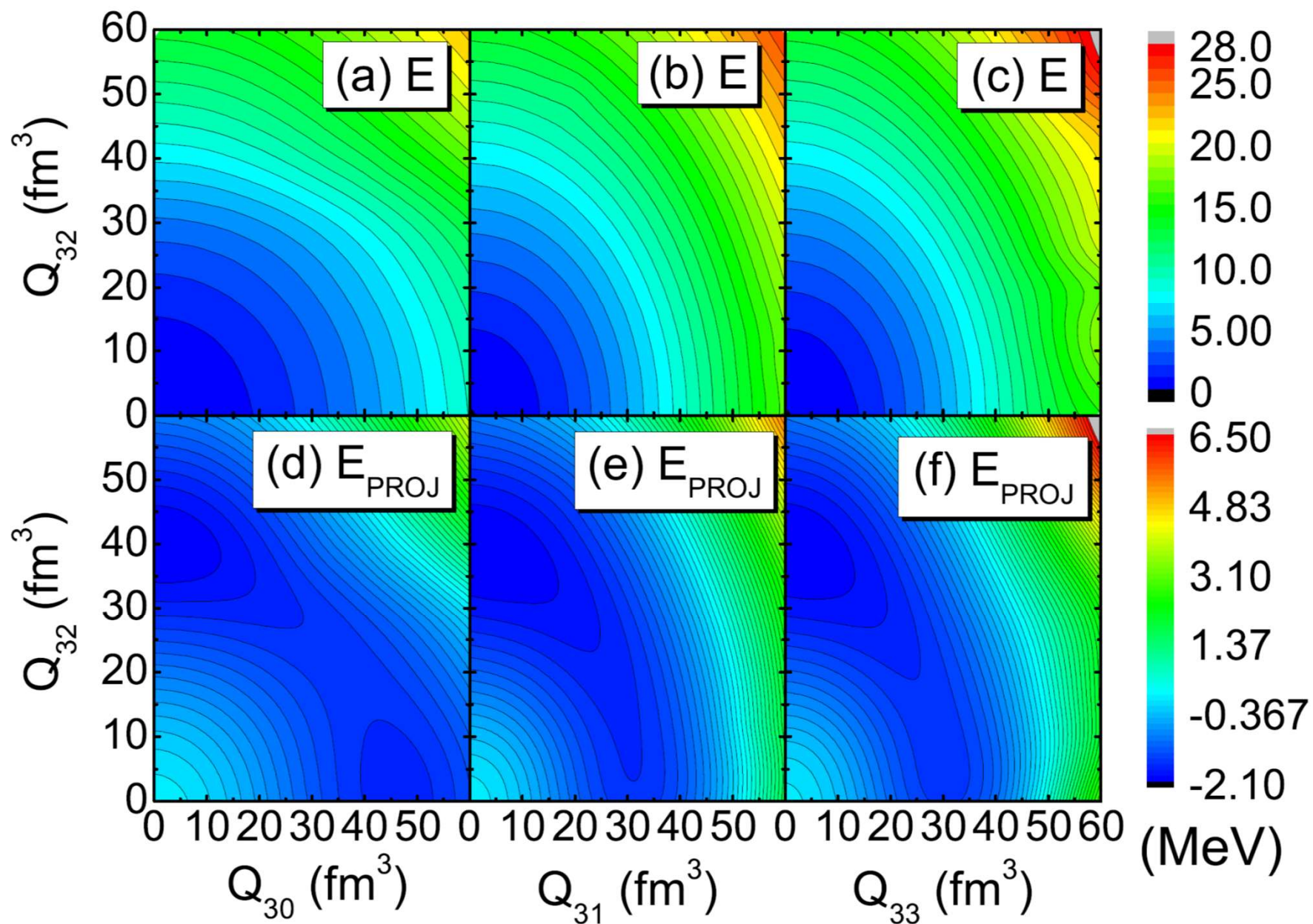


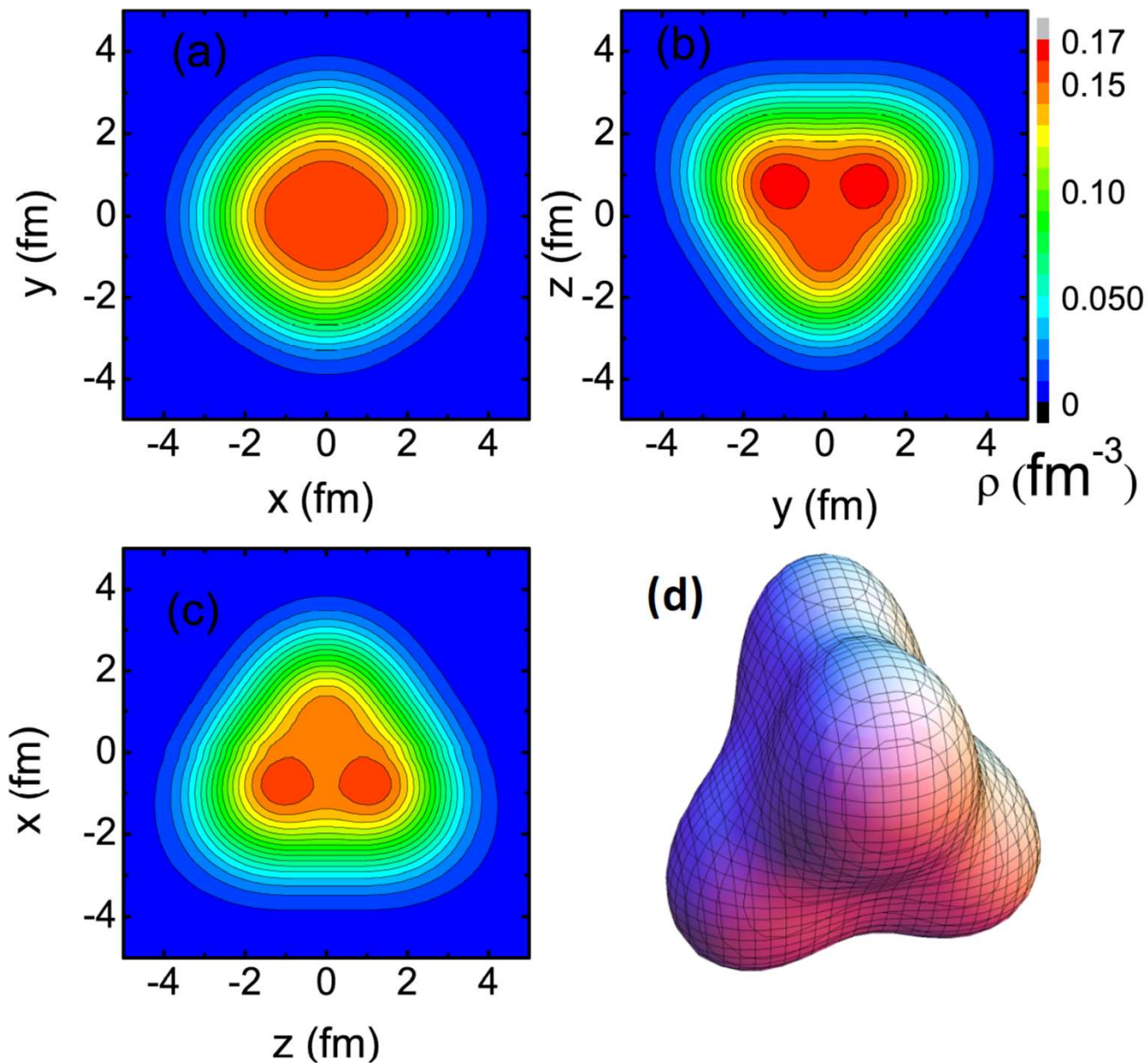
Q2形状自由度放开



Q2形状自由度放开

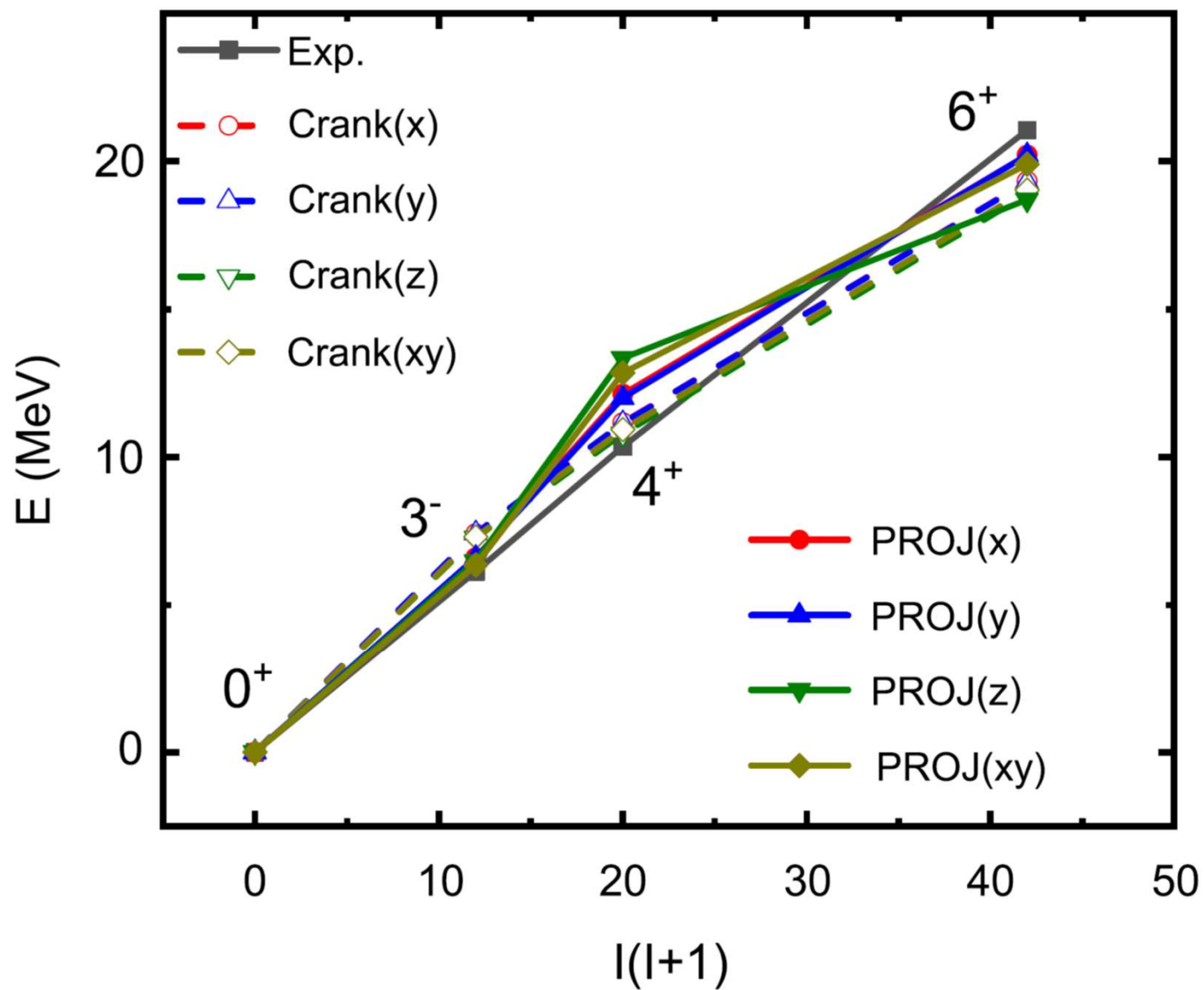






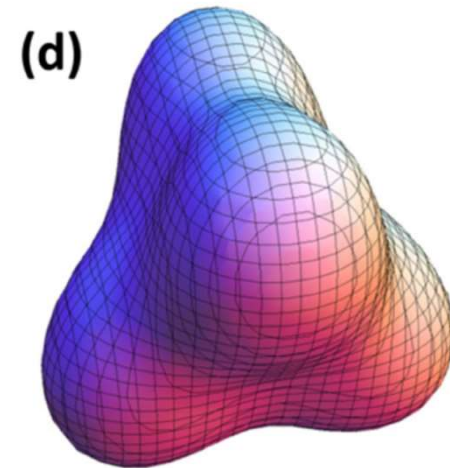
$$\hat{Q}_{32} = 40 \text{ fm}^3$$

$$(\beta_{32} = 0.339)$$



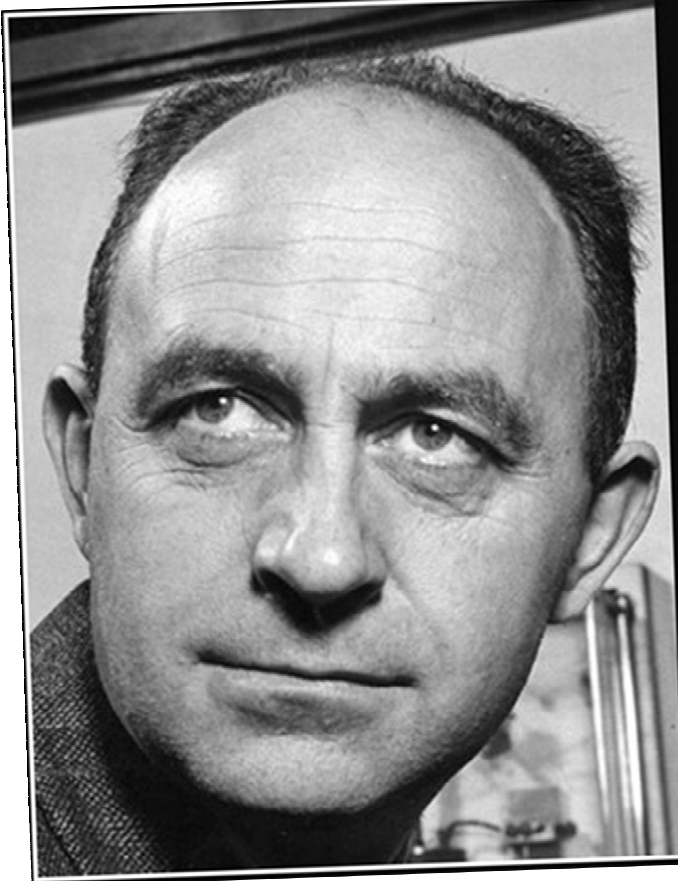
$$\hat{Q}_{32} = 40 \text{ fm}^3$$

$$\beta_{32} = 0.339$$



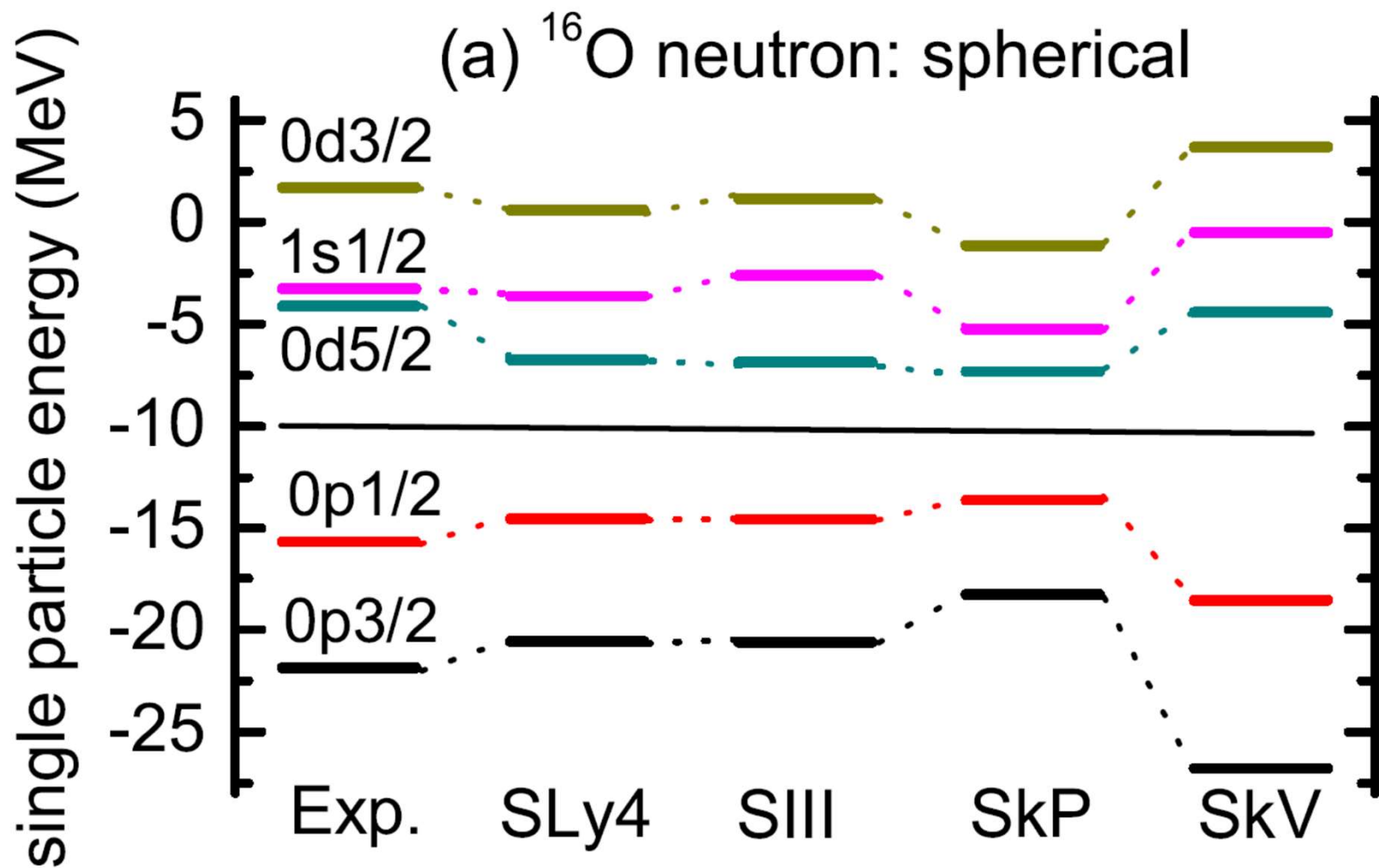
Take-away message

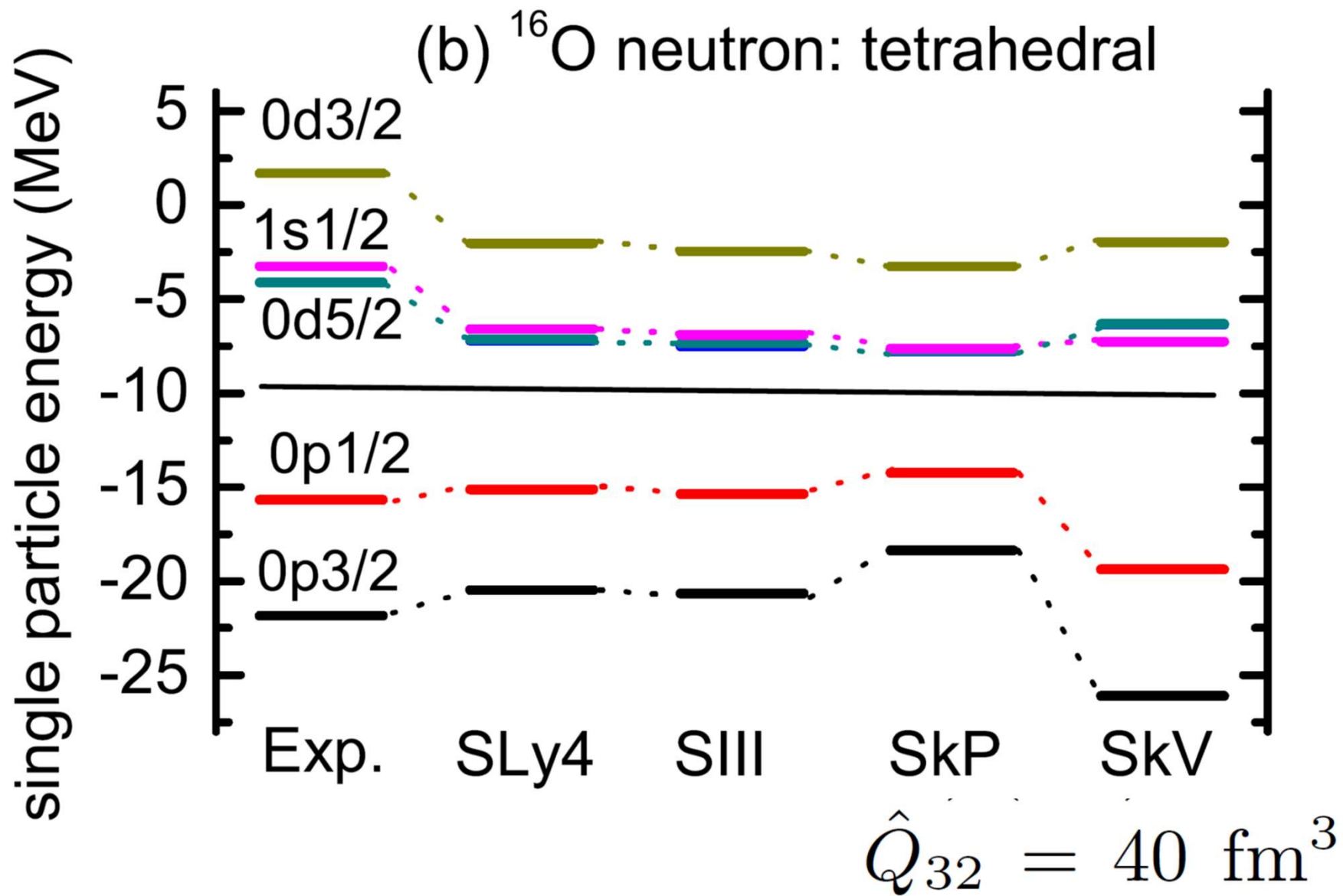
The DFT is a microscopic frame, which can be used to investigate the clustering phenomena without the assumption of cluster structure.



Before I came here I was confused
about this subject. Having listened
to your lecture I am still confused.
But on a higher level.

— *Enrico Fermi* —





Energy Density Functional in Hartree-Fock

$$H = \sum_i^A -\frac{\hbar^2}{2m} \nabla_i^2 + \sum_{i < j}^A V_{ij}$$

$$\begin{aligned} E &\equiv \int \mathcal{E} d^3r \\ &= \sum_{\alpha\beta} \langle \varphi_\alpha | -\frac{\hbar^2}{2m} \nabla^2 | \varphi_\beta \rangle \rho_{\alpha\beta} + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \varphi_\alpha \varphi_\beta | V_{12} (1 - P_{12}) | \varphi_\gamma \varphi_\delta \rangle \rho_{\alpha\gamma} \rho_{\delta\beta} \end{aligned}$$

Densities

- Normal density, or density matrix

$$\rho_{ij} = \langle \Phi | a_j^\dagger a_i | \Phi \rangle$$

$$\rho^\dagger = \rho$$

- Abnormal density, or pairing tensor

$$\mathbf{K}_{ij} = \langle \Phi | a_j a_i | \Phi \rangle$$

$$\mathbf{K}^T = -\mathbf{K}$$

One-body densities in Hartree-Fock

$$\rho_q(\mathbf{r}) = \sum_{i,s} |\varphi_i^q(\mathbf{r}, s)|^2 n_i^q, \quad \rho = \rho_n + \rho_p,$$

$$\tau_q(\mathbf{r}) = \sum_{i,s} |\nabla \varphi_i^q(\mathbf{r}, s)|^2 n_i^q, \quad \tau = \tau_n + \tau_p,$$

$$\mathbf{J}_q(\mathbf{r}) = \sum_{i,s,s'} \varphi_i^{q*}(\mathbf{r}, s') \nabla \varphi_i^q(\mathbf{r}, s) \times (s' | \boldsymbol{\sigma} | s) n_i^q,$$
$$\mathbf{J} = \mathbf{J}_n + \mathbf{J}_p.$$

The Energy Density Functional

$$\mathcal{E} = \frac{\hbar^2}{2m}\tau + \mathcal{E}_0 + \mathcal{E}_3 + \mathcal{E}_{eff} + \mathcal{E}_{fin} + \mathcal{E}_{so} + \mathcal{E}_{sg} + \mathcal{E}_{Coul} , \quad (4)$$

where

$$\begin{aligned} \mathcal{E}_0 &= \frac{1}{4}t_0 \left[(2 + x_0)\rho^2 - (2x_0 + 1)(\rho_n^2 + \rho_p^2) \right] , \\ \mathcal{E}_3 &= \frac{1}{24}t_3\rho^\alpha \left[(2 + x_3)\rho^2 - (2x_3 + 1)(\rho_n^2 + \rho_p^2) \right] , \\ \mathcal{E}_{eff} &= \frac{1}{8} \left[t_1(2 + x_1) + t_2(2 + x_2) \right] \tau\rho + \frac{1}{8} \left[t_2(2x_2 + 1) - t_1(2x_1 + 1) \right] \\ &\quad (\tau_n\rho_n + \tau_p\rho_p) , \\ \mathcal{E}_{fin} &= \frac{1}{32} \left[3t_1(2 + x_1) - t_2(2 + x_2) \right] |\nabla\rho|^2 - \frac{1}{32} \left[3t_1(2x_1 + 1) + t_2(2x_2 + 1) \right] \\ &\quad (|\nabla\rho_n|^2 + |\nabla\rho_p|^2) , \\ \mathcal{E}_{so} &= \frac{1}{2}W_0 \left[\mathbf{J} \cdot \nabla\rho + \mathbf{J}_n \cdot \nabla\rho_n + \mathbf{J}_p \cdot \nabla\rho_p \right] , \\ \mathcal{E}_{sg} &= -\frac{1}{16}(t_1x_1 + t_2x_2)\mathbf{J}^2 + \frac{1}{16}(t_1 - t_2)(\mathbf{J}_n^2 + \mathbf{J}_p^2) . \end{aligned} \quad (5)$$

The Skyrme-HF central potentials

$$\begin{aligned} U_q(\mathbf{r}) = & \frac{1}{2}t_0[(2+x_0)\rho - (1+2x_0)\rho_q] \\ & + \frac{1}{24}t_3\{(2+x_3)\rho^{\sigma+1} - (1+2x_3)[2\rho\rho_q + \sigma(\rho_n^2 + \rho_p^2)]\rho^{\sigma-1}\} \\ & + \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\tau - \frac{1}{8}[t_1(1+2x_1) - t_2(1+2x_2)]\tau_q \\ & - \frac{1}{16}[3t_1(2+x_1) - t_2(2+x_2)]\nabla^2\rho + \frac{1}{16}[3t_1(1+2x_1) + t_2(1+2x_2)]\nabla^2\rho_q \\ & - \frac{1}{2}W_0(\nabla \cdot \mathbf{J} + \nabla \cdot \mathbf{J}_q) , \end{aligned}$$

The spin-orbit and Coulomb potentials

$$\mathbf{W}_q(\mathbf{r}) = \frac{1}{2}W_0\nabla(\rho + \rho_q) + \frac{1}{8}(t_1 - t_2)\mathbf{J}_q - \frac{1}{8}(t_1x_1 + t_2x_2)\mathbf{J} .$$

The Coulomb potential requires an additional approximation for the exchange contribution in order to keep it local (the Coulomb interaction, unlike the Skyrme force, has a non-zero range). A local density approximation called the Slater approximation is used for expressing the Coulomb exchange contribution to the total energy:

$$E_C^{ex} = -\frac{3e^2}{4}\left(\frac{3}{\pi}\right)^{\frac{1}{3}} \int \rho_p^{\frac{4}{3}} d^3r .$$

This expression gives the exact result in infinite matter. With this approximation the one-body Coulomb potential becomes:

$$V_C(\mathbf{r}) = \frac{e^2}{2} \left[\int \frac{\rho_p(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3r' - \left[\frac{3}{\pi} \rho_p(\mathbf{r}) \right]^{\frac{1}{3}} \right] .$$

The center-of-mass correction

$$\begin{aligned} T &= \sum_i^A \frac{\mathbf{p}_i^2}{2m} - \frac{(\sum_i^A \mathbf{p}_i)^2}{2mA} \\ &= \frac{1}{2m} \left(1 - \frac{1}{A}\right) \sum_i^A \mathbf{p}_i^2 - \frac{1}{2mA} \sum_{i \neq j}^A \mathbf{p}_i \cdot \mathbf{p}_j . \end{aligned}$$

The first term on the second line is again a one-body kinetic term with a corrected mass $m' = m \frac{A}{A-1}$. This takes care of a large part of the center-of-mass correction on the total energy, and this is included in practically all Skyrme-HF calculations. The second term is a two-body correction much more difficult to incorporate and it is usually dropped in constructing Skyrme forces

Spherical case: radial equations in r-space

$$\varphi_{\alpha}^q(\mathbf{r}, \sigma) = \frac{u_{\alpha}^q(r)}{r} [Y_l(\hat{r}) \otimes \chi(\sigma)]_{jm} \chi_q(\tau) .$$

$$\frac{\hbar^2}{2m_q^*(r)} \left[-u_{\alpha}'' + \frac{l(l+1)}{r^2} u_{\alpha} \right] + V_q(r) u_{\alpha} - \left(\frac{\hbar^2}{2m_q^*} \right)' u_{\alpha}' = \epsilon_{\alpha} u_{\alpha}$$

$$V_q(r) = V_q^{cent}(r) + \delta_{q,1} V_C(r) + V_q^{s.o.}(r) \langle \mathbf{l} \cdot \boldsymbol{\sigma} \rangle .$$