Work Plan

Rest of Year 3

- Finish speed-up (and perhaps ADLB implementation) in next month or two
- Examine some drip-line resonances (pygmy and giant)
- Begin (at least) systematics for 2_2^+, 2_3^+ (0_2^+) states.
- Begin (at least) development of charge-changing code

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Year 4

- Apply charge-exchange code to *r*-process β-decay, $\beta\beta$ decay.
- Begin (at least) development of spherical 2nd RPA

Year 5?

- 2nd QRPA?

Charge-Exchange Code

Will be faster

- About half as many 2 quasiparticle states (1 neutron, 1 proton only), i.e. number of matrix elements smaller by 4.
- Fewer terms in Skyrme interaction participate (only np).
- No Coulomb interaction
- No spurious states
- Need only low-multipolarity states, below about 15 MeV.

Plus, straightforward to construct from like-particle code.

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But $\exists$ issues in application...

- Lots of nuclei figure in the r process (incl. odd nuclei)
- Issue of $T = 0$ pairing
- Additional overlap issue for $\beta\beta$ decay.

Time-Dependent DFT

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 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: small $G(t) \longrightarrow \lambda G(t)$ (λ small):

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

and also

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

Now let

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

for some nice f.

Then we have

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

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

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

So, since G is arbitrary, we have

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

Adiabatic approximation

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

if time evolution from ground state is very slow.

Recall exact definition

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

so in adiabatic approximation

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

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

and the equation for the response function becomes

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

i.e., the equation for the RPA response.

Beyond Adiabatic Approximation

Skyrme RPA is 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.

Zero-Frequency Response

Inverse-energy-weighted sum:

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

where $|0_\lambda\rangle$ is the ground state of $\hat{H} + \lambda \hat{G}$.

This holds in RPA if $|0_\lambda\rangle$ is the mean-field ground state. So if KS functional is exact, RPA gives exact sum rule, even though individual energies and transitions are not exact.

Second RPA apparently does not give the same zero-energy response as RPA. Can/should it be fixed?