The QRPA

J. Engel

University of North Carolina

June 18, 2008

Equations of motion method

$$\hat{H}\,|\Psi\rangle = E_\nu\,|\Psi_\nu\rangle$$

Let

$$Q_\nu^\dagger = |\nu\rangle\,\langle 0|\ , \quad \nu \neq 0$$

(so that, e.g., $Q_\nu\,|0\rangle = 0$). Then...

$$[\hat{H}, Q_\nu^\dagger]\,|0\rangle = (E_\nu - E_0)Q_\nu^\dagger\,|0\rangle \equiv \Omega^\nu\,Q_\nu^\dagger\,|0\rangle$$

and commuting both sides with any other operator $\hat{G}$ and "dotting" with $\langle 0|$

$$\langle 0|\,[G, [\hat{H}, Q_\nu^\dagger]\,|0\rangle = \Omega^\nu\,\langle 0|\,[\hat{G}, Q_\nu^\dagger]\,|0\rangle$$

Now let $G = a_m^\dagger a_i$ or $\hat{G} = a_i^\dagger a_m$, where we have assumed that in the crudest approximation the ground state is a Slater determinant $|SD\rangle$ (not the true ground state $|0\rangle$) and $\epsilon_m > \epsilon_F$, $\epsilon_i < \epsilon_F$. Then

$$\begin{aligned} \langle 0| \left[a_m^\dagger a_i, [\hat{H}, Q_\nu^\dagger]\right] |0\rangle &= \Omega^\nu \langle 0| \left[a_m^\dagger a_i, Q_\nu^\dagger\right] |0\rangle \\ \langle 0| \left[a_i^\dagger a_m, [\hat{H}, Q_\nu^\dagger]\right] |0\rangle &= \Omega^\nu \langle 0| \left[a_i^\dagger a_m, Q_\nu^\dagger\right] |0\rangle \end{aligned}$$

Finally, let $Q^\dagger$ be a only create particle-hole excitations of the ground state of a particular form:

$$Q_\nu^\dagger = \sum_{mi} X_{mi}^\nu a_m^\dagger a_i - \sum_{mi} Y_{mi}^\nu a_i^\dagger a_m$$

Crucial step (and reason for all the commutators). Assume that for one- and two-body operators $\hat{\mathcal{O}}$ *that result from commutations*:

$$\langle 0| \hat{\mathcal{O}} |0\rangle \approx \langle SD| \hat{\mathcal{O}} |SD\rangle$$

Then some algebra gives

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = \Omega^\nu \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix}$$

with

$$\begin{aligned} A_{mi,nj} &= (\epsilon_m - \epsilon_i)\,\delta_{mn}\delta_{ij} + \langle mj|\,\hat{V}\,|in\rangle_A \\ B_{mi,nj} &= \langle mn|\,\hat{V}\,|ij\rangle_A \end{aligned}$$

and

$$\langle ab|\,\hat{V}\,|cd\rangle_A = \langle ab|\,\hat{V}\,|cd\rangle - \langle ab|\,\hat{V}\,|dc\rangle$$

Finally,

$$\begin{aligned} \langle \nu|\,a_m^\dagger a_i\,|0\rangle &= \langle SD|\,[Q_\nu, a_m^\dagger a_i]\,|SD\rangle &= X_{mi}^{\nu *} \\ \langle \nu|\,a_i^\dagger a_m\,|0\rangle &= \langle SD|\,[Q_\nu, a_i^\dagger a_m]\,|SD\rangle &= Y_{mi}^{\nu *} \end{aligned}$$

So even without an explicit expression for $|0\rangle$, which must be different from $|SD\rangle$, we can calculate the transition matrix elements of any operator $G \equiv \sum_{mi}(G_{mi}a_m^\dagger a_i + G_{im}a_i^\dagger a_m)$:

$$\langle \nu|\,G\,|0\rangle = \sum_{mi}\left[X_{mi}^{\nu *}G_{mi} + Y_{mi}^{\nu *}G_{im}\right]$$

Review of Hartree Fock

Modern formulation of ordinary Hartree-Fock theory: Define

$$\rho_{ab} = \langle 0 | \, a_b^\dagger a_a \, | 0 \rangle$$

so that the expectation value of a one-body operator $\hat{G}$ is

$$\langle 0 | \, \hat{G} \, | 0 \rangle = \sum_{ab} G_{ab} \rho_{ba} = Tr(G\rho) \, .$$

For a slater determinant $|SD\rangle$, $\rho^2 = \rho$, and in the basis of single=particle eigenstates

$$\rho_{ab} = \begin{cases} \delta_{a,b} & a, b < F \\ 0 & a > F \text{ or } b > F \, . \end{cases}$$

One defines an *energy functional*

$$\begin{aligned} \mathcal{E}[\rho] &= \langle SD | \, \hat{H} \, | SD \rangle \\ &= \sum_{ab} T_{ab} \rho_{ba} + \frac{1}{2} \sum_{abcd} \rho_{ca} \, \langle ab | \, \hat{V} \, | cd \rangle \, \rho_{db} \\ &\equiv Tr(T\rho) + \frac{1}{2} \, Tr_1 \, Tr_1 (\rho V \rho) \end{aligned}$$

Setting $\delta\left[\mathcal{E} - \Lambda(\rho^2 - \rho)\right] = 0$ under small variations $\delta\rho$ (where Λ is a matrix of Lagrange multipliers) leads to the requirement that the *mean field*

$$h_{ab}[\rho] = \frac{\partial \mathcal{E}}{\partial \rho_{ba}} = t_{ab} + \sum_{bd} \langle ac| \, \hat{V} \, |bd\rangle_A \, \rho_{dc}$$

obeys

$$[h, \rho] = 0 \,,$$

i.e. h and ρ can be made simultaneously diagonal. Diagonalizing both leads to equations for a single-particle basis:

$$h_{ab}[\rho] = \epsilon_a \delta_{ab} \,,$$

where, in this basis,

$$h_{ab} = t_{ab} + \sum_{j<F} \langle aj| \, \hat{V} \, |bj\rangle_A \,.$$

Also in this basis, the constraint $\rho^2 = \rho$ becomes

$$\delta\rho_{ij} = \delta\rho_{mn} = 0 \,.$$

Linear response

One way to get properties of excited states is through the *linear response*. Add a weak time-dependent external one-body operator $\hat{G}$ to $\hat{H}$.Then for some function *response function* R,

$$\delta\rho_{ab}(t) = \int_{-\infty}^{\infty} dt'\, R_{ab,cd}(t-t')G_{cd}(t')$$

where R contains a factor $\theta(t-t')$. The Fourier transform is

$$\delta\rho_{ab}(\omega) = R_{ab,cd}(\omega)G_{cd}(\omega)$$

It's straightforward to show with perturbation theory that

$$R_{ab,cd}(\omega) = \sum_{\nu}\left(\frac{\langle 0|\, a_b^\dagger a_a\, |\nu\rangle\, \langle\nu|\, a_c^\dagger a_d\, |0\rangle}{\omega-\Omega^\nu+i\epsilon} - \frac{\langle 0|\, a_c^\dagger a_d\, |\nu\rangle\, \langle\nu|\, a_b^\dagger a_a\, |0\rangle}{\omega+\Omega^\nu+i\epsilon}\right)$$

The poles of R are at the excited-state energies and the residues are the squares of *transition densities*.Note also, even for states in continuum, where sum goes to integral:

$$\text{Rate}_{\,0\to\omega} = \frac{2\pi}{\hbar}\sum_{\nu} |\, \langle 0|\, \hat{G}\, |\nu\rangle\, |^2 \delta(\omega-\Omega_\nu) = \text{Im}[Tr(GR(\omega)G^*)]$$

RPA response

Simplest approximation R^{HF} to R: take $|0\rangle$ to be $|SD\rangle$, so that excited states are simple particle-hole excitations.

Better approximation through time-dependent HF:

$$i\dot{\rho} = [h[\rho] + G(t), \rho] \ .$$

Assuming G small and harmonic, so that $\rho(t) = \rho_0 + \delta\rho e^{-i\omega t} + \delta\rho^* e^{i\omega t}$:
Then

$$\omega\delta\rho = [h^0, \delta\rho] + \sum_{mi} \left[\frac{\partial h}{\partial \rho_{mi}} \delta\rho_{mi} + \frac{\partial h}{\partial \rho_{im}} \delta\rho_{im}, \rho^0 \right] + [G, \rho^0] \, ,$$

which with the explicit expressions for $\rho^0_{ab} = \sum_{i<F} \langle a|i\rangle \langle i|a\rangle$, $h^0_{ab} = \ldots$, and $\frac{\partial h_{ab}}{\partial \rho_{cd}} = \langle ad| \, V \, |bc\rangle_A$ becomes

$$\left\{ \begin{pmatrix} \omega & 0 \\ 0 & -\omega \end{pmatrix} - \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \right\} \begin{pmatrix} \delta\rho \\ \delta\rho^* \end{pmatrix} = \begin{pmatrix} G \\ G^* \end{pmatrix} \, ,$$

with the same A, B matrices as before!

Response function $R_{ab,cd}(\omega)$ in this approximation is just the inverse of the $\{\cdots\}$. It has poles at $\omega = \pm\Omega^{\nu}_{\mathrm{RPA}}$ (because RPA eigenvalues come in $\pm$ pairs). Residues are RPA eigenvectors.

Similar example:

$$\langle a| \left(\omega - \hat{H}\right)^{-1} |b\rangle = \sum_i \frac{\langle a|i\rangle \langle i|a\rangle}{\omega - E_i}$$

So small-amplitude motion around the ground state in TDHF leads to the RPA response function

$$R^{\mathrm{RPA}}_{ab,cd}(\omega) = \sum_{\nu} \left(\frac{\langle 0| a^{\dagger}_b a_a |\nu\rangle \langle \nu| a^{\dagger}_c a_d |0\rangle_{\mathrm{RPA}}}{\omega - \Omega^{\nu}_{\mathrm{RPA}} + i\epsilon} - \frac{\langle 0| a^{\dagger}_c a_d |\nu\rangle \langle \nu| a^{\dagger}_b a_a |0\rangle_{\mathrm{RPA}}}{\omega + \Omega^{\nu}_{\mathrm{RPA}} + i\epsilon} \right)$$

where now the energies and transition matrix elements are given by the RPA

Equation for RPA response

Note that if $\hat{H} = \hat{H}_0 + \hat{V}$, then

$$\begin{aligned}
\frac{1}{\omega - \hat{H}} &= \frac{1}{\omega - \hat{H}_0}[\omega - \hat{H}_0]\frac{1}{\omega - \hat{H}} = \frac{1}{\omega - \hat{H}_0}[\omega - \hat{H} + \hat{V}]\frac{1}{\omega - \hat{H}} \\
&= \frac{1}{\omega - \hat{H}_0}[1 + \hat{V}\frac{1}{\omega - \hat{H}}] \\
&= \frac{1}{\omega - \hat{H}_0} + \frac{1}{\omega - \hat{H}_0}\hat{V}\frac{1}{\omega - \hat{H}}\,.
\end{aligned}$$

Without the interaction $\hat{V}$ $(= \partial h/\partial\rho)$, the RPA A, B matrices correspond to their HF counterparts — only the average potential contributes — so there is a similar relation for the RPA response function:

$$R^{\mathrm{RPA}}_{ab,cd}(\omega) = R^{\mathrm{HF}}_{ab,cd}(\omega) + \sum_{ef,pq} R^{\mathrm{HF}}_{ab,ef}(\omega)\frac{\partial h_{ef}}{\partial \rho_{pq}} R^{\mathrm{RPA}}_{pq,cd}(\omega)\,.$$

or

$$R^{\mathrm{RPA}}(\omega) = R^{\mathrm{HF}}(\omega) + R^{\mathrm{HF}}(\omega)\frac{\partial h}{\partial \rho} R^{\mathrm{RPA}}(\omega)$$

for short.

Brief intro to DFT

Energy-Density-Functional theorems, adapted for nuclei, say, roughly:

Hohenberg-Kohn-Sham

Add an arbitrary one-body operator $\hat{G}$ to the nuclear Hamiltonian. There is a unique (complicated) mean-field Hamiltonian $h[\rho]$ that gives the *exact* ground-state energy and expectation values for one-body operators. It has the form

$$h[\rho] = h^{\mathrm{KS}}[\rho] + G\,,$$

where KS means Kohn-Sham. h^{KS}_{ab} can be written as $\frac{\partial \mathcal{E}^{\mathrm{KS}}}{\partial \rho_{ba}}$ for some complicated $\mathcal{E}^{\mathrm{KS}}$, just like in mean-field theory.

Nuclear theorists have ways of deriving/fitting/guessing $\mathcal{E}^{KS}$ (and therefore h^{KS}). When they do Skyrme mean-field theory, some of them are really trying to do Kohn-Sham theory. They want

$$h^{\mathrm{Sk}} \approx h^{KS}\,.$$

Skyrme DFT

$$\mathcal{E}^{\mathrm{Sk}} = \int d\mathbf{r}[\frac{\hbar^2}{2n}\tau + \frac{3}{8}t_0\rho^2 + \frac{1}{16}\rho^3 + \frac{1}{16}(3t_1+5t_2)\rho\tau + \frac{1}{64}(9t_1-5t_2)(\nabla\rho)^2 + \frac{3}{4}W_0\rho\nabla\cdot\mathbf{J} + \frac{1}{32}(t_1-t_2)\mathbf{J}^2]$$

$$\rho(\mathbf{r}) = \sum_s \rho_{\mathbf{r}s,\mathbf{r}'s} = \sum_{i\leq F,s} |\phi_i(\mathbf{r},s)|^2$$

$$\tau(\mathbf{r}) = \sum_{i\leq F,s} |\nabla\phi_i(\mathbf{r},s)|^2, \qquad \mathbf{J}(\mathbf{r}) = -i\sum_{i\leq F,s,s'} \phi_i(\mathbf{r},s)[\nabla\phi_i(\mathbf{r},s')\times\sigma_{ss'}]$$

Time-dependent version is a bit different:

Runge-Gross-Kohn-Sham-etc.

Add time-dependent operator $\hat{G}(t)$ to the nuclear Hamiltonian, and assume nucleus starts in ground state. There is a unique (complex) mean-field hamiltonian $h'[\rho, t]$ giving exact expectation values at each time for one-body operators, that can be written

$$h'[\rho](t) = h^{\mathrm{KS}}[\rho_0] + G^{\mathrm{KS}}[\rho](t)\,,$$

Important:

$$G^{\mathrm{KS}}[\rho](t) \neq G(t)\,.$$

Now consider linear response for small $G(t)$: In matrix form:

$$\delta\rho(\omega) = R(\omega)G(\omega)$$

and also

$$\delta\rho(\omega) = R^{\mathrm{KS}}(\omega)G^{\mathrm{KS}}(\omega)\,.$$

Now let

$$G^{\mathrm{KS}}(\omega) \equiv G(\omega) + \delta G(\omega)\,,$$

where

$$\delta G(\omega) = f(\omega)\delta\rho(\omega)\,.$$

for some nice f.
Then we have

$$\delta\rho(\omega) = R^{\mathrm{KS}}(\omega)\left[G(\omega) + f(\omega)\delta\rho(\omega)\right]$$

or, using $\delta\rho = RG$,

$$R(\omega)G(\omega) = R^{\mathrm{KS}}(\omega)\left[G(\omega) + f(\omega)R(\omega)G(\omega)\right]\,.$$

So, since G is arbitrary, we have

$$R(\omega) = R^{\mathrm{KS}}(\omega) + R^{\mathrm{KS}}(\omega)f(\omega)R(\omega)\,.$$

The problem is that we only have crude approximations for f, the simplest of which is the...

Adiabatic approximaton

$$h'[\rho](t) \approx h^{\mathrm{KS}}[\rho(t)] + G(t)$$

if time evolution from ground state is very slow.

Recall exact definition

$$h'[\rho](t) = h^{\mathrm{KS}}[\rho_0] + G^{\mathrm{KS}}[\rho](t)\,,$$

so in adiabatic approximation

$$G^{\mathrm{KS}}_{ab}(t) - G_{ab}(t) \approx h^{\mathrm{KS}}_{ab}[\rho(t)] - h^{\mathrm{KS}}_{ab}[\rho_0] \approx \sum_{cd} \frac{\partial h^{\mathrm{KS}}_{ab}[\rho]}{\partial \rho_{cd}}\Big|_{\rho_0} \delta\rho_{cd}(t)\,.$$

So

$$f(\omega) \approx \frac{\partial h^{\mathrm{KS}}}{\partial \rho}(\omega)$$

and the equation for the response function becomes

$$R = R^{KS} + R^{KS}\frac{\partial h^{KS}}{\partial \rho} R$$

Significance of Adiabatic Approximation

Now R^{KS} is a mean-field response function like R^{HF}. So the adiabatic approximation gives an RPA response function with $\partial h^{\mathrm{KS}}_{ab}/\partial \rho_{cd}$, which is not antisymmetric in general, in place of the matrix element $\langle ad|\, \hat{V}\, |bc\rangle_A$.

Skyrme RPA can be considered an attempt to approximate the adiabatic limit of the exact response function.

Going beyond the adiabatic limit would require a freqency-dependent f. You might think that this would be necessary for states with energies comparable to single-particle spacings.

Example of a theory with frequency-dependent f: Second RPA
But I don't think its response goes over to RPA response in $\omega = 0$ limit.

Sum rules

Two important sum rules:

- Energy-weigthed sum:

$$\sum_{\nu}(E_\nu - E_0)|\left\langle \nu\right| \hat{G}\left|0\right\rangle|^2 = \frac{1}{2}\left\langle 0\right|\left[[\hat{G},\hat{H}],\hat{G}\left|0\right\rangle\right]$$

  Can verify by inserting complete set of states

- Inverse-energy-weighted sum:

$$\sum_{\nu}\frac{1}{(E_\nu - E_0)}|\left\langle \nu\right| \hat{G}\left|0\right\rangle|^2 = -\frac{1}{2}\frac{d}{d\lambda}\left\langle 0_\lambda\right| \hat{G}\left|0_\lambda\right\rangle\Big|_{\lambda=0},$$

  where $|0_\lambda\rangle$ is the ground state of $\hat{H}+\lambda\hat{G}$.
  This one follows from first-order perturbation theory.

Fact: Both these hold in RPA if ground-states on right are HF vacua.

EW sum rule follows in equations of motion approach because double commutators were evaluated in mean-field ground states

IEW sum rule: TDHF derivation of RPA response function implies that for the HF state $|0^{\mathrm{HF}}_{\lambda}\rangle$

$$\delta\rho = \lambda R^{RPA}(\omega = 0) G$$

and

$$\langle 0^{\mathrm{HF}}_{\lambda}| \hat{G} |0^{\mathrm{HF}}_{\lambda}\rangle = Tr(G\rho_0) + Tr(G\delta\rho) + \mathcal{O}(\lambda^2)$$

so

$$-\frac{1}{2}\frac{d}{d\lambda} \langle 0^{\mathrm{HF}}_{\lambda}| \hat{G} |0^{\mathrm{HF}}_{\lambda}\rangle \big|_{\lambda=0} = -\frac{1}{2}\sum_{abcd} G_{ba} R^{\mathrm{RPA}}_{ab,cd}(0) G_{cd}$$

$$= \sum_{abcd} G_{ba} \sum_{\nu} \frac{\langle 0| a^{\dagger}_b a_a |\nu\rangle \langle \nu| a^{\dagger}_c a_d |0\rangle_{\mathrm{RPA}}}{\Omega^{\nu}_{\mathrm{RPA}}} G_{cd} = \sum_{\nu} \frac{\langle 0| \hat{G} |\nu\rangle \langle \nu| \hat{G} |0\rangle_{\mathrm{RPA}}}{\Omega^{\nu}_{\mathrm{RPA}}}$$

IEW sum in DFT

Note that if we use a Kohn-Sham DFT in place of HF, then the identity becomes

$$-\frac{1}{2}\frac{d}{d\lambda}\left\langle 0_\lambda^{\mathrm{KS}}\right|\hat{G}\left|0_\lambda^{\mathrm{KS}}\right\rangle\Big|_{\lambda=0}=\sum_\nu\frac{\left\langle 0\right|\hat{G}\left|\nu\right\rangle\left\langle \nu\right|\hat{G}\left|0\right\rangle_{\text{“RPA”}}}{\Omega^\nu_{\text{“RPA”}}}$$

where “RPA” means the adiabatic approximation discussed earlier.

If the KS functional on the LHS is exact, then so is the RHS. Even though the energies and matrix elements are only adiabatic approximations, the sum above is exact because it contains the response function at $\omega = 0$, i.e. at the adiabatic limit.

Symmetries

Mean-field theory spontaneously breaks symmetries, producing set of ground states related to each other by the symmetry. Mean-field ground states are localized in space, for example. Bad because

- true ground state is not localized,
- When one state is picked as ground state, others can mix with excited states unless you're really careful.

Fortunately, RPA handles this second problem automatically.

Consider an operation $\hat{U} = e^{-i\lambda\hat{S}}$, with $[\hat{H}, \hat{S}] = 0$. If the ground state is not an eigenstate of $\hat{S}$, then the operation produces another ground state. In mean-field (or KS) theory, the new density ρ' must obey the same equation as the original one:

$$\left[[h[\rho'], \rho'\right] = 0\,.$$

For small λ, it turns out

$$\rho'_{ab} = \langle 0'| a_b^\dagger a_a |0'\rangle = \langle 0| U^\dagger a_b^\dagger U U^\dagger a_a U |0\rangle = \sum_{cd} U^*_{ac} \rho_{cd} U_{db}$$

$$\longrightarrow \rho_{ab} + \lambda [S, \rho]_{ab} + \ldots$$

Now repeat the small-oscillations derivation of the RPA, except with no applied field, $\omega = 0$ and $\delta\rho_{mi} = \lambda[S,\rho]_{mi} = S_{mi}$, $\delta\rho_{im} = \lambda[S,\rho]_{im} = -S_{im}$. The result, instead of

$$\left\{ \begin{pmatrix} \omega & 0 \\ 0 & -\omega \end{pmatrix} - \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \right\} \begin{pmatrix} \delta\rho \\ \delta\rho^* \end{pmatrix} = \begin{pmatrix} G \\ G^* \end{pmatrix},$$

is

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} S \\ -S^* \end{pmatrix} = 0$$

So there is an RPA eigenstate with:

$$\Omega_{\rm sp} = 0\,, \qquad X^{\rm sp}_{mi} = S_{mi}\,, \qquad Y^{\rm sp}_{mi} = -S_{im}\,,$$

where "sp" means "spurious"

Numerical implementations of RPA

Two basic routes:

- Diagonalize $\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix}$ in some convenient basis.
  Requires discretizing the continuum, usually by putting the system in a harmonic oscillator or "spherical box".
- Solve response equation in coordinate space, which is frelatively with zero-range effective interactions: you only need $R(\vec{r}_1, \vec{r}_1'; \vec{r}_2, \vec{r}_2')$ at $\vec{r}_1 = \vec{r}_1'$, $\vec{r}_2 = \vec{r}_2'$.
  Then solve

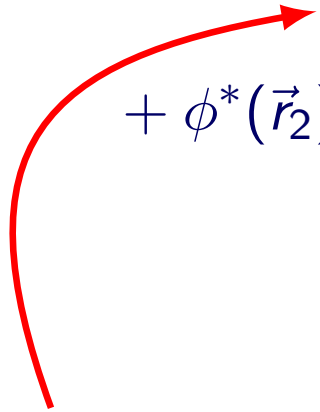
$$R^{\mathrm{RPA}}(\vec{r}_1, \vec{r}_2; \omega) = R^{\mathrm{HF}}(\vec{r}_1, \vec{r}_2; \omega) + \int d\vec{r}' \, R^{\mathrm{HF}}(\vec{r}_1, \vec{r}'; \omega) \tilde{V}(\vec{r}') R^{\mathrm{RPA}}(\vec{r}', \vec{r}_2; \omega)$$

  where $\tilde{V}$ is just a constant if you have a pure delta function interaction, by discretizing integral over space and treating as matrix equation.
  Helped by: nice expression for R^{HF}. This method treats outgoing boundary conditions of continuum particles correctly (gets nonzero "escape width").

HF response

$$R^{\mathrm{HF}}(\vec{r}_1,\vec{r}_2;\omega) = \sum_{mi}\left(\frac{\phi_m(\vec{r}_1)\phi_i^*(\vec{r}_1)\phi_m^*(\vec{r}_2)\phi_i(\vec{r}_2)}{\omega-\epsilon_m+\epsilon_i+i\eta} + \frac{\phi_i^*(\vec{r}_2)\phi_m(\vec{r}_2)\phi_m^*(\vec{r}_1)\phi_i(\vec{r}_1)}{-\omega-\epsilon_m+\epsilon_i+i\eta}\right)$$

$$= \sum_{i}\left(\phi^*(\vec{r}_1)\langle\vec{r}_1|\frac{1}{\omega+\epsilon_i-h+i\eta}|\vec{r}_2\rangle\phi_i(\vec{r}_2) + \phi^*(\vec{r}_2)\langle\vec{r}_2|\frac{1}{-\omega+\epsilon_i-h+i\eta}|\vec{r}_1\rangle\phi_i(\vec{r}_1)\right)$$



This is the the Greens function for a particle scattering from the potential in h.

Pairing and quasiparticles

Note that $|SD\rangle$ is a vacuum for the complete set of operators

$$\alpha_a = \begin{cases} a_a^\dagger & a < F \\ a_a & a > F \end{cases} .$$

Making mean-field theory more general can incorporate important pairing correlations, in which a nucleon in orbit a correlate strongly with a nucleon in the time-reversed orbit $\bar{a}$ The (number nonconserving) state

$$|BCS\rangle \equiv \mathcal{N} e^{\frac{v_a}{u_a} a_a^\dagger a_{\bar{a}}^\dagger} |\mathrm{vac}\rangle$$

can be represented as a vacuum of *quasiparticles*

$$\alpha_a \equiv u_a a_a - v_a a_{\bar{a}}^\dagger , \quad [\alpha_a, \alpha_b^\dagger] = \delta_{ab} \quad \text{if} \quad |u_a|^2 + |v_a|^2 = 1 .$$

Generalization of HF and BCS: HFB

HFB is the most general "mean-field" theory in these kinds of operators:

$$\alpha_a = \sum_c \left(\mathcal{U}^*_{ac} a_c + \mathcal{V}^*_{ac} a^\dagger_c \right) , \qquad \alpha^\dagger_a = \sum_c \left(\mathcal{U}_{ac} a_c + \mathcal{V}_{ac} a_c \right) ,$$

with appropriate constraints on matrices $\mathcal{U}$ and $\mathcal{V}$.

Representation like that we used for HF earlier:

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^* \end{pmatrix} , \qquad \kappa_{ab} \equiv \langle 0 | \, a_b a_a \, | 0 \rangle \equiv \text{"pairing tensor"}$$

HFB energy functional:

$$E[\rho, \kappa] = Tr(t\rho) + \frac{1}{2} Tr_1 Tr_1 \rho V \rho + \frac{1}{4} Tr_2 Tr_2 \kappa^* V \kappa$$

or a more general KS-like functional if you want to try to do better.

Varying $\mathcal{E} - \lambda N - Tr\left(\Lambda[\mathcal{R}^2 - \mathcal{R}]\right)$ with respect to R gives HFB eqation:

$$[\mathcal{H}[\mathcal{R}], \mathcal{R}] = 0\,,$$

where

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

with

$$\Delta_{ab} \equiv \frac{1}{2} \sum_{cd} \langle ab|\, \hat{V}\, |cd\rangle_A\, \kappa_{cd}\,,$$

or something more general if you're doing (generalized) KS theory. The simultaneous diagonalization of $\mathcal{H}$ and $\mathcal{R}$ leads to the explicit equation

$$\begin{pmatrix} h - \lambda & \Delta \\ -\Delta^* & -h^* + \lambda \end{pmatrix} \begin{pmatrix} \mathcal{U}_a \\ \mathcal{V}_a \end{pmatrix} = E_a \begin{pmatrix} \mathcal{U}_a \\ \mathcal{V}_a \end{pmatrix},$$

where $\mathcal{U}_a$, $\mathcal{V}_a$ are the a^{th} columns of the transformation matrices $\mathcal{U}$ and $\mathcal{V}$.

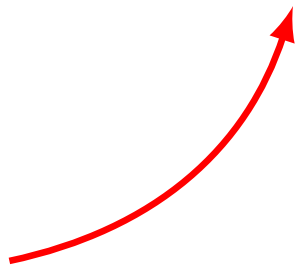
Bases

The basis that diagonalizes $\mathcal{H}$ is called the "quasiparticle basis"
There is another "canonical" basis that diagonalizes ρ, $\mathcal{U}$, and $\mathcal{V}$ so that, e.g.

$$\mathcal{V}_{ab} = v_a \delta_{ab} \,.$$

In this basis HFB looks almost like BCS, except for the fact that $\mathcal{H}$ is not diagonal:

$$H_{ab} \equiv E_{ab} \neq E_a \delta_{ab}$$



Name for later use

QRPA through equations-of-motions method

Same idea as with ph RPA, except now

$$\begin{aligned} \langle 0| \alpha_a^\dagger \alpha_b^\dagger, [\hat{H}, Q_\nu^\dagger] |0\rangle &= \Omega^\nu \langle 0| [\alpha_a^\dagger \alpha_b^\dagger, Q_\nu^\dagger] |0\rangle \\ \langle 0| [\alpha_a \alpha_b, [\hat{H}, Q_\nu^\dagger] |0\rangle &= \Omega^\nu \langle 0| [\alpha_a \alpha_b, Q_\nu^\dagger] |0\rangle \end{aligned}$$

and

$$Q_\nu^\dagger = \sum_{a>b} X_{ab}^\nu \alpha_a^\dagger \alpha_b^\dagger - \sum_{a>b} Y_{ab}^\nu \alpha_a \alpha_b \,,$$

Now assume that can substitute $|HFB\rangle$ for $|0\rangle$ after doing commutators. Again get

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix} = \Omega^\nu \begin{pmatrix} X^\nu \\ Y^\nu \end{pmatrix}$$

but now with more complicated expressions for A and B (what, don't believe me?), which can be derived from TDHFB

A matrix...

In the canonical basis:

$$
\begin{aligned}
A_{ab,cd} \;=\;& E_{ac}\delta_{bd} - E_{bc}\delta_{ad} - E_{ad}\delta_{bc} + E_{bd}\delta_{ac} \\
& - V^{\mathrm{ph}}_{a\bar{c}\bar{b}d}\, u_d v_c u_a v_b + V^{\mathrm{ph}}_{b\bar{c}\bar{a}d}\, u_d v_c u_b v_a \\
& + V^{\mathrm{ph}}_{a\bar{d}\bar{b}c}\, u_c v_d u_a v_b - V^{\mathrm{ph}}_{b\bar{d}\bar{a}c}\, u_c v_d u_b v_a \\
& - V^{\mathrm{pp}}_{\bar{c}\bar{d}\bar{b}\bar{a}}\, v_c v_d v_b v_a - V^{\mathrm{pp}}_{abdc}\, u_a u_b u_c u_d \\
& - V^{\mathrm{3p1h}}_{\bar{c}\bar{d}a\bar{b}}\, v_c v_d u_a v_b + V^{\mathrm{3p1h}}_{\bar{c}\bar{d}b\bar{a}}\, v_c v_d u_b v_a \\
& - V^{\mathrm{3p1h}}_{ab\bar{c}d}\, u_a u_b u_d v_c + V^{\mathrm{3p1h}}_{ab\bar{d}c}\, u_a u_b u_c v_d \\
& - V^{\mathrm{1p3h}}_{\bar{c}d\bar{b}\bar{a}}\, u_d v_c v_b v_a + V^{\mathrm{1p3h}}_{\bar{d}c\bar{b}\bar{a}}\, u_c v_d v_b v_a \\
& - V^{\mathrm{1p3h}}_{a\bar{b}dc}\, u_a v_b u_c u_d + V^{\mathrm{1p3h}}_{b\bar{a}dc}\, u_b v_a u_c u_d ,
\end{aligned}
$$

$$
V^{\mathrm{ph}}_{acbd} = \frac{\delta^2 E[\rho,\kappa,\kappa^*]}{\delta\rho_{ba}\delta\rho_{dc}},
$$

$$
V^{\mathrm{pp}}_{badc} = \frac{\delta^2 E[\rho,\kappa,\kappa^*]}{\delta\kappa^*_{ba}\delta\kappa_{dc}}, \qquad V^{\mathrm{3p1h}}_{badc} = \frac{\delta^2 E[\rho,\kappa,\kappa^*]}{\delta\kappa^*_{ba}\delta\rho_{cd}} = V^{\mathrm{1p3h}\ *}_{cdba},
$$

and B...

$$
\begin{aligned}
B_{ab,cd} \;=\; & V^{\mathrm{ph}}_{bd\bar{a}\bar{c}}\, u_d v_c u_b v_a - V^{\mathrm{ph}}_{ad\bar{b}\bar{c}}\, u_d v_c u_a v_b \\
& - V^{\mathrm{ph}}_{bc\bar{a}\bar{d}}\, u_c v_d u_b v_a + V^{\mathrm{ph}}_{ac\bar{b}\bar{d}}\, u_c v_d u_a v_b \\
& + V^{\mathrm{pp}}_{ba\bar{c}\bar{d}}\, v_c v_d u_a u_b + V^{\mathrm{pp}}_{dc\bar{a}\bar{b}}\, v_a v_b u_c u_d \\
& + V^{\mathrm{3p1h}}_{bad\bar{c}}\, u_d v_c u_a u_b - V^{\mathrm{3p1h}}_{bac\bar{d}}\, u_c v_d u_a u_b \\
& + V^{\mathrm{3p1h}}_{dcb\bar{a}}\, u_b v_a u_c u_d - V^{\mathrm{3p1h}}_{dca\bar{b}}\, u_a v_b u_c u_d \\
& + V^{\mathrm{1p3h}}_{b\bar{a}\bar{c}\bar{d}}\, v_c v_d u_b v_a - V^{\mathrm{1p3h}}_{a\bar{b}\bar{c}\bar{d}}\, v_c v_d u_a v_b \\
& + V^{\mathrm{1p3h}}_{d\bar{c}\bar{a}\bar{b}}\, v_a v_b u_d v_c - V^{\mathrm{1p3h}}_{c\bar{d}\bar{a}\bar{b}}\, v_a v_b u_c v_d,
\end{aligned}
$$

Implementation

- Matrices are much larger than in regular RPA since indices run over *all* quasiparticle states. Set of states must be truncated at some point, using energy or occupation as a criterion (Note that zero-range pairing must be renormalized at HFB level, usually by putting upper limit on the continuum)
- Discretization of continuum introduces uncertainty in energy. It takes about $t = 2R_{\mathrm{box}}/c$ for an emitted particle to bounce of wall of box and come back (rather than escaping). This introduces uncertainty in energy of about

$$\Delta E \approx \frac{\hbar}{t} \approx \frac{100\ \mathrm{fm}}{R_{\mathrm{box}}} = 5\ \mathrm{MeV} \quad \text{for } R_{\mathrm{box}} = 20\ \mathrm{fm}$$

  Need "smoothing function" to account for this.
- We have a completely self-consistent code for box boundary conditions in spherical nuclei — extending it now to deformed nuclei

Response function and equation for it generalize. In external field $\hat{G} = \sum_{ab} G_{ab} a_a^\dagger a_b + \tilde{G} a_a^\dagger a_b^\dagger + c.c$

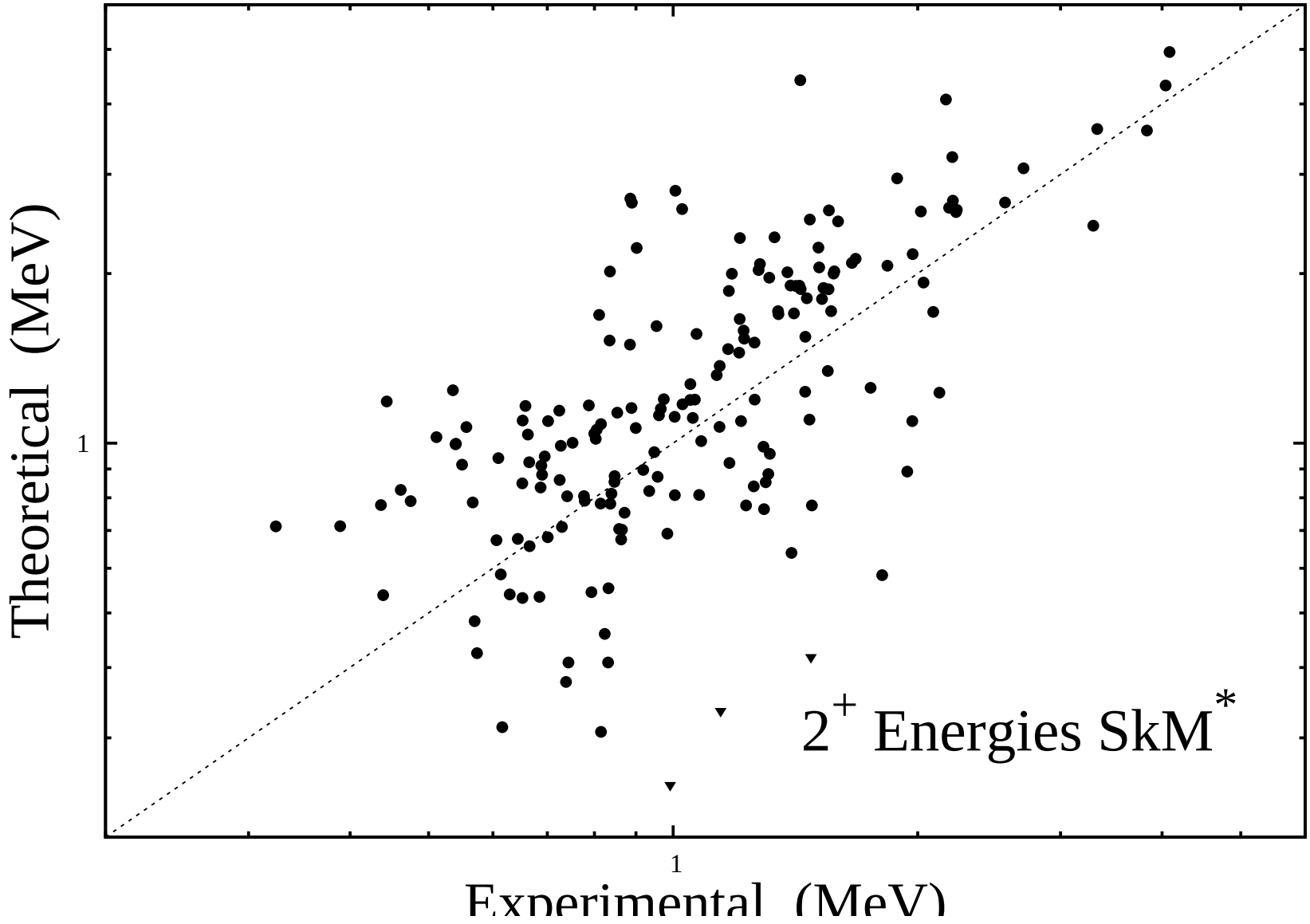
$$\begin{pmatrix} \delta\rho(\omega) \\ \delta\kappa(\omega) \end{pmatrix} = R(\omega) \begin{pmatrix} G \\ \tilde{G} \end{pmatrix}$$

$$R^{\mathrm{QRPA}}(\omega) = R^{\mathrm{HFB}}(\omega) + R^{\mathrm{HFB}}(\omega) \frac{\partial \mathcal{H}}{\partial \mathcal{R}} R^{\mathrm{QRPA}}(\omega)$$

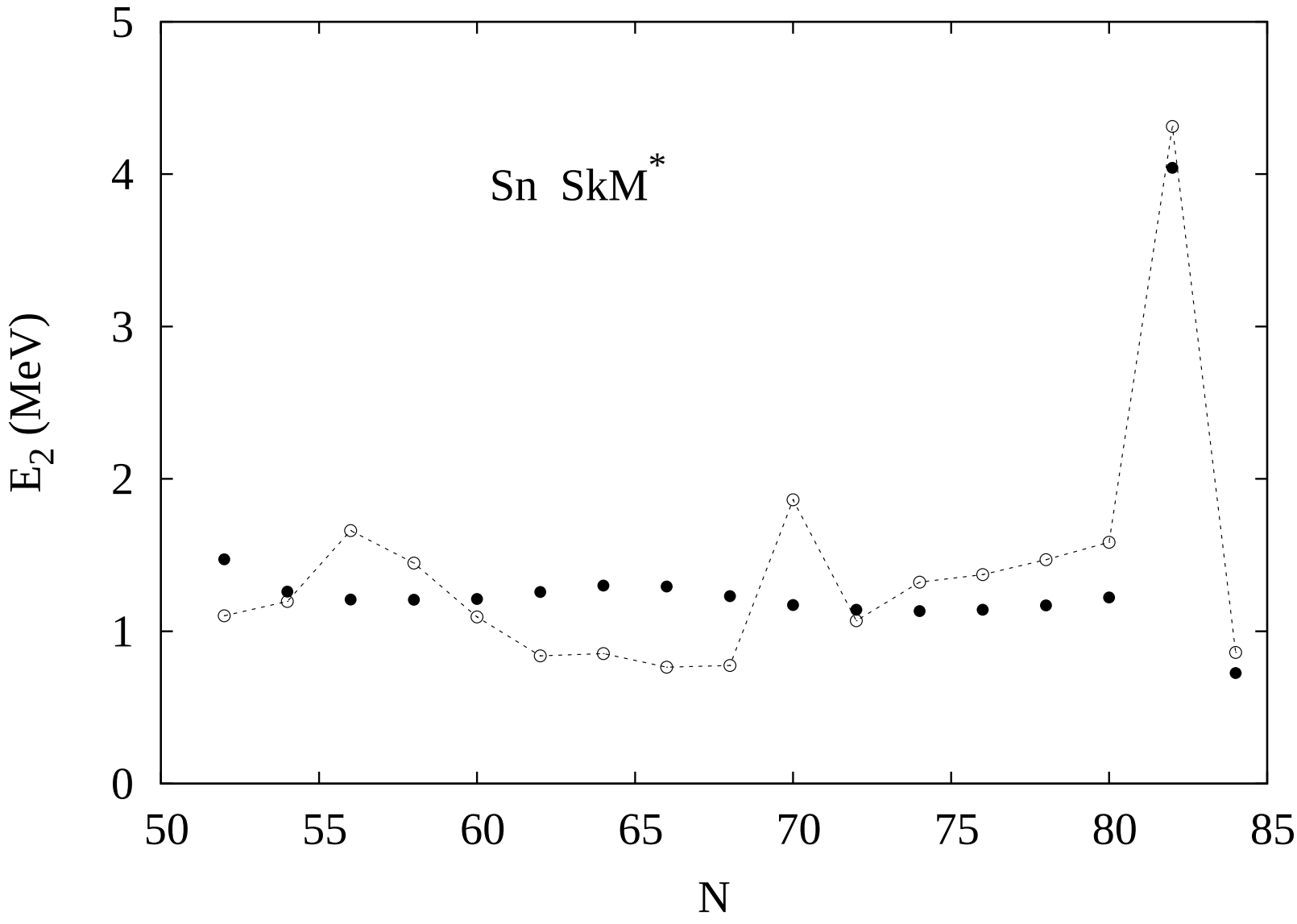
Getting R^{HFB} as a starting point is harder than getting R^{HF} because spectral representation isn't much use.

Completely self-consistent setup of Green's function Skyrme HFB+QRPA isn't quite there yet even in spherical nuclei

2^+-energy systematics

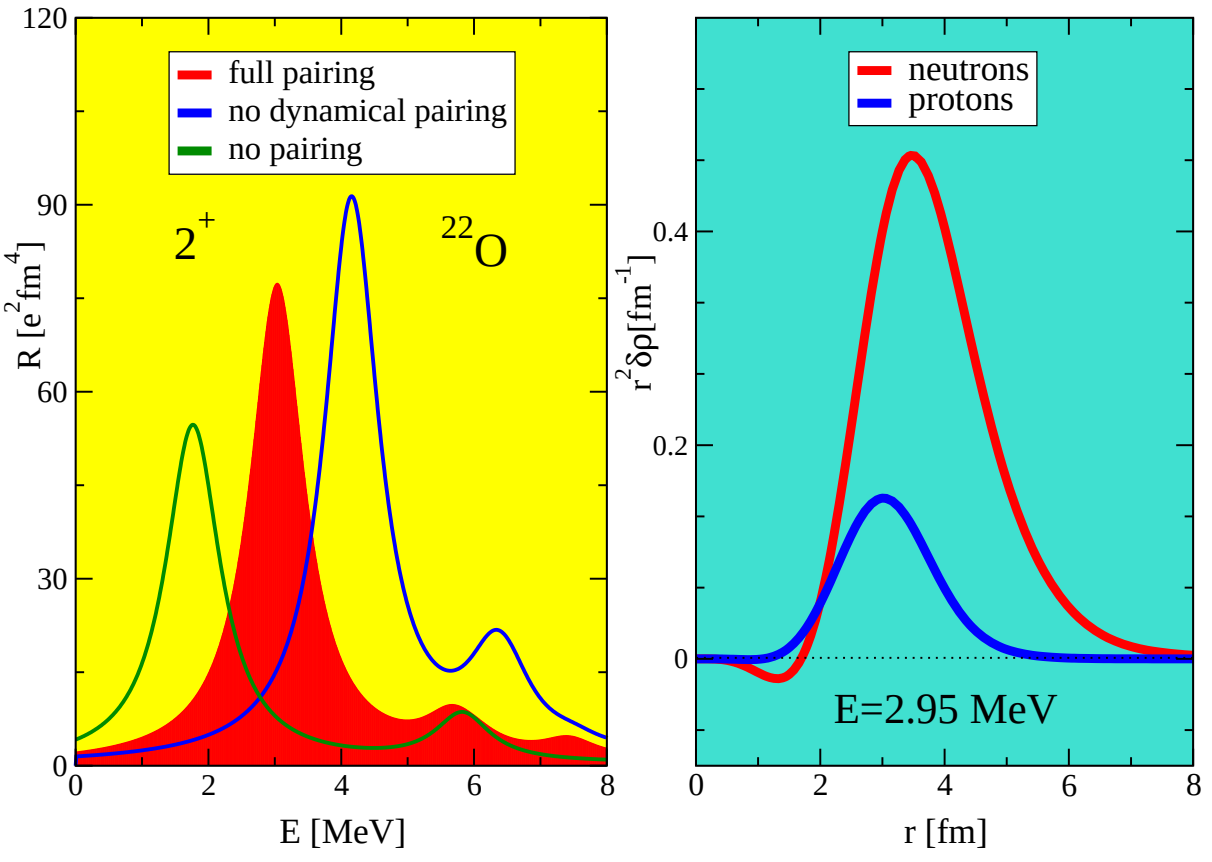


2^+ energies for Sn isotopes



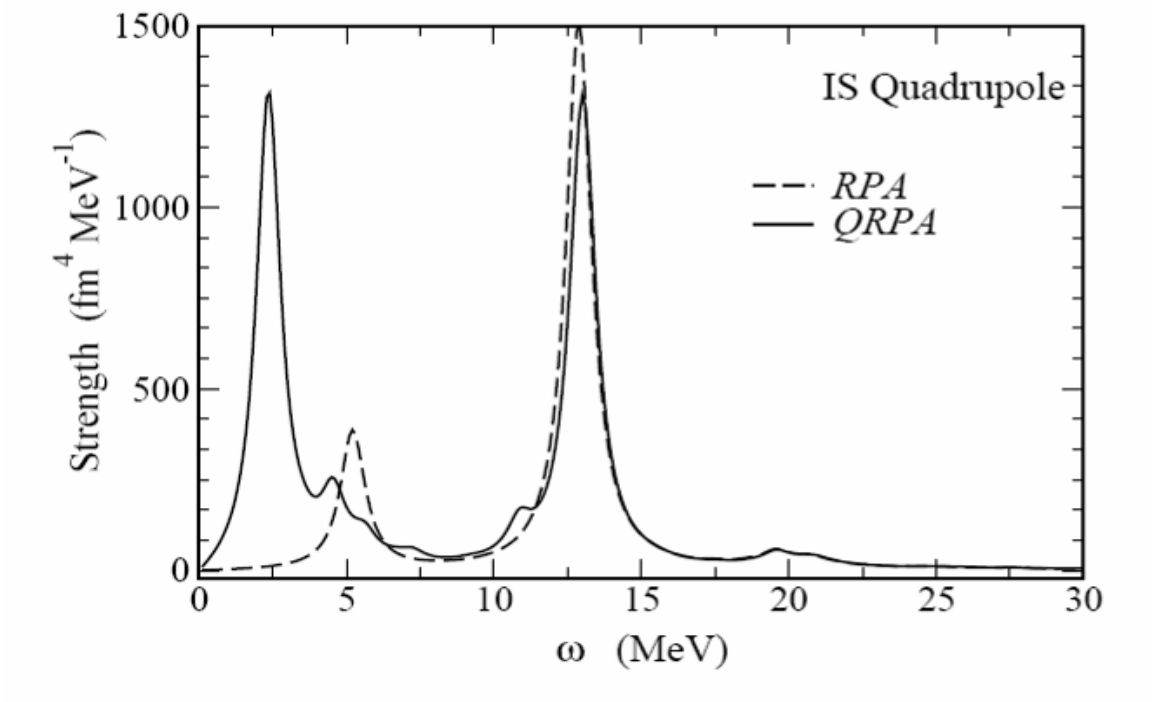
Effects of dynamical pairing on 2^+ state

- **Pairing effect on the low-lying T=0 2^+ state**

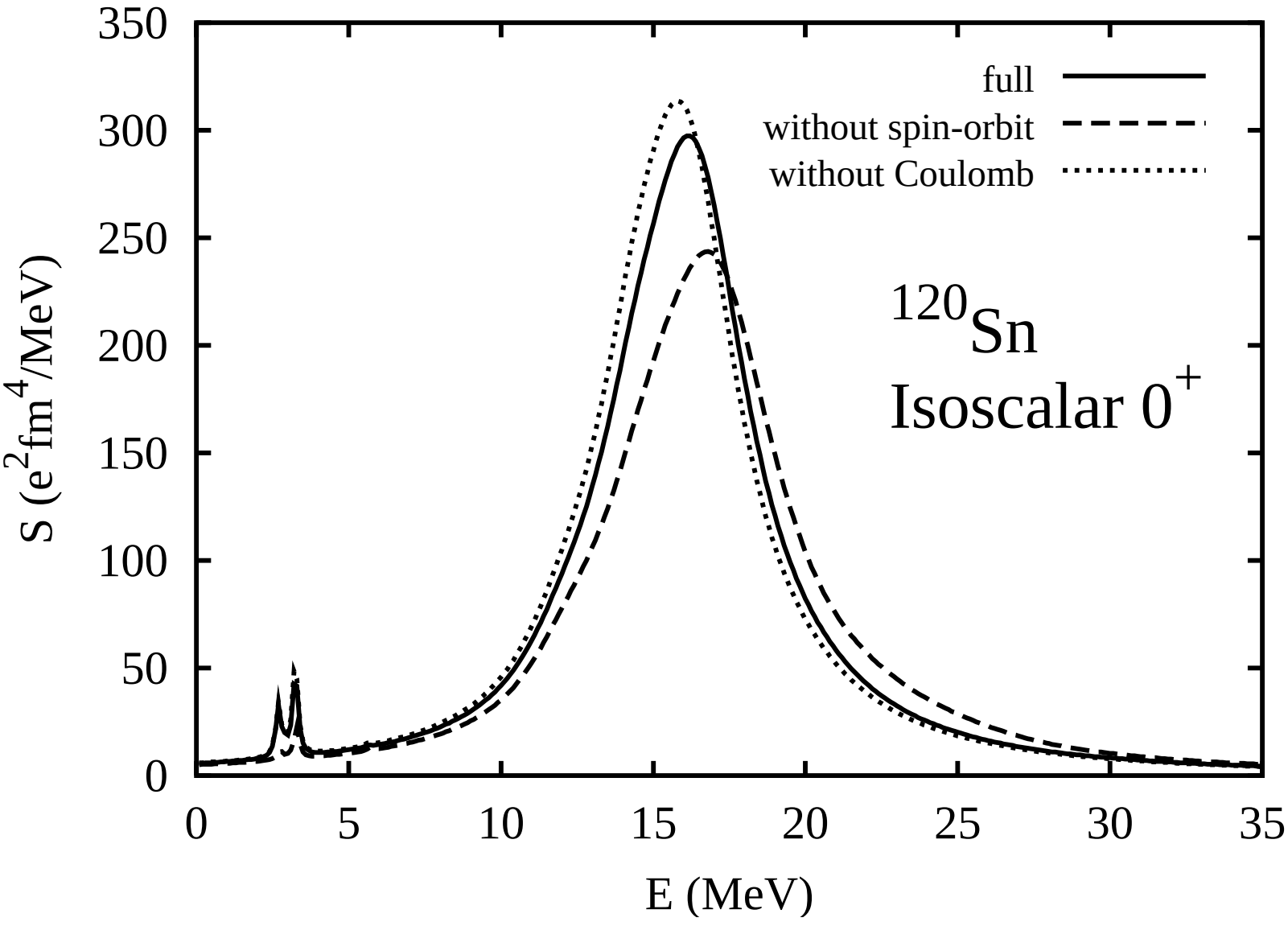


RPA vs. QRPA

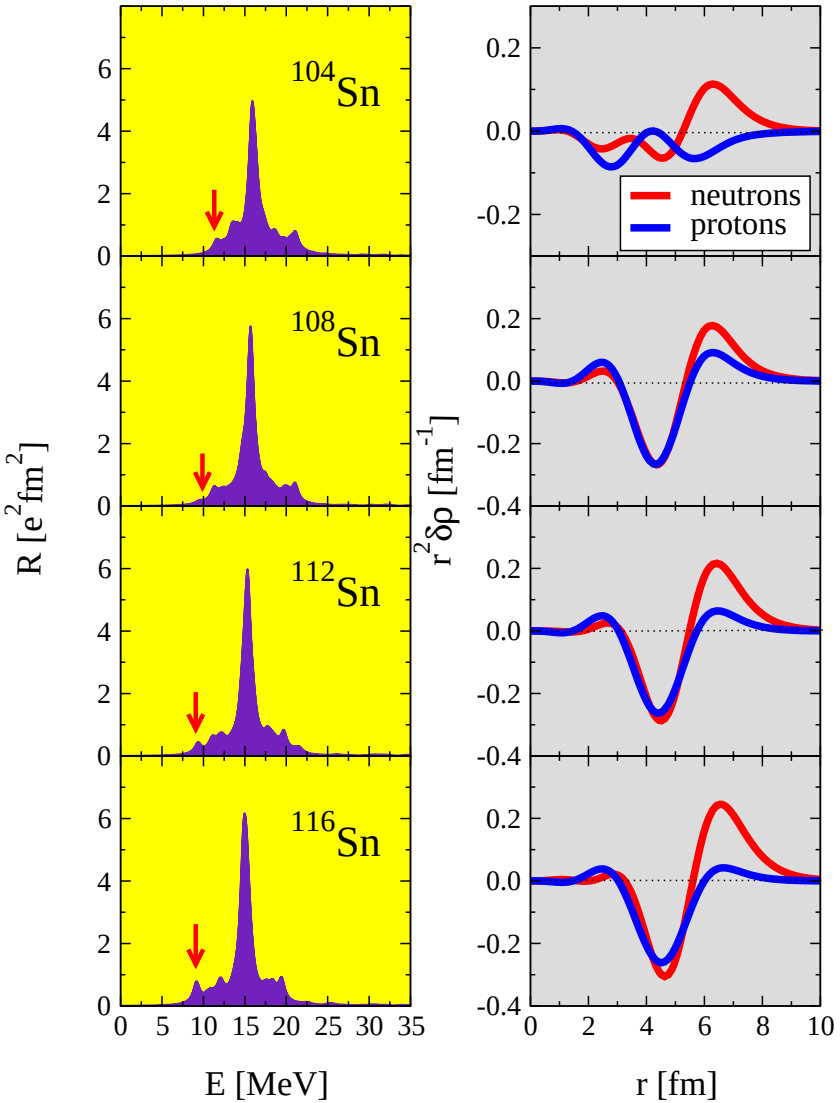
2+ states in 120Sn, with smearing



Monopole strength with some Skyrme terms omitted

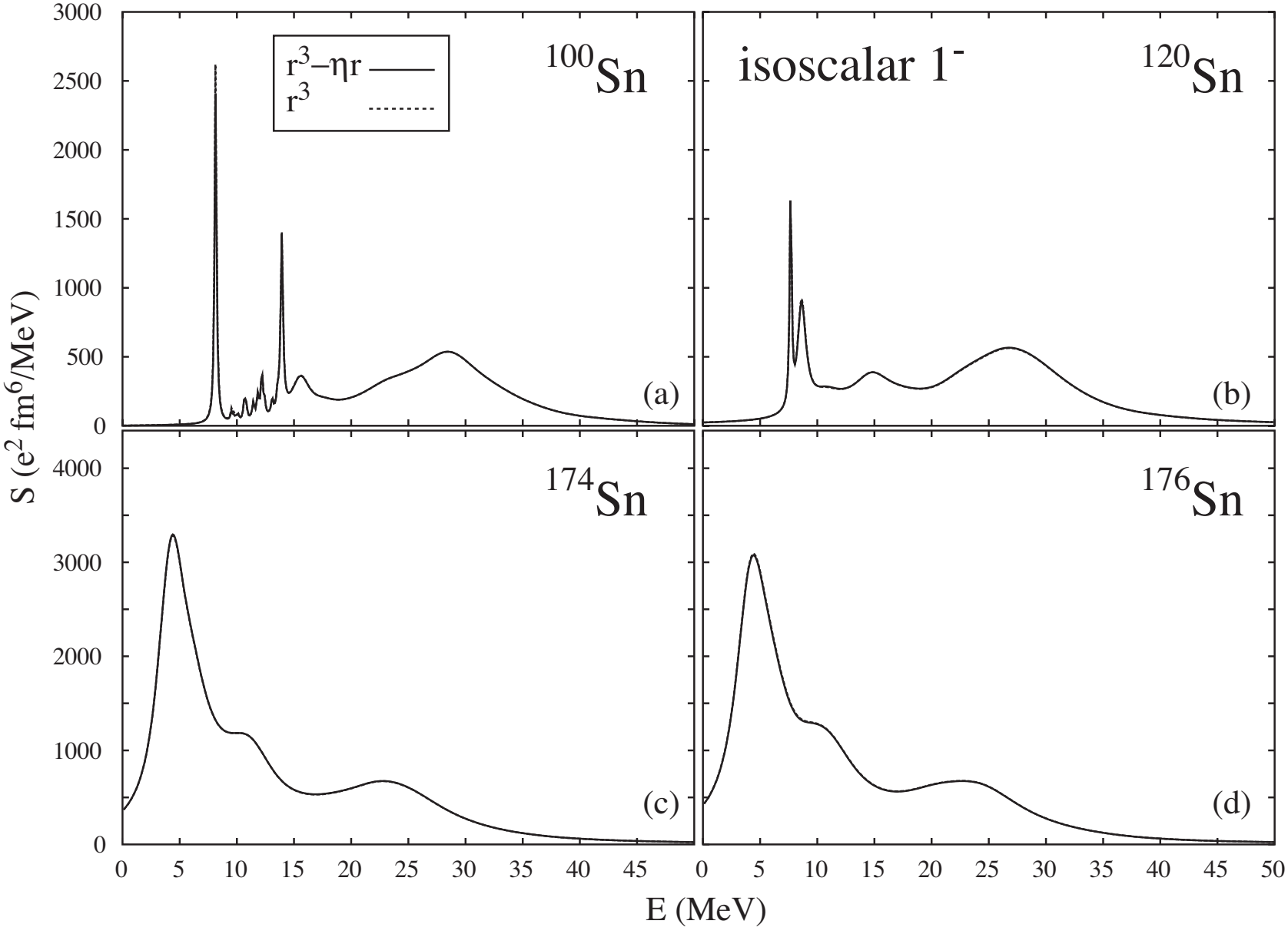


Evolution of isovector dipole strength

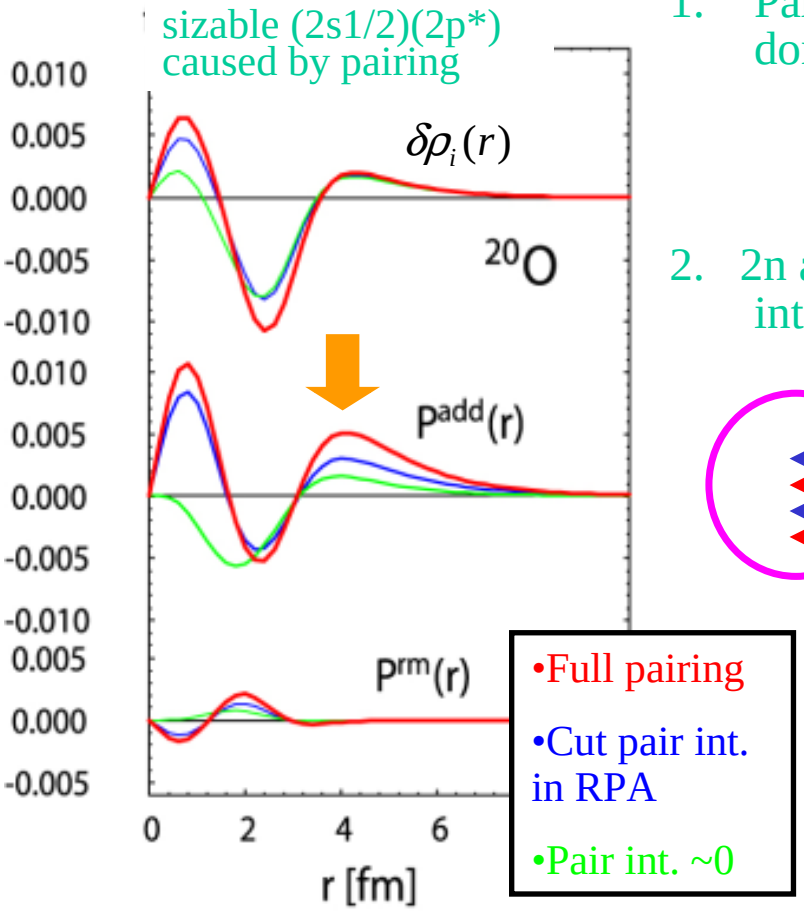


From talk by D. Vretenar

Isoscalar dipole strength near the drip line



Di-neutron correlation in soft dipole mode

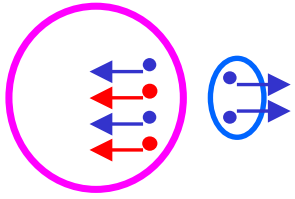


1. Particle-particle amplitude (Pair-add) is dominating in r>3fm (surface & outside)

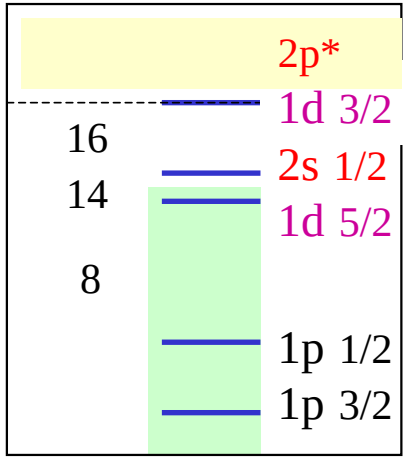
$$P^{add}(r) > \delta\rho_i(r) >> P^{rm}(r)$$

^{18}O(gs) + 2n character

2. 2n amplitude is strongly enhanced by pairing interaction: nn-correlation in excited states



Di-neutron correlation



From talk by M. Matsuo

Now

$$Q_\nu^\dagger = \sum_{pn} X_{pn}^\nu \alpha_p^\dagger \alpha_n^\dagger - Y_{pn} \alpha_p \alpha_n$$

Canonical basis again:

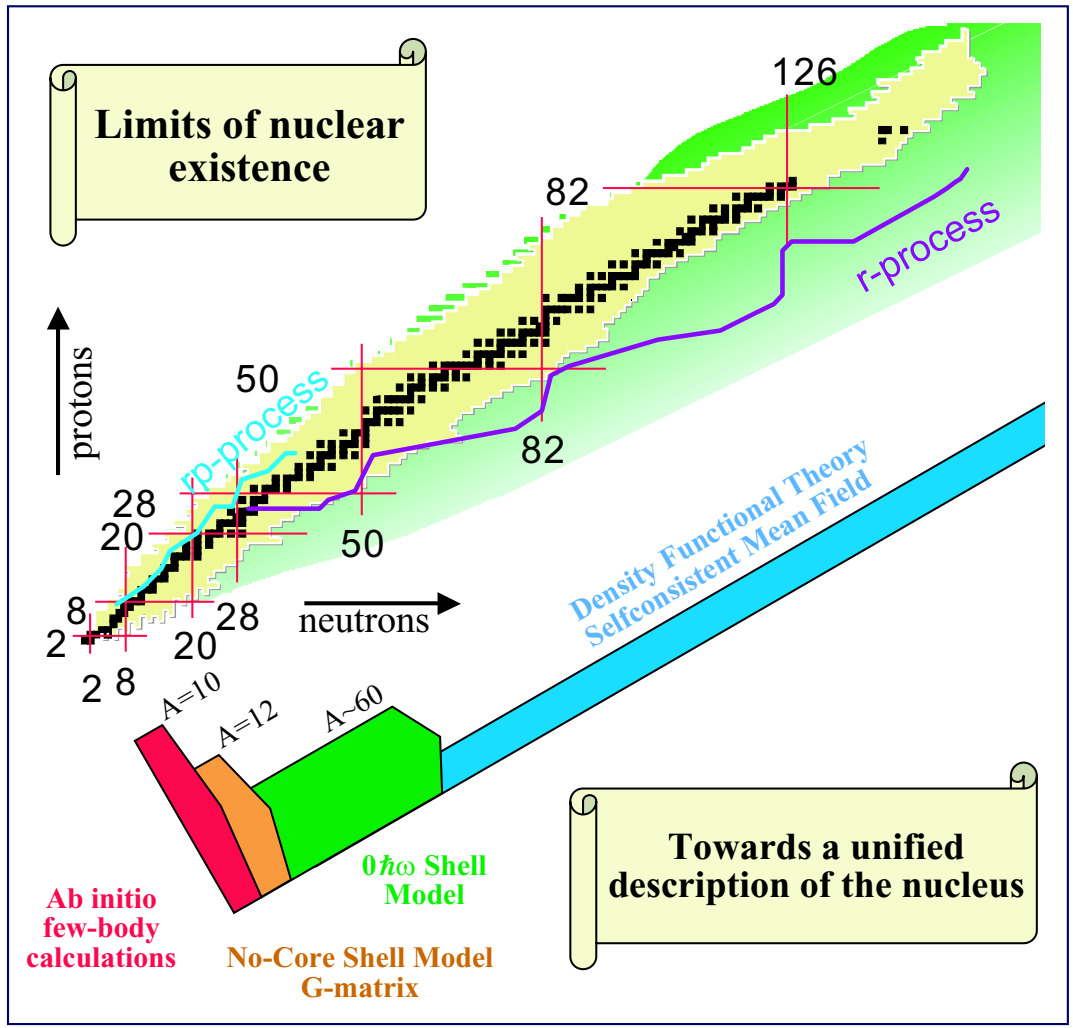
$$\begin{aligned} A_{pn,p'n'} &= E_{p,p'}\ \delta_{n,n'} + E_{n,n'}\ \delta_{p,p'} \\ &\quad + V^{\rm ph}_{pn,p'n'}(u_p v_n u_{p'} v_{n'} + v_p u_n v_{p'} u_{n'}) \\ &\quad + V^{\rm pp}_{pn,p'n'}(u_p u_n u_{p'} u_{n'} + v_p v_n v_{p'} v_{n'}) \end{aligned}$$

and

$$\begin{aligned} B_{pn,p'n'} &= V^{\rm ph}_{pn,p'n'}(v_p u_n u_{p'} v_{n'} + u_p v_n v_{p'} u_{n'} \\ &\quad - V^{\rm pp}_{pn,p'n'}(u_p u_n v_{p'} v_{n'} + v_p v_n u_{p'} u_{n'}) \end{aligned}$$

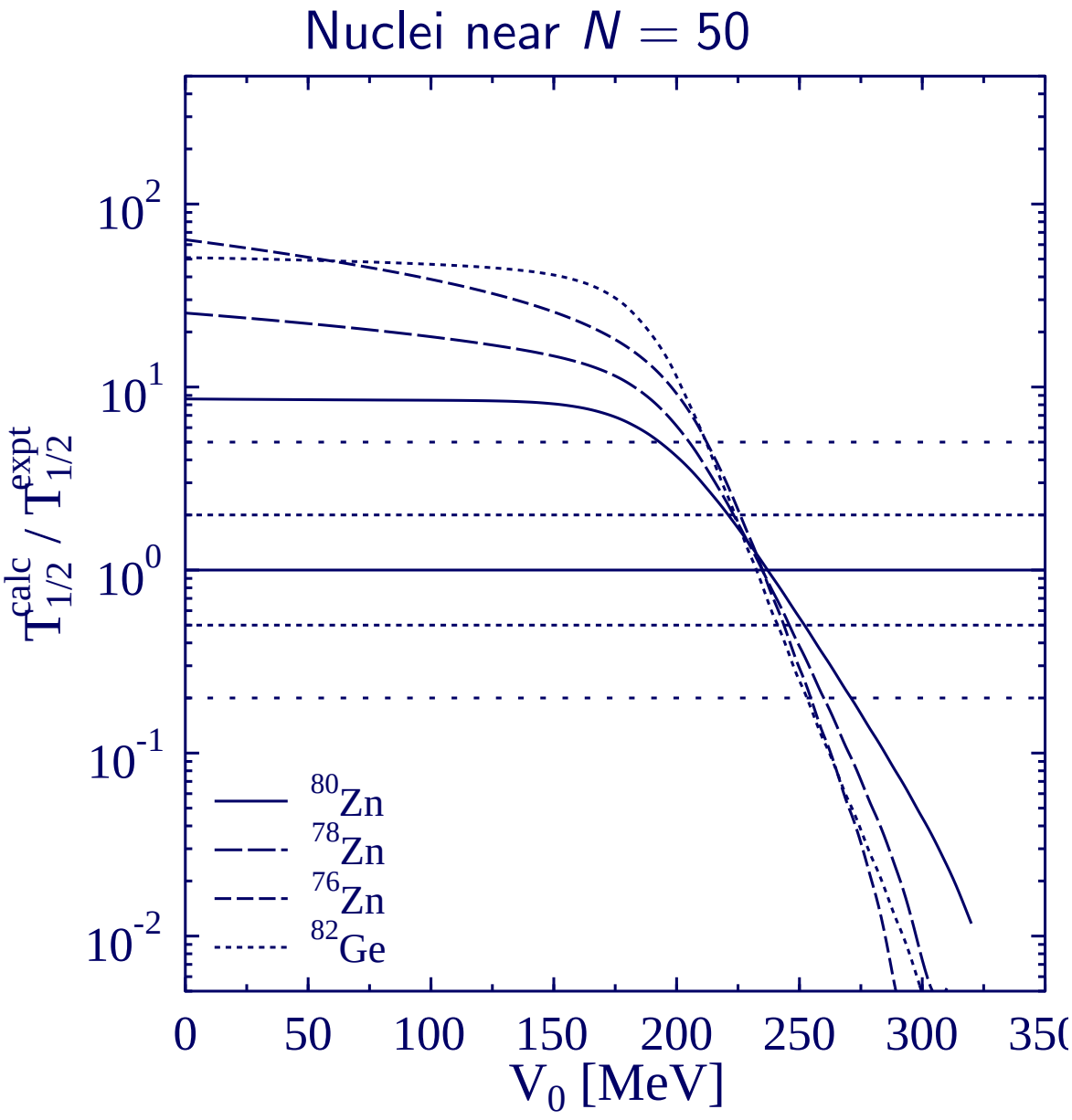
if energy functional contains no $\rho\kappa$ parts.

R-process beta decay

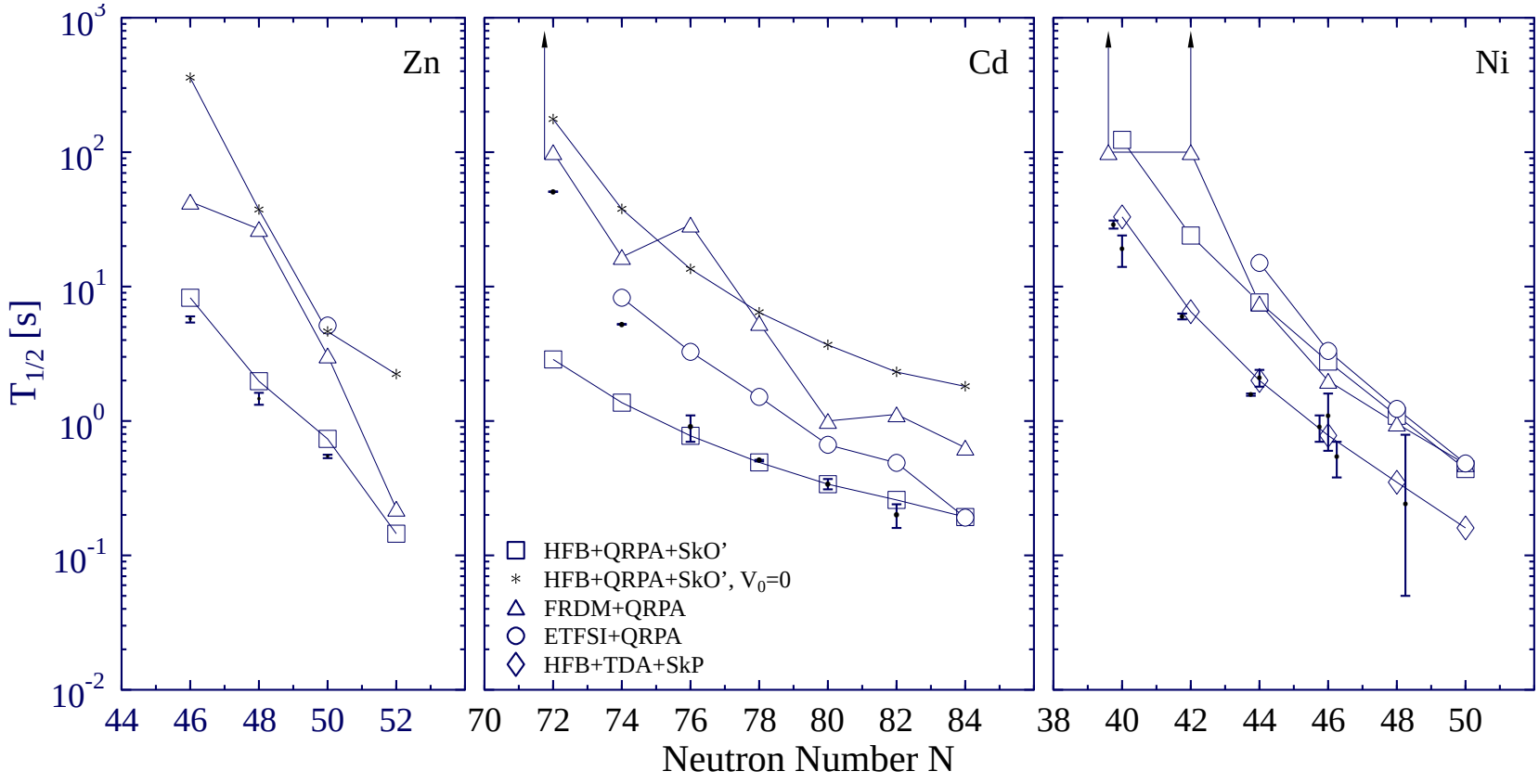


We want to evaluate matrix elements of $\vec{\sigma}\tau_+$ for nuclei along the r-process path.

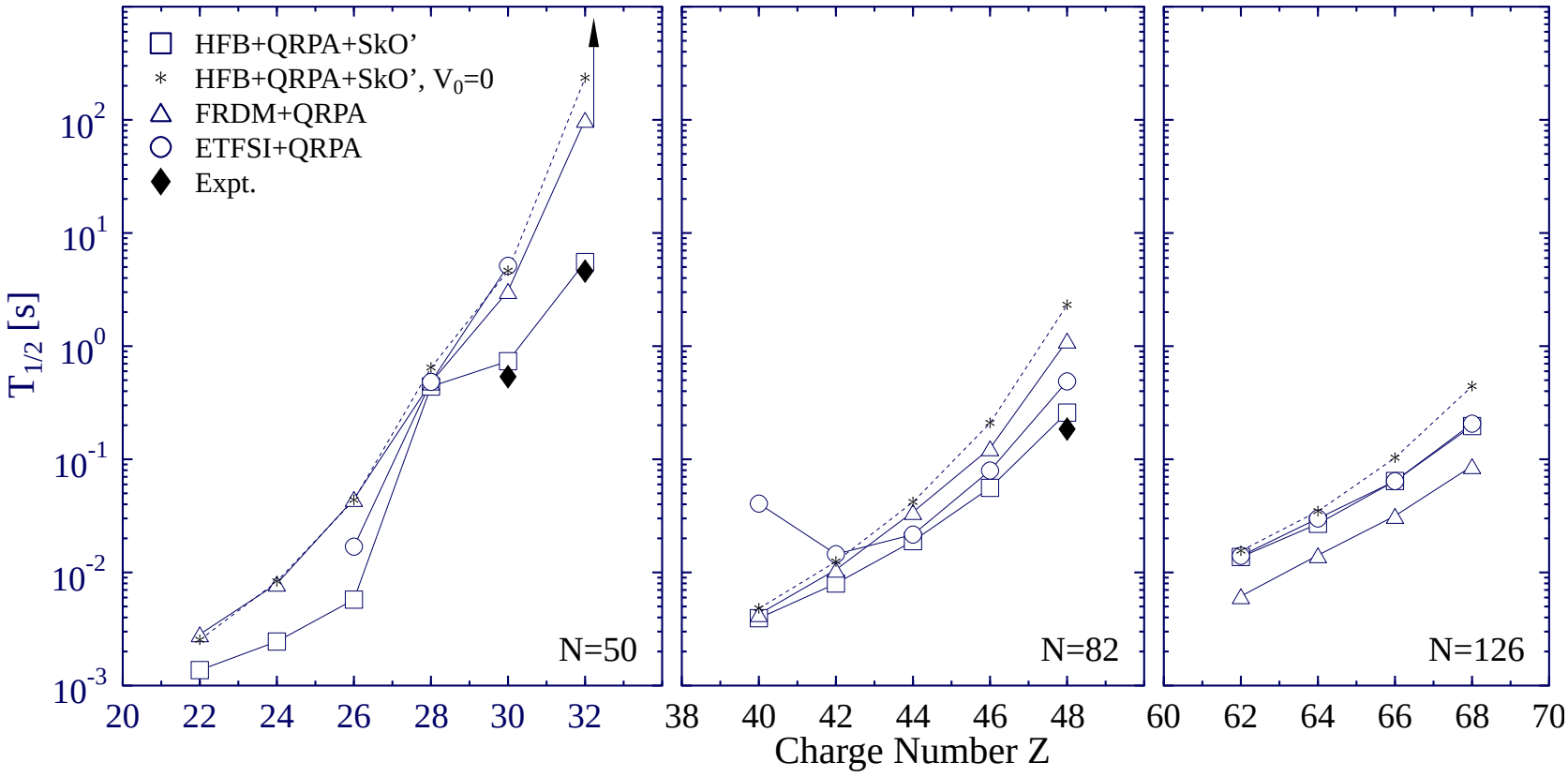
Effects of $T = 0$ pairing



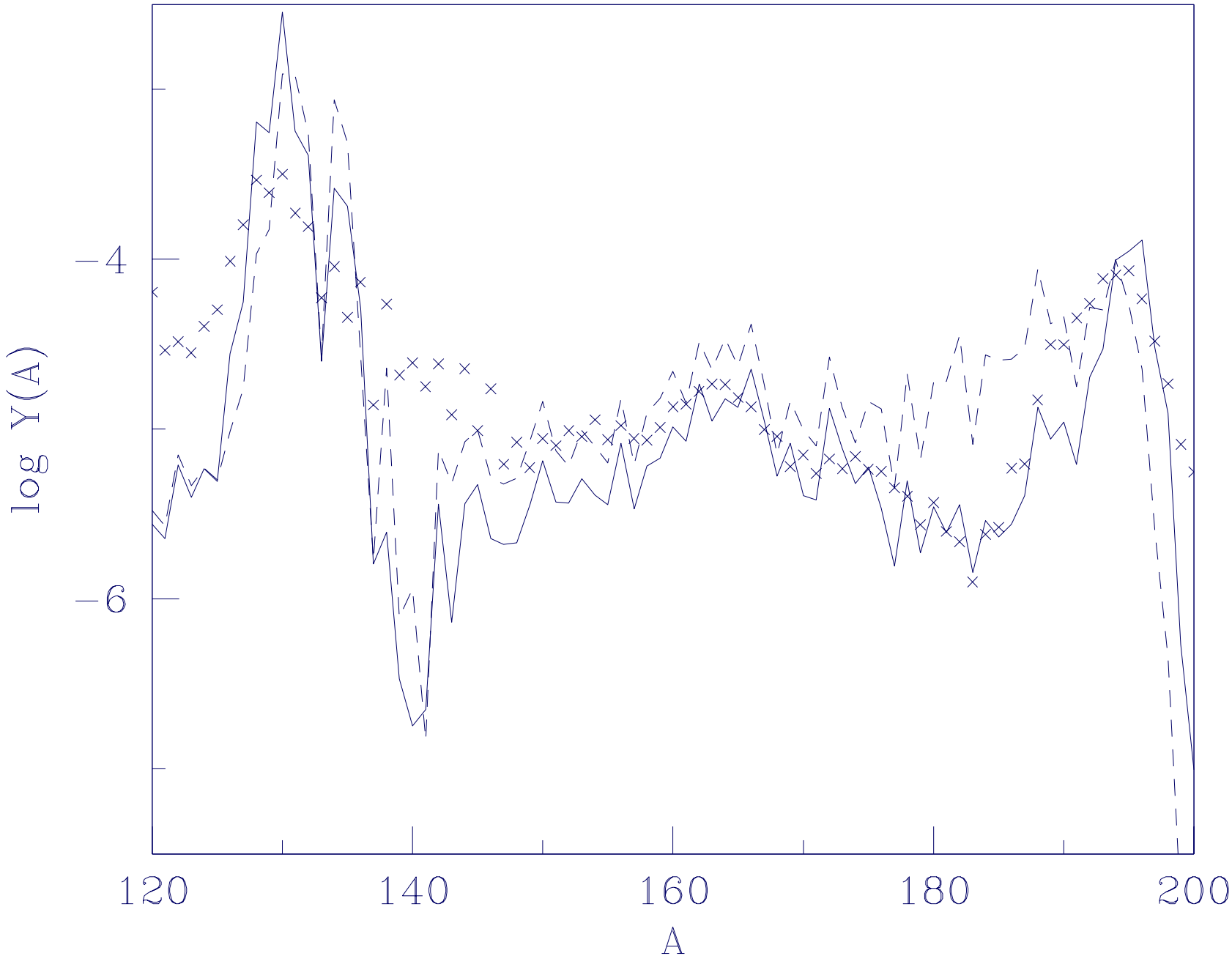
Half-life comparison



Half lives for r-process nuclei



Effect on abundances?



What We Know About Neutrinos

Come in three "flavors", none of which have definite mass.

$$\begin{pmatrix} \nu_e \\ e \end{pmatrix} \quad \begin{pmatrix} \nu_\mu \\ \mu \end{pmatrix} \quad \begin{pmatrix} \nu_\tau \\ \tau \end{pmatrix}$$

$$\begin{pmatrix} \nu_e \\ \nu_\mu \\ \nu_\tau \end{pmatrix} = \begin{pmatrix} \\ U_\nu \\ \\ \end{pmatrix} \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{pmatrix} \Longleftarrow \text{mass eigenstates}$$

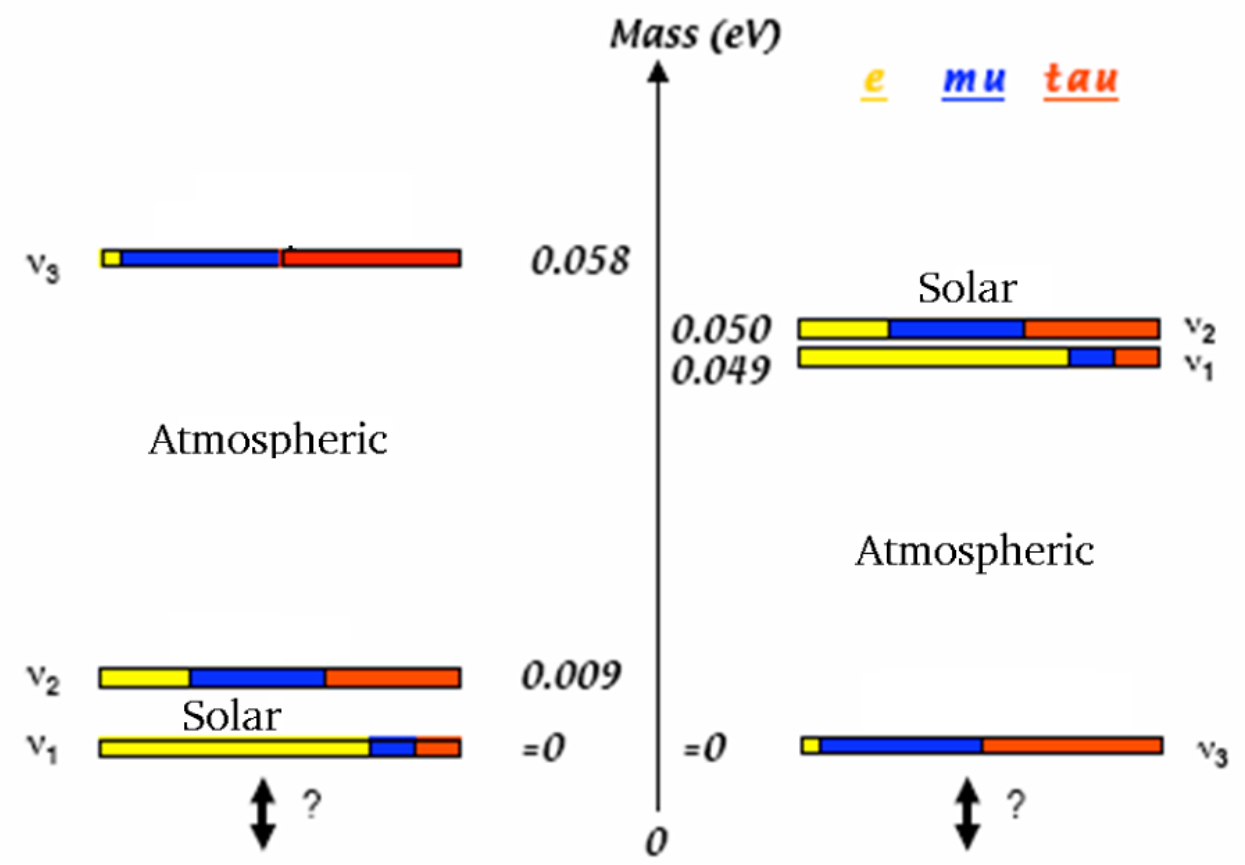
$$m_i \lesssim 1 \text{ eV}$$

U contains three mixing angles (and a few phases).

From recent "oscillation" experiments:

- Solar-ν's: $\Delta m^2_{\rm sol} \approx 7 \times 10^{-5}$ eV^2 $\quad \theta_{\rm sol} \approx 33^\circ$
- Atmospheric-ν's: $\Delta m^2_{\rm atm} \approx 2 \times 10^{-3}$ eV^2 $\quad \theta_{\rm atm} \approx 45^\circ$
- Reactor ν's: Third mixing angle is small.
  Atmospheric ν_e's don't oscillate.

What We Still Don't Know



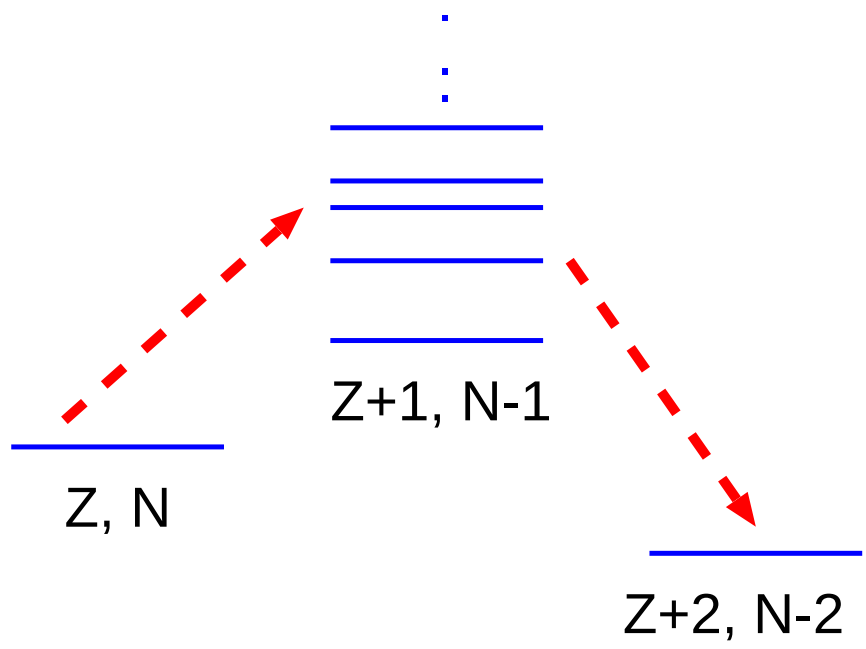
- "Hierarchy": normal or inverted?
- Overall mass scale
- Are neutrinos their own antiparticles?

Oscillation experiments cannot answer these questions.

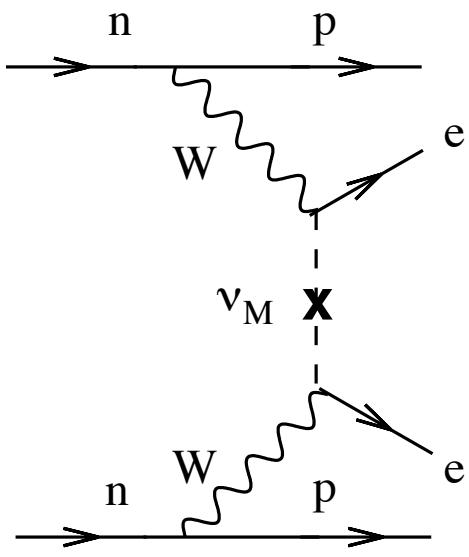
Neutrinoless double-beta decay can help

Neutrinoless Double-Beta Decay

If energetics are right (ordinary beta decay forbidden)...

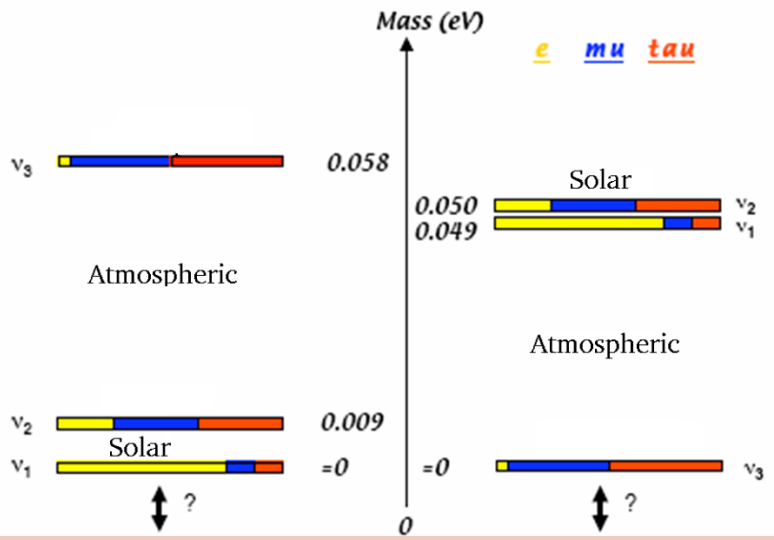


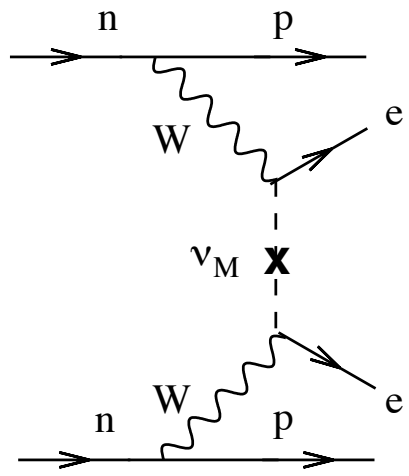
and neutrinos are their own antiparticles...



then two neutrons inside a nucleus can turn into two protons, emitting two electrons and nothing else (unlike the already observed two-neutrino process).

How It Helps



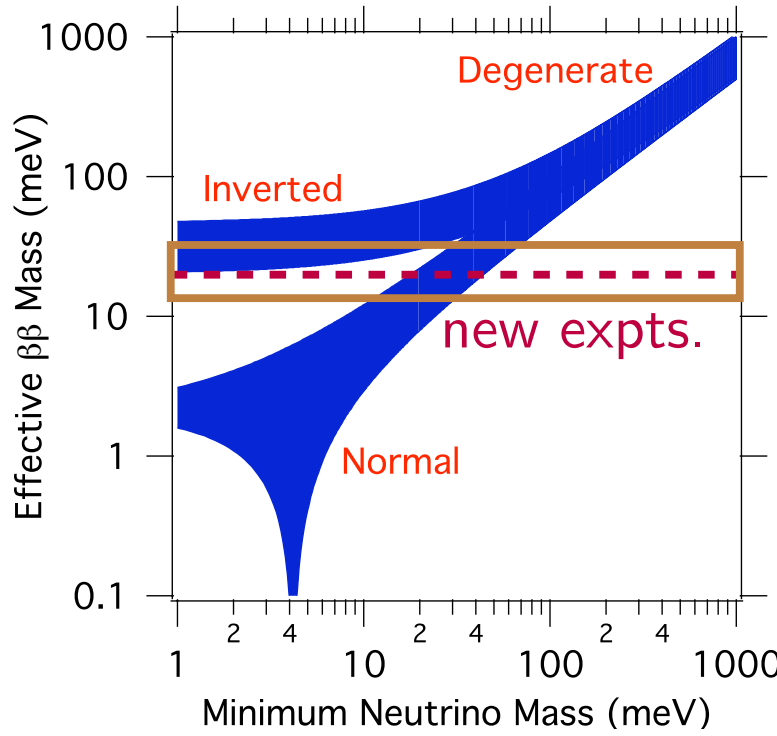


Rate proportional to square of "effective neutrino mass"

$$m_{\text{eff}} \equiv \sum_i m_i U_{ei}^2$$

If lightest neutrino is light:

- $m_{\text{eff}} \approx \sqrt{\Delta m^2_{\text{sol}}} \sin^2 \theta_{\text{sol}}$ (normal)
- $m_{\text{eff}} \approx \sqrt{\Delta m^2_{\text{atm}}} \cos 2\theta_{\text{sol}}$ (inverted)



Calculating the Rate

$$[T^{0\nu}_{1/2}]^{-1} = \sum_{\text{spins}} \int |Z_{0\nu}|^2 \delta(E_{e1} + E_{e2} - Q_{\beta\beta}) \frac{d^3p_1}{2\pi^3} \frac{d^3p_2}{2\pi^3}$$

$Z_{0\nu}$, the decay amplitude, contains lepton part

$$\sum_k \; \overline{e}(x)\gamma_\mu(1-\gamma_5)U_{ek}\phi_k(x) \; \overline{e}(y)\gamma_\nu(1-\gamma_5)U_{ek}\phi_k(y)$$

$$= \; -\sum_k \; \overline{e}(x)\gamma_\mu(1-\gamma_5)U_{ek}\phi_k(x) \; \overline{\phi^c_k}(y)\gamma_\nu(1+\gamma_5)U_{ek}e^c(y) \; ,$$

where ϕ's are Majorana mass eigenstates. After contraction, get 5

$$-\frac{i}{4}\int \sum_k \frac{d^4q}{(2\pi)^4} e^{-iq\cdot(x-y)} \overline{e}(x)\gamma_\mu(1-\gamma_5)\frac{q^\rho\gamma_\rho + m_k}{q^2 - m_k^2}\gamma_\nu(1+\gamma_5)e^c(y) \; U^2_{ek} \; ,$$

The $q^\rho\gamma_\rho$ part vanishes, leaving a factor proportional to

$$m_{\text{eff}} \equiv \textstyle\sum_k m_k U^2_{ek}.$$

Hadronic part

Contains product of weak hadronic currents J_L:

$$\langle f|J_L^\mu(x)J_L^\nu(y)|i\rangle = \sum_n \langle f|J_L^\mu(\vec{x})|n\rangle\langle n|J_L^\nu(\vec{y})|i\rangle e^{-i(E_f-E_n)x_0} e^{-i(E_n-E_i)y_0} \ ,$$

which, after integration over times, gives a factor

$$2\pi\delta(E_f + E_{e1} + E_{e2} - E)\sum_n \left[\frac{\langle f|J_L^\mu(\vec{x})|n\rangle\langle n|J_L^\nu(\vec{y})|i\rangle}{q^0(E_n + q^0 + E_{e2} - E_i)} + \frac{\langle f|J_L^\nu(\vec{x})|n\rangle\langle n|J_L^\mu(\vec{y})|i\rangle}{q^0(E_n + q^0 + E_{e1} - E_i)}\right] ,$$

with the hadronic current given by

$$\langle p|J_L^\mu(x)|p'\rangle = e^{iqx}\overline{u}(p)\Big(g_V(q^2)\gamma^\mu - g_A(q^2)\gamma_5\gamma^\mu - ig_M(q^2)\frac{\sigma^{\mu\nu}}{2m_p}q_\nu + g_P(q^2)\gamma_5 q^\mu\Big)\tau_+ u(p')$$

$$\longrightarrow g_A\delta_{\mu\neq 0}\sigma_\mu\tau_+ + g_V\delta_{\mu 0}\tau_+ + \ldots$$

Simplified Form

Neglecting the induced-pseudoscalar term and momentum dependence in the weak current, and summing over intermediate states in closure (a good approximation) gives

$$M_{0\nu} \approx M_{0\nu}^{GT} - \frac{g_V^2}{g_A^2} M_{0\nu}^{F}$$

with

$$M_{0\nu}^{F} = \langle f | \sum_{a,b} H(r_{ab}, \overline{E}) \tau_a^+ \tau_b^+ | i \rangle$$

$$M_{0\nu}^{GT} = \langle f | \sum_{a,b} H(r_{ab}, \overline{E}) \vec{\sigma}_a \cdot \vec{\sigma}_b \tau_a^+ \tau_b^+ | i \rangle$$

$$H(r, \overline{E}) \approx \frac{2R}{\pi r} \int_0^\infty dq \frac{\sin qr}{q + \overline{E} - (E_i + E_f)/2}$$

Phenomenolgical QRPA

1. Start with pheonomoneological Wood-Saxon potential and G-matrix 2-body interaction.
2. BCS for both nuclei in space containing all single-particle states within 10 or 20 MeV of the Fermi surface.
3. Matrix charge-changing QRPA (in same space) from both nuclei — creates two sets of intermediate states $|n_i\rangle$ and $|n_f\rangle$.
4. Write, e.g.,

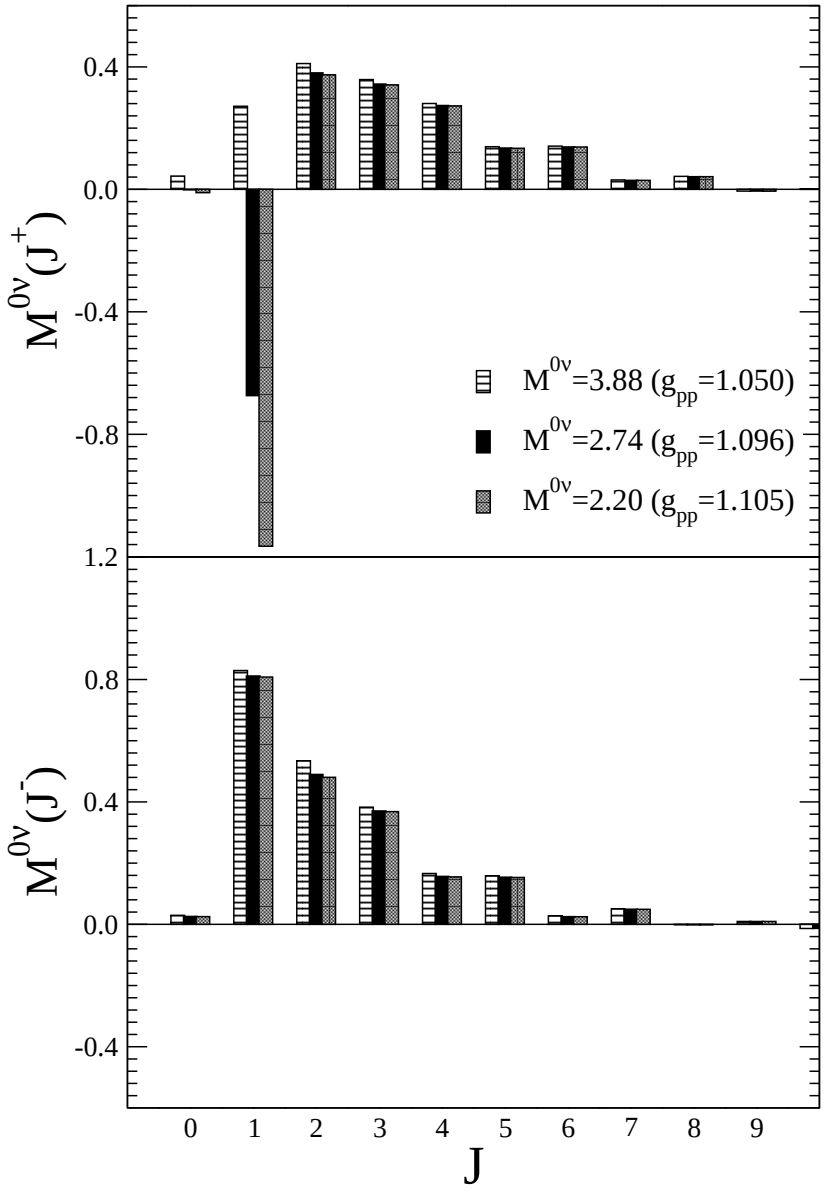
$$\sum_n \frac{\langle f|J_L^\mu(\vec{x})|n\rangle\langle n|J_L^\nu(\vec{y})|i\rangle}{q^0(E_n + q^0 + E_{e2} - E_i)} = \sum_{n_i,n_f} \frac{\langle f|J_L^\mu(\vec{x})|n_f\rangle\langle n_f\,|n_i\rangle\,\langle n_i|\,J_L^\nu(\vec{y})|i\rangle}{q^0(\frac{1}{2}[E_{n_i} + E_{n_f}] + q^0 + E_{e2} - E_i)}$$

5. Use *recipe* for overlap of intermediate states:

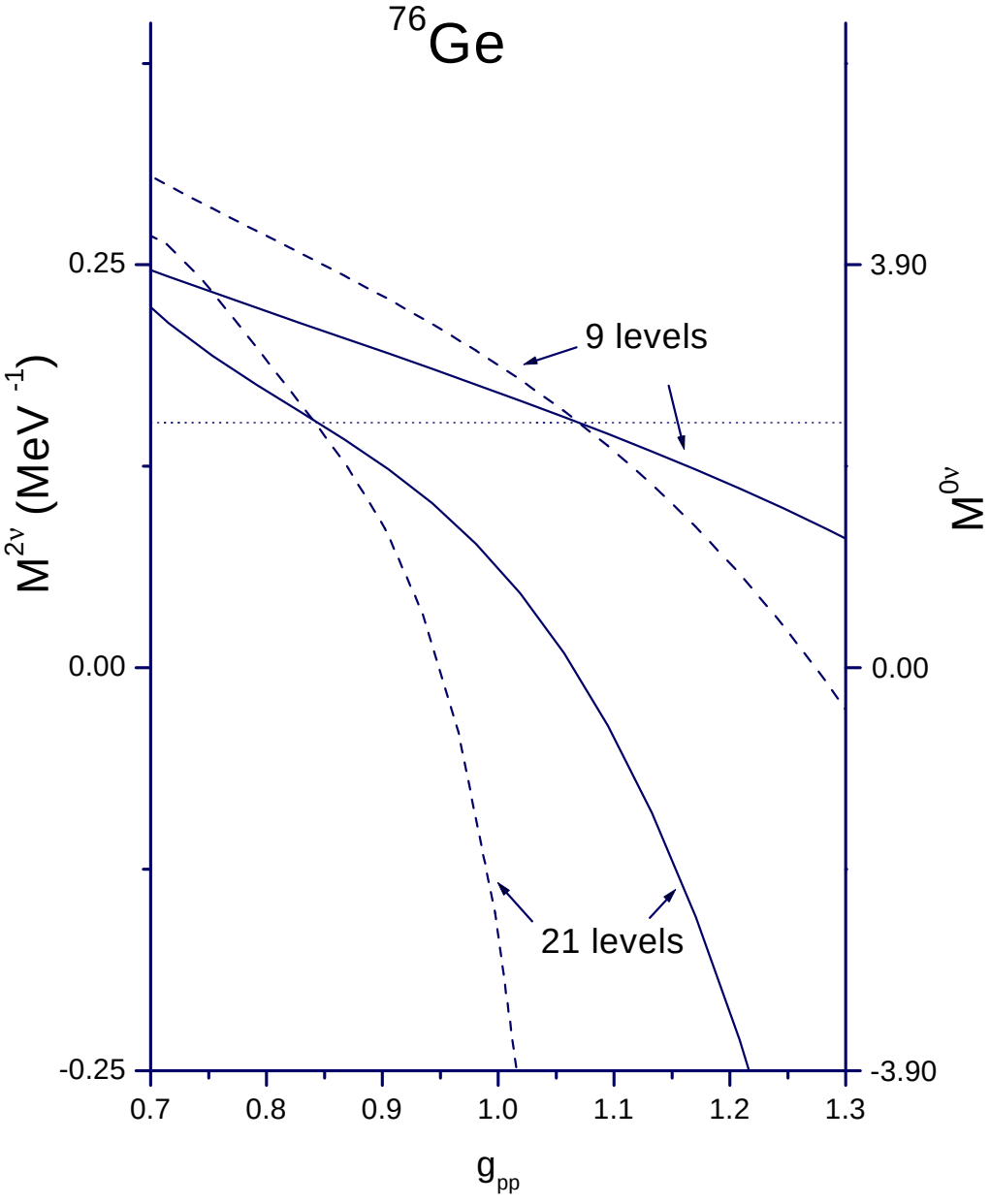
$$\langle n_f|n_i\rangle = \sum_{ab} \left(X_{ab}^{n_f *} X_{ab}^{n_i} - Y_{ab}^{n_f *} Y_{ab}^{n_i}\right)$$

Just like in single-beta decay, result sensitive to $T = 0$ pairing (especially for 2ν decay).

Intermediate-state contributions



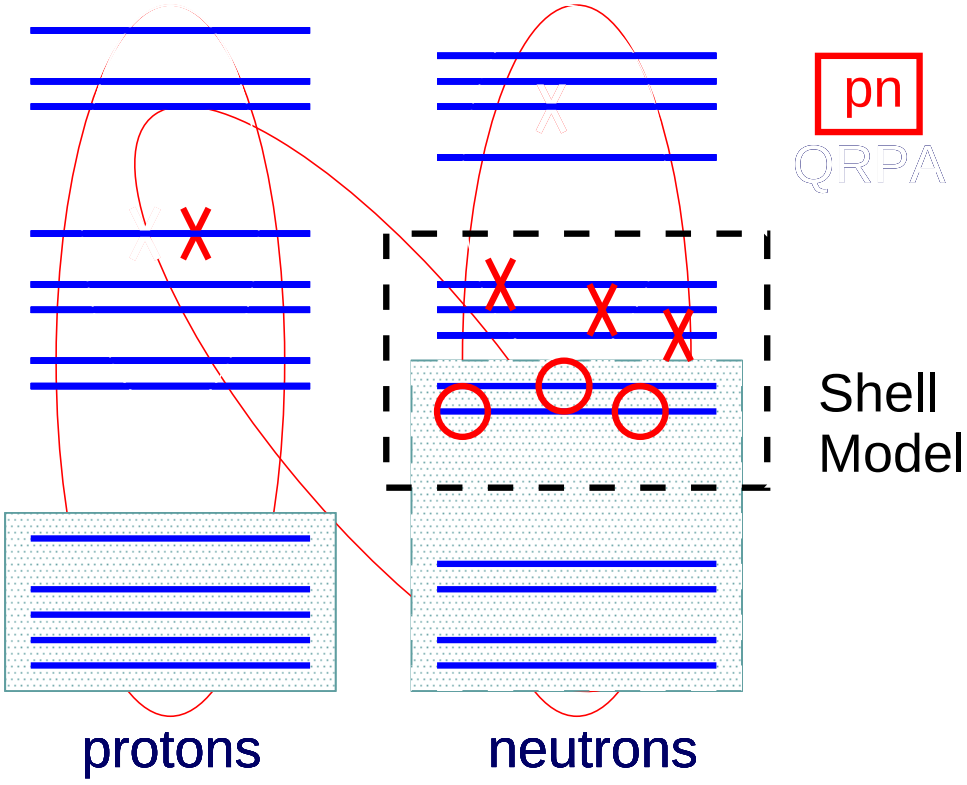
Fiddling with the QRPA



Existing Calculations

Lots done since 1987, most in QRPA, some in shell model.

QRPA vs. Shell Model:



Large single-particle space; simple correlations within it.
Small single-particle space; arbitrarily complex correlations within it.

Shell-Model vs. QRPA Results

Results can differ by factor of 2 or more