Density Functional Theory with spatial-symmetry breaking and configuration mixing

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FIDIPRO–NESQ workshop, Jyväskylä, 2013-11-19

Outline

Nuclear structure: methods

- Unified, microscopic theory ?
  - Perturbation theory: fail (repulsive core)
  - Ladder resummation (Brueckner): fail
    (involved, 3N force needed)
  - Effective NN+3N interactions: fail
    (pairing, INM EoS, ferromagnetism, parameters)
  - ➡ Effective density-dependent "interactions": density functionals
  - "Beyond-Mean-field" scheme (Hill-Wheeler-Griffin)

$$E_{\rm mf}(q) = \min_{\Phi_0(q)} \langle \Phi_0(q)| \hat{T} + \hat{V}_{\rm eff} - \lambda \hat{Q} |\Phi_0(q)\rangle \quad \rightarrow \quad |\Phi_0(q)\rangle$$

$$E = \min_f \int dq\, dq'\, f^*(q) f(q') \langle \Phi_0(q)| \left(\hat{T} + \hat{V}_{\rm eff}\right) \hat{P}_{NZJMK} |\Phi_0(q')\rangle$$

  - Deformed rotor/vibrator but $[\hat{H}, \hat{J}^2] = 0$:
    break then restore symmetries
    M. Bender, P.-H. Heenen, P.-G. Reinhard,
    Rev. Mod. Phys. 75, 121 (2003)
  - ...but theory is ill defined: back to interactions ?

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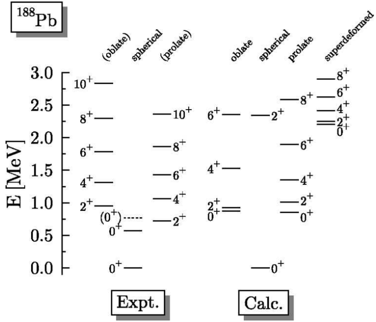
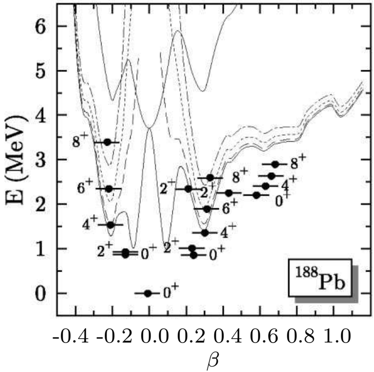
MR-EDF: Capabilities





M. Bender, P. Bonche, T. Duguet, and P.-H. Heenen, PRC 69, 064303 (2004)

- Describe A-body correlations
- + Fission, reactions (TD extension), neutron star crusts...

Hohenberg-Kohn-Sham scheme (quick version)

- Consider a system with Hamiltonian $\hat{H} = \hat{T} + \hat{U} + \hat{V}$ with $\hat{T}$ kinetic, $\hat{U}$ interaction (NN+3N+...), $\hat{V} \sim v(\vec{r})$ ext. potential

$$F[v] = \min_{\Psi} \langle \Psi | \hat{T} + \hat{U} + \hat{V} | \Psi \rangle$$

- Legendre transform with $\rho(\vec{r}) = \partial E / \partial v(\vec{r})$

$$E[\rho] = \min_{v} \left[F[v] - \int d^3\vec{r}\, v(\vec{r})\, \rho(\vec{r}) \right] = \min_{\Psi \to \rho} \langle \Psi | \hat{T} + \hat{U} | \Psi \rangle$$

- $E[\rho]$ "universal" w.r.t choice of v
- Kohn-Sham scheme: write

$$E[\rho] = T_{\mathrm{s}}[\rho] + E_H[\rho] + E_{\mathrm{xc}}[\rho]$$
$$T_{\mathrm{s}}[\rho] = \min_{\{\phi_i\} \to \rho} \left[-\frac{1}{2} \int d^3\vec{r} \sum_{i=1}^{N} \phi_i^*(\vec{r})\, \Delta\, \phi_i(\vec{r}) \right]$$

- G.s.: minimum of $E[\rho]$

Definitions

- Consider a system of N particles with Hamiltonian $\hat{H} = \hat{T} + \hat{U} + \hat{V}$ (kinetic, interaction, ext.)

$$\mathbf{R} \equiv (\vec{r}_1, \ldots, \vec{r}_N), \quad d^{3N}\mathbf{R} \equiv d^3\vec{r}_1 \ldots d^3\vec{r}_N$$

- Now consider real functions $Q_\mu(\vec{r})$, $\mu = 1 \ldots n$, $\underline{q} = (q_1, \ldots, q_n)$

$$\hat{Q}_\mu(\mathbf{R}) \equiv \sum_i Q_\mu(\vec{r}_i)$$

$$\hat{P}(\underline{q}, \mathbf{R}) \equiv \prod_\mu \delta(\hat{Q}_\mu(\mathbf{R}) - q_\mu)$$

- $\hat{P}$ projects on an eigenspace of $\hat{Q}$

- Define the generalized density

$$D(\underline{q}, \vec{r}) \equiv N \int d^{3N}\mathbf{R}\, \delta^{(3)}(\vec{r} - \vec{r}_1)\, \hat{P}(\underline{q}, \mathbf{R})\, \Psi^*(\mathbf{R})\, \Psi(\mathbf{R})$$

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External potential

- Let $w(\underline{q},\vec{r})$ be a real (bounded) function and

$$w(\underline{q},\mathbf{R}) = \sum_i w(\underline{q},\vec{r}_i) \qquad \hat{W}(\mathbf{R}) = \int d^n\underline{q}\; w(\underline{q},\mathbf{R})\;\hat{P}(\underline{q},\mathbf{R})$$

- We have

$$\langle\Psi|\hat{W}|\Psi\rangle = \int d^n\underline{q}\int d^3\vec{r}\; w(\underline{q},\vec{r})\; D(\underline{q},\vec{r})$$

- First, define the functional (assume non-degenerate)

$$F[w] = \min_{\Psi}\langle\Psi|\hat{T}+\hat{U}+\hat{W}|\Psi\rangle$$

- then

$$\begin{aligned} E[D] &= \min_{w}\left[F[w] - \int d^n\underline{q}\int d^3\vec{r}\; w(\underline{q},\vec{r})D(\underline{q},\vec{r})\right] \\ &= \min_{\Psi\to D}\langle\Psi|\hat{T}+\hat{U}|\Psi\rangle \end{aligned}$$

- Universality: $\hat{V}$ is a special case of $\hat{W}$ $(w(\underline{q},\vec{r}) = v(\vec{r}))$

Energy functional

- Define the collective w.f., and $\underline{q}$-dependent density

$$
\begin{aligned}
f(\underline{q}) &\equiv e^{i\theta(\underline{q})} \left[\frac{1}{N} \int d^3\vec{r}\, D(\underline{q},\vec{r}) \right]^{1/2} \\
d(\underline{q},\vec{r}) &\equiv |f(\underline{q})|^{-2} D(\underline{q},\vec{r})
\end{aligned}
$$

➡ $E[D] = E[f,d]$

- $\underline{q}$-dependent wave function ("slice")

$$
\begin{aligned}
\Psi(\underline{q},\mathbf{R}) &= f^{-1}(\underline{q})\, \hat{P}(\underline{q},\mathbf{R})\, \Psi(\mathbf{R}) \\
\int d^{3N}\mathbf{R}\, \Psi^*(\underline{q},\mathbf{R})\, \Psi(\underline{q}',\mathbf{R}) &= \delta^{(n)}(\underline{q}-\underline{q}')
\end{aligned}
$$

- $d(\underline{q},\vec{r})$ is the density of $\Psi(\underline{q},\mathbf{R})$

$$
\int d^{3N}\mathbf{R}\, \delta^{(3)}(\vec{r}-\vec{r}_1)\, \Psi^*(\underline{q},\mathbf{R})\, \Psi(\underline{q}',\mathbf{R}) = \delta^{(n)}(\underline{q}-\underline{q}')\, d(\underline{q},\vec{r})
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Properties

- Normalisation

$$\begin{aligned}
\int d^n\underline{q}\, f^*(\underline{q})f(\underline{q}) &= 1 \\
\forall \underline{q}, \int d^3\vec{r}\; d(\underline{q},\vec{r}) &= N \\
\forall \vec{r}, \int d^n\underline{q}\; D(\underline{q},\vec{r}) &= \rho(\vec{r}) \\
\int d^n\underline{q} \int d^3\vec{r}\; D(\underline{q},\vec{r}) &= N
\end{aligned}$$

- Verify that

$$\int d^3\vec{r}\; Q_\mu(\vec{r})\, d(\underline{q},\vec{r}) = q_\mu$$

Collective coordinates

- Assume...
  - f given by symmetry
  - $d(\underline{q},\vec{r})$ and $d(\underline{q}',\vec{r})$ related by sym. transformation

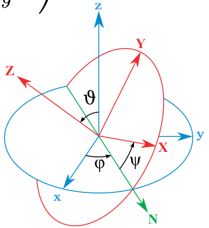
- ...then $E[f,d] = E[\rho_{\mathrm{int}}]$, with $\rho_{\mathrm{int}}(\vec{r}) = d(\underline{0},\vec{r})$
  - Functional of the density of "pinned down" w.f.
  - $(Q_1, Q_2, Q_3)(\vec{r}) = \frac{1}{N}(x, y, z)$: internal-frame DFT
  - ➡ Messud, Bender, Suraud, Phys.Rev.C 80 054314 (2009)

- Note: $D(\underline{q},\vec{r})$ conserves symmetries !

Collective coordinates cont'd

- $(Q_1, Q_2, Q_3)(\vec{r}) = \frac{1}{N}(x, y, z)$, call $(q_1, q_2, q_3) \equiv \vec{R}$
- Now, add to (q_μ) the inertia tensor

$$\mathbb{J} \quad \equiv \quad \int d^3\vec{r} \begin{pmatrix} y^2+z^2 & -xy & -xz \\ -yx & x^2+z^2 & -yz \\ -zx & -zy & x^2+y^2 \end{pmatrix} d(\vec{R}, \mathbb{J}, \vec{r})$$



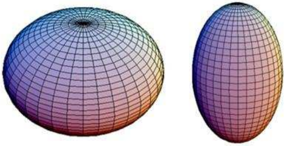
- Huygens-Steiner theorem for intrinsic inertia tensor

$$\mathbb{J}_0 \quad = \quad \mathbb{J} - N(R^2\mathbb{I} - \vec{R} \otimes \vec{R})$$

- $(\vec{R}, \mathbb{J}) \;\rightarrow\; (\vec{R}, r_{\text{rms}}, \beta, \gamma, \varphi, \vartheta, \psi)$: Rotation + quadrupole vibrations

$$\beta\cos\gamma \quad = \quad \sqrt{\frac{\pi}{5}}\frac{\langle 2z^2 - x^2 - y^2\rangle_{\text{int}}}{N\, r_{\text{rms}}^2}$$

$$\beta\sin\gamma \quad = \quad \sqrt{\frac{3\pi}{5}}\frac{\langle x^2 - y^2\rangle_{\text{int}}}{N\, r_{\text{rms}}^2}$$



oblate spheroid *prolate spheroid*

Internal/intrinsic density

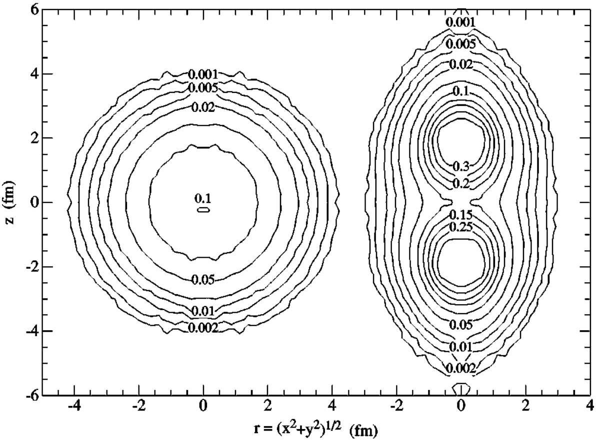


FIG. 15. Contours of constant density, plotted in cylindrical coordinates, for ^{8}Be(0^{+}). The left side is in the "laboratory" frame while the right side is in the intrinsic frame.

- ^{8}Be, AV18+UIX GFMC
  - Left: $\vec{R}$
  - Right: $\vec{R}, \varphi, \vartheta$
- Wiringa, Pieper, Carlson, Pandharipande, Phys. Rev. C 62, 014001 (2000)

Collective equation ?

- Rewrite w.f. $\Psi(\mathbf{R})$ as

$$\Psi(\mathbf{R}) = \int d^n\underline{q}\, f(\underline{q})\Psi(\underline{q},\mathbf{R})$$

- Assume $\hat{U}$ local

$$E[f,d] = \langle\Psi[f,d]|\hat{T}+\hat{U}+\hat{V}|\Psi[f,d]\rangle$$

$$E[f,d] = \int d^n\underline{q}\, f^*(\underline{q})\Big[-\frac{1}{2}\sum_{\mu\nu}\partial_\mu \mathcal{A}_{\mu\nu}(\underline{q})\partial_\nu + \mathcal{U}(\underline{q}) - \frac{i}{2}\sum_{\mu}\left(\partial_\mu \mathcal{V}_\mu(\underline{q}) + \mathcal{V}_\mu(\underline{q})\partial_\mu\right)\Big] f(\underline{q})$$

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- Collective mass

$$\mathcal{A}_{\mu\nu}(\underline{q}) = \frac{1}{\langle \hat{P}(\underline{q}) \rangle} F_{\mu\nu}(\underline{q})$$

$$F_{\mu\nu}(\underline{q}) = \int d^{3N}\mathbf{R}\, \hat{P}(\underline{q},\mathbf{R})[\vec{\nabla}\hat{Q}_\mu(\mathbf{R})]\cdot[\vec{\nabla}\hat{Q}_\nu(\mathbf{R})]\,\Psi^*(\mathbf{R})\,\Psi(\mathbf{R})$$

- Collective potential

$$\begin{aligned}\mathcal{U}(\underline{q}) \equiv & \sum_{\mu\nu} F_{\mu\nu}(\underline{q}) \left[\frac{1}{2} \frac{\partial_\mu \theta(\underline{q})\, \partial_\nu \theta(\underline{q})}{\langle \hat{P}(\underline{q}) \rangle} + \frac{1}{8} \frac{\partial_\mu \langle \hat{P}(\underline{q}) \rangle\, \partial_\nu \langle \hat{P}(\underline{q}) \rangle}{\langle \hat{P}(\underline{q}) \rangle^3} \right] \\ & + \frac{1}{4} \sum_{\mu\nu} \partial_\mu \left[\frac{F_{\mu\nu}(\underline{q})}{\langle \hat{P}(\underline{q}) \rangle^2} \partial_\nu \langle \hat{P}(\underline{q}) \rangle \right] - \frac{1}{2} \sum_\mu \frac{J_\mu(\underline{q})\, \partial_\mu \theta(\underline{q})}{\langle \hat{P}(\underline{q}) \rangle} \\ & + \frac{1}{\langle \hat{P}(\underline{q}) \rangle} \int d^{3N}\mathbf{R}\, \hat{P}(\underline{q},\mathbf{R}) \Psi^*(\mathbf{R}) \left[-\tfrac{1}{2}\hat{\Delta} + \hat{U}(\mathbf{R}) \right] \Psi(\mathbf{R}) \\ & + \int d^3\vec{r}\, v_{\text{ext}}(\vec{r})\, d(\underline{q},\vec{r})\end{aligned}$$

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Collective equation ?

- Current term

$$\mathcal{V}_\mu(\underline{q}) \equiv \sum_\nu F_{\mu\nu}(\underline{q}) \frac{\partial_\nu \theta(\underline{q})}{\langle \hat{P}(\underline{q}) \rangle} + \frac{J_\mu(\underline{q})}{\langle \hat{P}(\underline{q}) \rangle}.$$

$$J_\mu(\underline{q}) \equiv \frac{i}{2} \int d^{3N}\mathbf{R}\, \hat{P}(\underline{q},\mathbf{R}) \vec{\nabla} \hat{Q}_\mu(\mathbf{R}) \cdot \left[\vec{\nabla}\Psi^*(\mathbf{R})\,\Psi(\mathbf{R}) - \Psi^*(\mathbf{R})\,\vec{\nabla}\Psi(\mathbf{R}) \right].$$

- Choose $\theta(\underline{q})$ to make f continuous, and/or cancel $\mathcal{V}$ with

$$\sum_\nu F_{\mu\nu}(\underline{q})\, \partial_\nu \theta(\underline{q}) = -J_\mu(\underline{q}),$$

➡ Minimize energy: collective Schrödinger equation

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- For ex. if $\underline{q}$ is $\vec{R}$, $\mathcal{A}_{\mu\nu}[f,d](\underline{q}) = \frac{1}{N}$ and $\mathcal{U}[f,d](\underline{q}) = E_{\rm int}$

Collective equation ?

- Current term

$$\mathcal{V}_\mu(\underline{q}) \equiv \sum_\nu F_{\mu\nu}(\underline{q}) \frac{\partial_\nu \theta(\underline{q})}{\langle \hat{P}(\underline{q}) \rangle} + \frac{J_\mu(\underline{q})}{\langle \hat{P}(\underline{q}) \rangle}.$$

$$J_\mu(\underline{q}) \equiv \frac{i}{2} \int d^{3N}\mathbf{R}\, \hat{P}(\underline{q},\mathbf{R}) \vec{\nabla} \hat{Q}_\mu(\mathbf{R}) \cdot \left[\vec{\nabla}\Psi^*(\mathbf{R})\,\Psi(\mathbf{R}) - \Psi^*(\mathbf{R})\,\vec{\nabla}\Psi(\mathbf{R}) \right].$$

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Kohn-Sham scheme

- Write the collective potential $\mathcal{U}$ as (def $\rho_{\underline{q}}(\vec{r}) \equiv d(\underline{q},\vec{r})$)

$$\mathcal{U}[f,d](\underline{q}) = T_{\mathrm{s}}[\rho_{\underline{q}}] + \mathcal{U}^{\mathrm{ext}}[f,d](\underline{q}) + \mathcal{U}^{\mathrm{ic}}[f,d](\underline{q})$$

$$T_{\mathrm{s}}[\rho_{\underline{q}}] = \min_{\{\phi_i\}\to\rho_{\underline{q}}} \left[-\frac{1}{2}\int d^3\vec{r} \sum_{i=1}^{N} \phi_i^*(\underline{q};\vec{r})\,\Delta\,\phi_i(\underline{q};\vec{r}) \right]$$

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$$\frac{\delta\left[E - |f(\underline{q})|^2 \varepsilon_k(\underline{q})(\underline{q}k|\underline{q}k) - |f(\underline{q})|^2 \sum_\mu \lambda_\mu (Q_\mu|\rho_{\underline{q}})\right]}{\delta\phi_k^*(\underline{q};\vec{r})} =$$

$$|f(\underline{q})|^2\left[-\tfrac{1}{2}\Delta + v_{\mathrm{s}}(\underline{q};\vec{r}) + v_{\mathrm{ext}}(\vec{r}) - \lambda_\mu Q_\mu(\vec{r}) - \varepsilon_k(\underline{q})\right]\phi_k(\underline{q};\vec{r}) = 0$$

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Summary and outlook

- Generalized DFT: we can obtain a model with
  - A collective Hamiltonian
  - ...coupled to single particle degrees of freedom
  - ...potentially exact
  - ...from first principles
  - ...that looks just like a Bohr Hamiltonian
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