Density functional theory with spatial-symmetry breaking and configuration mixing

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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

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

  - Deformed rotor/vibrator but $[\hat{H}, \hat{J}^2] = 0$: break/restore sym. M. Bender, P.-H. Heenen, P.-G. Reinhard, RMP 75, 121 (2003)
  - Beyond-Mean-field scheme (Hill-Wheeler-Griffin) for mixing (quasi-)degenerate minima

- ...but theory with functionals is ill defined:
  1. Back to interactions (or “pseudopotentials”) ?
  2. Approximate schemes (Lipkin, GOA+collective Hamiltonian)

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Outline

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 $\rho(\vec{r}) = \partial E / \partial v(\vec{r})$

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

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

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

- 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.)

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

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

$$\begin{aligned} \hat{Q}_\mu(\mathbf{R}) &\equiv \sum_i Q_\mu(\vec{r}_i) \\ \hat{P}(\underline{q}, \mathbf{R}) &\equiv \prod_\mu \delta(\hat{Q}_\mu(\mathbf{R}) - q_\mu) \end{aligned}$$

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

$$\hat{P}(\underline{q}, \mathbf{R}) \hat{P}(\underline{q}', \mathbf{R}) = \delta^{(n)}(\underline{q} - \underline{q}') \hat{P}(\underline{q}, \mathbf{R})$$

- 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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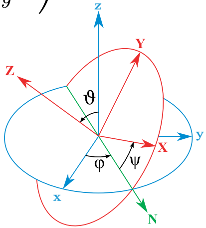
Collective coordinates

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

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

- Huygens-Steiner theorem for intrinsic inertia tensor

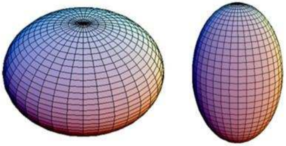
$$\mathbb{J}_0 = \mathbb{J} - N(R^2\mathbb{I} - \vec{R} \otimes \vec{R})$$



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

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

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



oblate spheroid *prolate spheroid*

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

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

Internal/intrinsic density

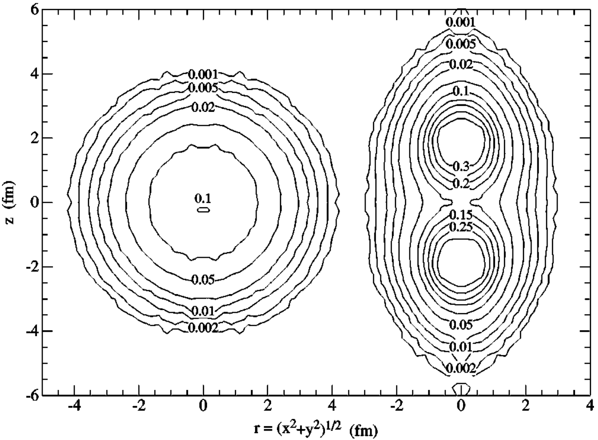

FIG. 15. Contours of constant density, plotted in cylindrical coordinates, for ^{8}Be(0^+). The left side is in the ‘‘laboratory’’ frame while the right side is in the intrinsic frame.

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

Outline

Collective coordinates and symmetries

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

- . . . then $E[f, d] = E[\rho_{\text{int}}]$, with $\rho_{\text{int}}(\vec{r}) = d(\underline{0}, \vec{r})$
  - 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 !

$$D\left(\underline{\mathcal{S}}(\underline{q}), \vec{\mathcal{S}}(\vec{r})\right) \quad = \quad D(\underline{q}, \vec{r})$$

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

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

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

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Collective equation ?

- Collective mass

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

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

- Current term ($\langle \hat{P}(\underline{q})\rangle = |f(\underline{q})|^2$)

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

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

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

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

Collective equation ?

- Collective potential

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

➡ Minimize energy: collective Schrödinger equation

$$
\left[-\frac{1}{2} \sum_{\mu\nu} \partial_\mu \mathcal{A}_{\mu\nu}[f,d](\underline{q}) \partial_\nu + \mathcal{U}[f,d](\underline{q}) + \mathcal{U}_{\text{ra}}[f,d](\underline{q}) - E' \right] f(\underline{q}) = 0
$$

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

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- Collective potential

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

➡ Minimize energy: collective Schrödinger equation

$$\left[-\frac{1}{2} \sum_{\mu\nu} \partial_\mu \mathcal{A}_{\mu\nu}[f,d](\underline{q}) \partial_\nu + \mathcal{U}[f,d](\underline{q}) + \mathcal{U}_{\text{ra}}[f,d](\underline{q}) - E' \right] f(\underline{q}) = 0$$

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

Collective equation ?

- Collective potential

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\begin{aligned}
\mathcal{U}(\underline{q}) \quad \equiv \quad & \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] \\
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& + \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}) \\
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\end{aligned}
$$

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Outline

Kohn-Sham scheme

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

$$
\begin{aligned}
\mathcal{U}[f,d](\underline{q}) &= T_{\mathrm{s}}[\rho_{\underline{q}}] + \mathcal{U}^{\mathrm{ext}}[f,d](\underline{q}) + \mathcal{U}^{\mathrm{ic}}[f,d](\underline{q}) \\
T_{\mathrm{s}}[\rho_{\underline{q}}] &= \min_{\{\phi_i\}\to\rho_{\underline{q}}} \left[-\frac{1}{2} \int d^3\vec{r} \sum_{i=1}^{N} \phi_i^*(\underline{q};\vec{r})\, \Delta\, \phi_i(\underline{q};\vec{r}) \right]
\end{aligned}
$$

- Kohn-Sham equation

$$
\begin{aligned}
\frac{\delta\left[E - |f(\underline{q})|^2 \varepsilon_k(\underline{q})(\underline{q}k|\underline{q}k) - |f(\underline{q})|^2 \sum_\mu \lambda_\mu (Q_\mu|\rho_{\underline{q}})\right]}{\delta\phi_k^*(\underline{q};\vec{r})} &= \\
|f(\underline{q})|^2 \left[-\tfrac{1}{2}\Delta + v_{\mathrm{s}}(\underline{q};\vec{r}) + v_{\mathrm{ext}}(\vec{r}) - \lambda_\mu Q_\mu(\vec{r}) - \varepsilon_k(\underline{q}) \right] \phi_k(\underline{q};\vec{r}) &= 0
\end{aligned}
$$

- $v(\underline{q};\vec{r})$ optimizes energy: functional derivatives of $\mathcal{U}$, $\mathcal{A}$

$$
v_{\mathrm{s}}(\underline{q};\vec{r}) = |f(\underline{q})|^{-2} \int d^n\underline{q}'\, f^*(\underline{q}') \left[-\partial'_\mu \frac{1}{2} \frac{\delta\mathcal{A}_{\mu\nu}(\underline{q}')}{\delta d(\underline{q},\vec{r})} \partial'_\nu + \frac{\delta\mathcal{U}^{\mathrm{ic+ext}}(\underline{q}')}{\delta d(\underline{q},\vec{r})} \right] f(\underline{q}')
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- Nothing new ! Collective Hamiltonian
  Review: Próchniak, Rohoziński, J. Phys. G 36, 123101 (2009)
  - Equation for quantum vibrating droplet (Bohr)
  - $\mathcal{A}_{\mu\nu}$? Inglis(-Belyaev), ATDHFB,...
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- $\delta\mathcal{A}_{\mu\nu}(\underline{q}')/\delta d(\underline{q},\vec{r})$ term: use OEP

- Assume...
  - Weak feedback from f (neglect above)
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    - ➨ $\mathcal{U}^{\mathrm{ic}}[\rho_{\underline{q}}]$: Skyrme/Gogny/relativistic/... functional
    - ➨ Collective equation can be solved a posteriori

- But in general, coupling between slow (collective) and fast (s.p.) d.o.f.
  Beyond adiabatic approximation
- NB(1): Any prescription for $\mathcal{A}$, $\mathcal{U}$ is part of the functional definition
- NB(2): Minimum of $\mathcal{U}$ of no physical significance.

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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
  - ➡ TL, arXiv:1301.0807 (2013)

- Determine the functional $(\mathcal{A},\mathcal{U})[f,d]$?...