Effective mass: discussion (1)

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Effective mass: basic ideas

I. Free wave-packet centered around $\vec{k}$ with dispersion relation: $\epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m}$

$\Rightarrow d\epsilon_k/d\vec{k} = \nabla_{\vec{k}}\epsilon_k = \hbar\,\vec{V}_G = \frac{\hbar^2\vec{k}}{m} \Leftrightarrow$ density of states in momentum space $\propto m$

II. Infinite nuclear matter or condensed matter: in medium-effects $\Rightarrow \epsilon_k \neq \frac{\hbar^2 k^2}{2m}$

$\Rightarrow$ Effective mass m_k^* defined by analogy BUT already some ambiguity:

a) Condensed matter: through curvature $\frac{d^2\epsilon_k}{dk^2} = \frac{\hbar^2}{m_k^*}$ / $m_k^* \frac{d\vec{V}_G}{dt} = \vec{F}$

*$0 \leq m_k^* \leq m$ at the bottom of the conduction band

*$-m \leq m_k^* \leq 0$ at the top of the valence band

b) Infinite nuclear matter: through density of states $\frac{d\epsilon_k}{dk} = \frac{\hbar^2 k}{m_k^*}$

$m_k^* \leq m$? depends...

$m^* =$ useful to characterize the propagation of quasi-particles in a medium

III. m_k^* characterizes the non-locality of the single-particle potential

a) Condensed matter: (approximate) Bloch wave: $\Psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}.\vec{r}}\, u_0(\vec{r})$

b) Infinite matter: plane wave $\Psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}.\vec{r}}$

The one-body eigen-equation reads as:

$$-\frac{\hbar^2\nabla^2}{2m}\, e^{i\vec{k}.\vec{r}} + \int d\vec{r}\,'V(\vec{r},\vec{r}\,')\, e^{i\vec{k}.\vec{r}\,'} = \epsilon_k\, e^{i\vec{k}.\vec{r}} \quad \Longrightarrow \quad \frac{\hbar^2 k^2}{2m} + \underbrace{\int d\vec{s}\, V(\vec{s})\, e^{i\vec{k}.\vec{s}}}_{\bar{V}(k)\rightarrow \text{constant if V local}} = \epsilon_k$$

$$\Longrightarrow \quad \frac{1}{m_k^*} = \frac{1}{m} + \frac{1}{\hbar^2 k}\frac{d\bar{V}(k)}{dk} \longrightarrow = \frac{1}{m} \text{ if V is local}$$

Effective mass: Infinite nuclear matter

I. Effective mass is a one-body concept within a many-body system!

*Independent quasi-nucleons: good starting point to describe bulk properties of nuclei

*Beyond that, the residual interaction is crucial to do detailed spectroscopy ...

$\Rightarrow m_k^*$ will depend on the level of approximation

II. Notion of one-body nuclear field can be extended to correlated systems: self-energy $\Sigma(k;\omega)$

*Non-hermitian and energy-dependent potential: $\lim_{\eta\to 0}\Sigma(k;\omega-\imath\eta)\equiv V(k;\omega)+\imath W(k;\omega)$

*Introduced through one-body green-functions: $G_k(k;t-t') - i\langle\phi_0^A|\mathcal{T}[c_k(t)c_k^\dagger(t')]|\phi_0^A\rangle$

$$G_k(k;\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} d\omega e^{-\imath\omega(t-t')}G_k(k;t-t') = \sum_n \frac{\langle\phi_0^A|c_k|\phi_n^{A+1}\rangle\langle\phi_n^{A+1}|c_k^\dagger|\phi_0^A\rangle}{\omega-(E_n^{A+1}-E_0^A)+\imath\eta} + \sum_m \frac{\langle\phi_0^A|c_k^\dagger|\phi_m^{A-1}\rangle\langle\phi_m^{A-1}|c_k}{\omega-(E_0^A-E_m^{A-1})+}$$

$$\equiv \frac{1}{\omega-\hbar^2k^2/2m-\Sigma(k;\omega)}$$

*Poles of $G_k(k;\omega)$ = spectrum in $A=\pm 1$ system = roots of $\epsilon_k = \hbar^2 k^2/2m + \Sigma(k;\epsilon_k)$

*Several roots for one $\vec{k}$ $\Leftrightarrow$ fragmented strength

$\Leftrightarrow$ nucleons do not have a well defined energy in the many-body system

*Hole-line expansion of $\Sigma(k;\omega)$ (BHF, EBHF, collective 1p-2h ...)

*Quasi-particle approximation: keep the largest residue $\Rightarrow$ impose an on-shell dispersion relation ϵ_k

keep ϵ_k such that $G_k(k;\omega) = \frac{S_k}{\omega-\epsilon_k} +$ slowly varying funtion of ω

*"Mean-field" approximation = take spectroscopic factors = 1

II. Definition of the effective mass

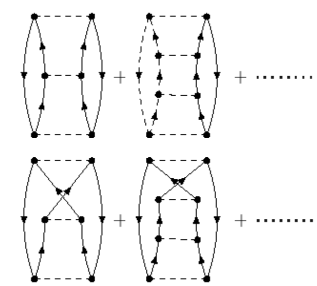
*Originates from non-locality (k-mass) and energy-dependence (e-mass) of $V(k;\omega)$

*Themselves due to finite-range and non-locality of force in space as well as non-locality in time

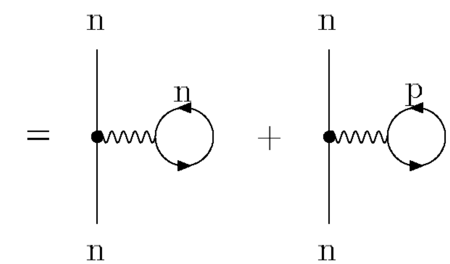
$$\frac{m}{m_k^*} = 1 + \frac{m}{\hbar^2 k}\frac{d\bar{V}(k;\omega)}{dk}\bigg|_{\omega=\epsilon_k} = \underbrace{\left[1 + \frac{m}{\hbar^2 k}\frac{\partial\bar{V}(k;\omega)}{\partial k}\right]}_{1/m_k^{k*}} \underbrace{\left[1 - \frac{\partial\bar{V}(k;\omega)}{\partial\omega}\right]^{-1}}_{m/m_k^{e*}}\Bigg|_{\omega=\epsilon_k}$$

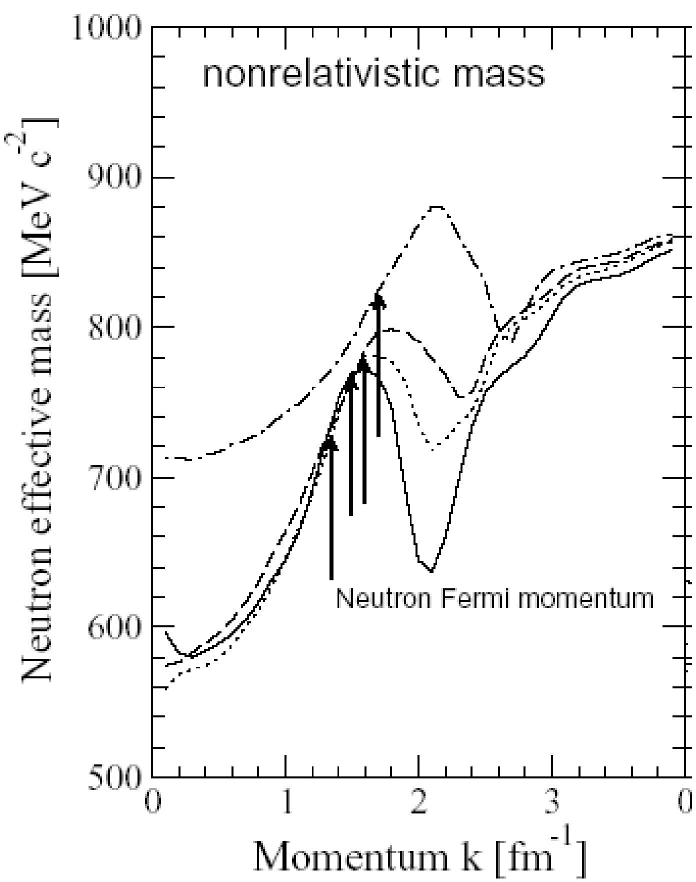
III. Brueckner-Hartree-Fock = "Mean-field" approx

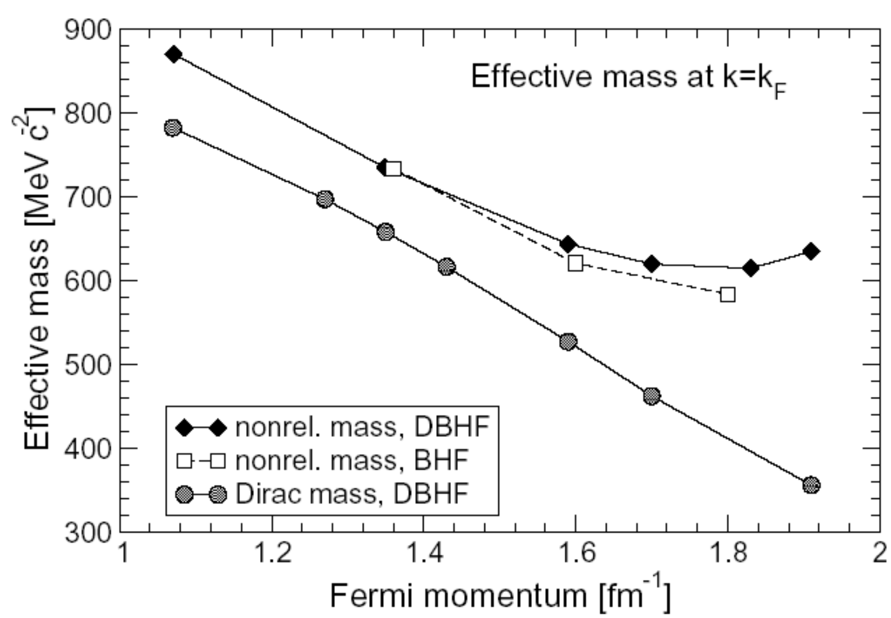
*Effective NN interaction in the medium G resums 2-body correlations



*The self-energy becomes $\Sigma_q^{BHF}(k;\omega) = \sum_{\vec{k}',q' \leq k_F^{q'}} \langle \vec{k}q\vec{k}'q'|G(\omega + \epsilon_{k'}^{q'})|\vec{k}q\vec{k}'q'\rangle_A$







E. van Dalen et al. (2005)

Finite nuclei: self-consistent Skyrme Hartree-Fock calculations

I. Skyrme "effective nucleon-nucleon interaction"

$$
\begin{aligned}
v_{Skyrme}(\vec{R},\vec{r},\overrightarrow{k},\overleftarrow{k'}) \;=\; & t_0\,(1+x_0P_\sigma)\;\delta(\vec{r}) + \frac{1}{6}\,t_3\;(1+x_3P_\sigma)\;\rho^\alpha(\vec{R})\;\delta(\vec{r}) \\
& + \frac{1}{2}\,t_1\;(1+x_1P_\sigma)\;(\delta(\vec{r})\;\overrightarrow{k}^2 + \overleftarrow{k'}^2\;\delta(\vec{r})) \\
& + t_2\;(1+x_2P_\sigma)\;\overleftarrow{k'}.\;\delta(\vec{r})\;\overrightarrow{k} \\
& + iW_0\;(\hat{\vec{\sigma}}_1 + \hat{\vec{\sigma}}_2)\;\overleftarrow{k'}\wedge\;\delta(\vec{r})\;\overrightarrow{k}\quad ,
\end{aligned}
$$

with $\overrightarrow{k} = \hbar(\nabla_1 - \nabla_2)/2i$

*Mimic energy-averaged G-matrix + Density-Matrix-Expansion + 3-body-force $\Rightarrow$ average m_k^{e*}

II. Skyrme-HF functional

$$
\begin{aligned}
\mathcal{E}_{\text{Skyrme}} = \int d\vec{r}\,\Big\{ & \frac{b_0}{2}\rho^2 - \frac{b_0'}{2}\sum_q \rho_q^2 + b_1\left(\rho\tau - \vec{j}^2\right) - b_1'\sum_q\left(\rho_q\tau_q - \vec{j}_q^2\right) - \frac{b_2}{2}\rho\Delta\rho + \frac{b_2'}{2}\sum_q \rho_q\Delta\rho_q \\
& + \frac{b_3}{3}\rho^{\alpha+2} - \frac{b_3'}{3}\rho^\alpha\sum_q \rho_q^2 - b_4\Big[\rho\,\nabla\cdot\vec{J} + \vec{s}\cdot\nabla\times\vec{j} + \sum_q\Big(\rho_q\nabla\cdot\vec{J}_q + \vec{s}_q\cdot\nabla\times\vec{j}_q \\
& - \frac{1}{16}(t_1x_1 + t_2x_2)\left(\vec{J}^2 - 2\,\vec{s}\cdot\vec{\tau}\right) + \frac{1}{16}(t_1 - t_2)\sum_q\left(\vec{J}_q^2 - 2\,\vec{s}_q\cdot\vec{\tau}_q\right)\Big\}\quad ,
\end{aligned}
\tag{1}
$$

III. One-body local densities from the full one-body density matrix $\rho(\vec{r}sq, \vec{r}\,'s'q')$

$$
\begin{aligned}
\rho_q(\vec{r}) &= \rho_q(\vec{r},\vec{r}) = \sum_{k\in q} |\varphi_k(\vec{r})|^2 \\
\tau_q(\vec{r}) &= \nabla\cdot\nabla\,'\rho_q(\vec{r},\vec{r}\,')\Big|_{\vec{r}=\vec{r}\,'} = \sum_{k\in q} |\nabla\varphi_k(\vec{r})|^2 \\
\vec{s}_q(\vec{r}) &= \vec{s}_q(\vec{r},\vec{r}) = \sum_{k\in q} \varphi_k^\dagger(\vec{r})\,\hat{\vec{\sigma}}\,\varphi_k(\vec{r}) \\
\vec{j}_q(\vec{r}) &= -\frac{\imath}{2}(\nabla-\nabla')\rho_q(\vec{r},\vec{r}\,')\Big|_{\vec{r}=\vec{r}\,'} = -\frac{\imath}{2}\sum_{k\in q}\left\{\varphi_k^\dagger(\vec{r})\nabla\varphi_k(\vec{r}) - \left[\nabla\varphi_k^\dagger(\vec{r})\right]\varphi_k(\vec{r})\right\} \\
\vec{J}_q(\vec{r}) &= -\frac{\imath}{2}(\nabla-\nabla')\times\vec{s}_q(\vec{r},\vec{r}\,')\Big|_{\vec{r}=\vec{r}\,'} = -\frac{\imath}{2}\sum_{k\in q}\left\{\varphi_k^\dagger(\vec{r})\nabla\times\hat{\vec{\sigma}}\,\varphi_k(\vec{r}) - \left[\nabla\times\hat{\vec{\sigma}}\,\varphi_k^\dagger(\vec{r})\right]\varphi_k(\vec{r})\right\} \\
\vec{\tau}_q(\vec{r}) &= \nabla\cdot\nabla'\vec{s}_q(\vec{r},\vec{r}\,')\Big|_{\vec{r}=\vec{r}\,'} = \sum_{k\in q}\left[\nabla\varphi_k^\dagger(\vec{r})\right]\cdot\nabla\left[\hat{\vec{\sigma}}\varphi_k(\vec{r})\right] \\
\nabla\cdot\vec{J}_q(\vec{r}) &= -\frac{\imath}{2}\sum_{k\in q}\left\{\left[\nabla\varphi_k^\dagger(\vec{r})\right]\cdot\nabla\times\hat{\vec{\sigma}}\,\varphi_k(\vec{r}) - \left[\nabla\times\hat{\vec{\sigma}}\,\varphi_k^\dagger(\vec{r})\right]\cdot\nabla\varphi_k(\vec{r})\right\}
\end{aligned}
$$

IV. Action of the one-body HF field on φ_{iq}

$$
\begin{aligned}
h^q\,\varphi_{iq}(\vec{r}) &= \frac{\delta\mathcal{E}}{\delta\varphi^\dagger_{iq}(\vec{r})}\,\varphi_{iq}(\vec{r}) = \int d\vec{r}\,'\left\{\frac{\delta\mathcal{E}}{\delta\tau_q(\vec{r}\,')}\,\frac{\delta\tau_q(\vec{r}\,')}{\delta\varphi^\dagger_i(\vec{r})} + \frac{\delta\mathcal{E}}{\delta\rho_q(\vec{r}\,')}\,\frac{\delta\rho_q(\vec{r}\,')}{\delta\varphi^\dagger_{iq}(\vec{r})} + \dots\right\}\varphi_{iq}(\vec{r}\,') \\
&= \left\{-\nabla\cdot\left[\frac{\delta\mathcal{E}}{\delta\tau_q(\vec{r})} + \hat{\vec{\sigma}}\cdot\frac{\delta\mathcal{E}}{\delta\vec{\tau}_q(\vec{r})}\right]\nabla + \frac{\delta\mathcal{E}}{\delta\rho_q(\vec{r})} + \frac{\delta\mathcal{E}}{\delta\vec{s}_q(\vec{r})}\cdot\hat{\vec{\sigma}} - \frac{\imath}{2}\left[\frac{\delta\mathcal{E}}{\delta\vec{J}_q(\vec{r})} - \nabla\frac{\delta\mathcal{E}}{\delta\nabla\cdot\vec{J}_q(\vec{r})}\right]\cdot\nabla\times\hat{\vec{\sigma}}\right. \\
&\quad \left. -\frac{\imath}{2}\nabla\cdot\left(\frac{\delta\mathcal{E}}{\delta\vec{j}_q(\vec{r})} - \frac{\delta\mathcal{E}}{\delta\vec{J}_q(\vec{r})}\times\hat{\vec{\sigma}}\right) - \frac{\imath}{2}\left(\frac{\delta\mathcal{E}}{\delta\vec{j}_q(\vec{r})} + \nabla\frac{\delta\mathcal{E}}{\delta\nabla\cdot\vec{J}_q(\vec{r})}\times\hat{\vec{\sigma}}\right)\cdot\nabla\right\}\varphi_{iq}(\vec{r})
\end{aligned}
$$

*The non-locality of the HF field appears only through gradient terms

*From a finite range/non-local interaction, one would obtain:

$$
h^q\,\varphi_{iq}(\vec{r}) = -\frac{\hbar^2}{2m}\,\triangle\,\varphi_{iq}(\vec{r}) + \int d\vec{r}\,'\,u_1(-\imath\hbar\nabla_{\vec{r}})\,v(\vec{r},\vec{r}\,')\,u_2(-\imath\hbar\nabla_{\vec{r}\,'})\,\varphi_{iq}(\vec{r}\,')
$$

where $u_1(-\imath\hbar\nabla_{\vec{r}})$ and $u_2(-\imath\hbar\nabla_{\vec{r}\,'})$ are functional of the gradient operator.

V. Single-particle spectrum $\{\epsilon_{iq}\}$ for a given nucleus

$\Rightarrow$ solve HF eigen-equation iteratively $\quad h^q\,\varphi_{iq}(\vec{r}) = \epsilon_{iq}\,\varphi_{iq}(\vec{r})$

$\Rightarrow$ Koopmans Theorem: $\epsilon_{iq} = E^{A+1}_{iq} - E^{A}_{0}$

$\rightarrow$ Deformation, polarization effects, pairing effects, density dependence; T. Duguet et al. (2002)

$\rightarrow$ Mean-field level vs experiment: ordering (yes), absolute value (MUST NOT)

$\rightarrow$ Beyond mean-field effects explicitely; M. Bender et al (in the future...)

VI. Effective mass in the Skyrme framework is usually simply defined through the scalar part of:

$$-\nabla\cdot\left[\frac{\hbar^2}{2m^*_{iq}(\vec{r})}\right]\nabla \equiv -\nabla\cdot\left[\frac{\delta\mathcal{E}}{\delta\tau_q(\vec{r})} + \hat{\vec{\sigma}}\cdot\frac{\delta\mathcal{E}}{\delta\vec{\tau}_q(\vec{r})}\right]\nabla \quad\Longrightarrow\quad \frac{m}{m^*_q(\vec{r})} = 1 + \frac{2m}{\hbar^2}\Big(b_1\rho(\vec{r}) - b'_1\rho_q(\vec{r})\Big)$$

*Identical for all s.p. states because expansion in the non-locality limited to second order in $\vec{k}$

*Density dependence has no explicit influence. However, m^*, α and K strongly correlated in INM

*Vector part rarely discussed and never constrained:

$$\frac{\delta\mathcal{E}}{\delta\vec{\tau}_q(\vec{r})} = \frac{1}{8}\,(t_1x_1 + t_2x_2)\,\vec{s}(\vec{r}) - \tfrac{1}{8}\,(t_1 - t_2)\,\vec{s}_q(\vec{r}) \qquad (2)$$

$\rightarrow$ Ok for time-reversal invariant systems (even-even ground-states)

VI. Effective mass at the mean-field level: some facts from phenomenology

*Isoscalar quadrupole resonance in (heavy) doubly magic nuclei (exp vs RPA)

$\rightarrow$ in favor of $m^*/m = 0.7 - 0.8$

$\rightarrow$ consistent with $m^*_{k_F}(\rho_{sat}, 0)$ from (D)BHF in INM before coupling to collective modes

*s.p. spectra in odd neighbors when including particle-vibration coupling; V. Bernard et al (1980)

$\rightarrow m^*/m \geq 1$ around the Fermi surface once particle-vibration coupling = $\nearrow$ due to $\nearrow$ e-mass!

$\rightarrow$ Now close to what experiment requires

*Mass "formulas"

$\rightarrow$ have always been in favor of $m^*/m = 1$ to fit masses of open-shell nuclei

$\rightarrow$ changed lately... due to effect from pairing; S. Goriely et al. (2003)

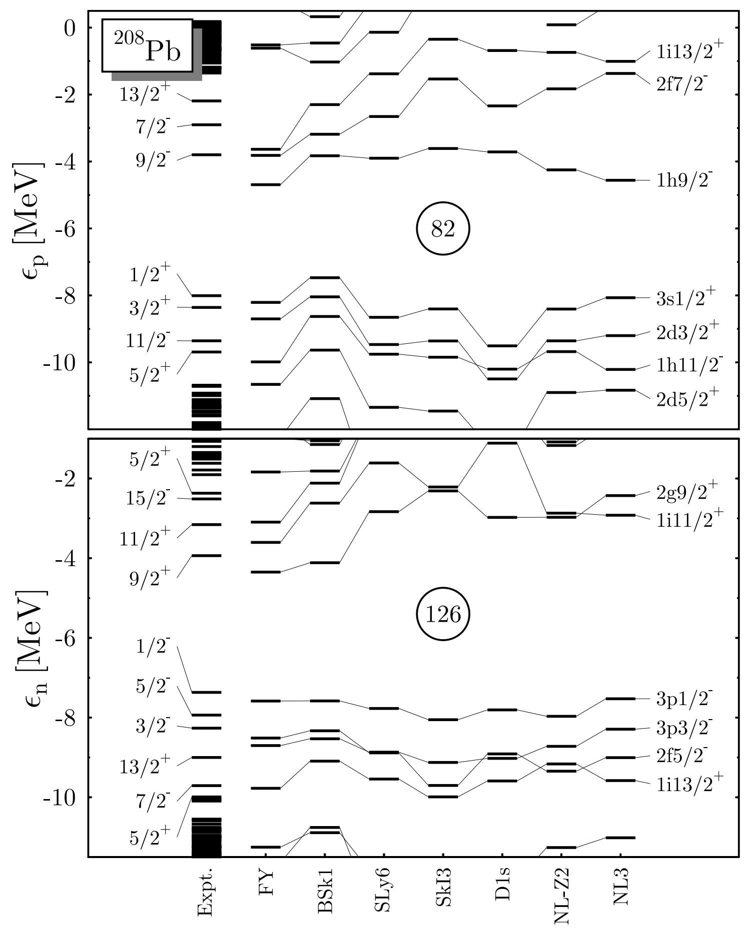
*Skyrme effective mass is independent of k in IM

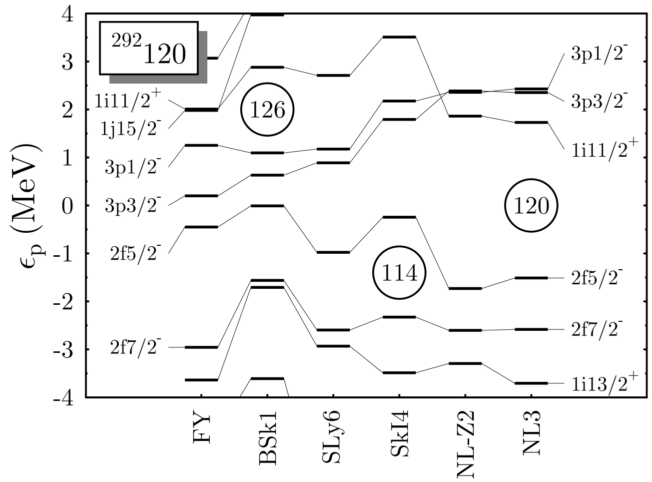
$$\frac{m}{m^*_q}(\rho, \beta) = 1 + \frac{2m}{\hbar^2}(b_1\rho - b'_1\rho_q) \equiv (1 \pm \beta)\,\frac{m}{m^*_s} \mp \beta\,\frac{m}{m^*_v}$$

where $\rho = \rho_n + \rho_p$ and $\beta = (\rho_n - \rho_p)/\rho$

*$m^*_q(\rho_{sat}, 0)$ in INM always part of Skyrme forces fitting procedure

VI. Density of states: parametrisations with $\neq m^*$ in symmetric INM; M. Bender et al. (2003)





*Ordering of levels is correct for all forces. Less true in ^{132}Sn for instance

*In ^{208}Pb, strong correlations between m^* and the size of the magic gaps at the Fermi surface

*However, no clear correlation within hole or particle states

*No clear correlation in superheavy nuclei; mainly due to high-density of states vs spin-orbit.