3rd International Workshop on P(ND)^2-3 (Paris, March 9-13, 2026)

Constraining Direct and Pre-equilibrium Models through Microscopic Approaches

Phys. Rev. C, 112 054607 (2025)

Hirokazu Sasaki[1], Toshihiko Kawano[1], Marc Dupuis[2]

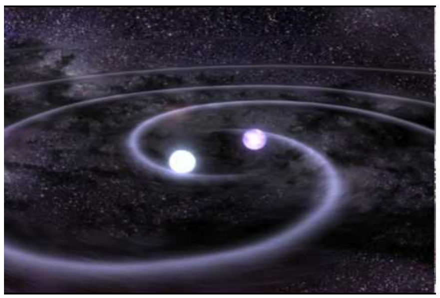
1. Los Alamos National Laboratory
2. CEA, DAM, DIF

Universit ´e Paris-Saclay, CEA, Laboratoire Mati ` ere sous Conditions Extr ˆ emes

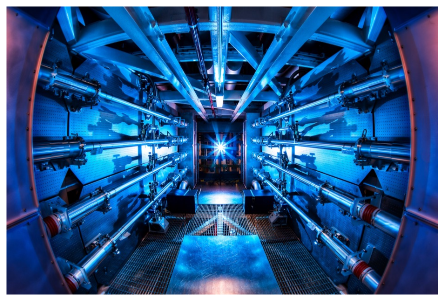
LA-UR-26-21609

Neutron-induced reactions

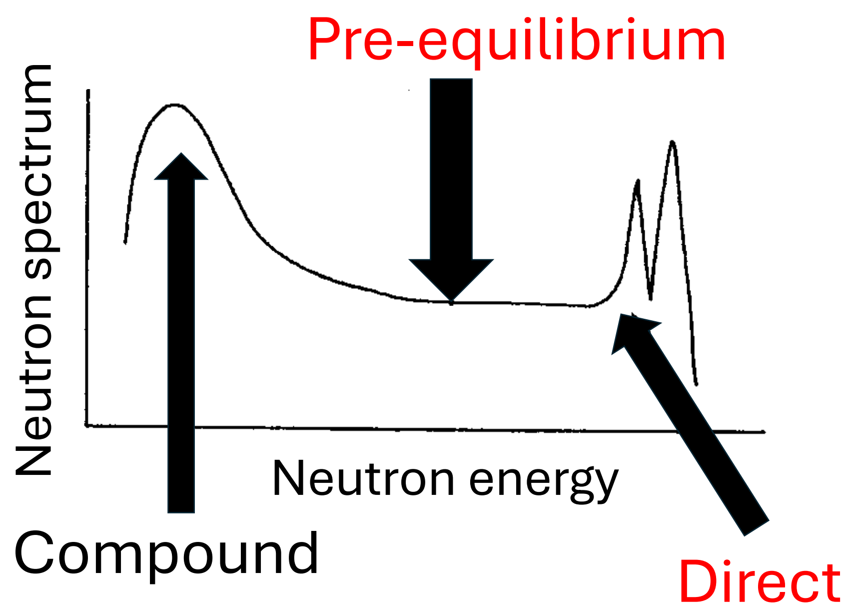
Advanced nuclear reaction theory for neutron-induced reactions is indispensable for producing reliable nuclear data used for both basic science and practical applications



Astrophysics



Nuclear reactors



Neutron spectrum of (n,xn) is characterized by three processes (Compound , Direct, and Pre-equilibrium)

Microscopic approaches incorporating nuclear structure information have predictive capabilities for direct and pre-equilibrium processes

Microscopic approach to derive cross sections

1. Linear response of the time-dependent Hartree Fock (HF) equations

$$(\epsilon_m - \epsilon_i - \omega)X_{mi}(\omega) + \langle\phi_m|\,\delta h(\omega)\,|\phi_i\rangle = -\,\langle\phi_m|\,V_{\rm ext}(\omega)\,|\phi_i\rangle$$

$$(\epsilon_m - \epsilon_i + \omega)Y_{mi}(\omega) + \langle\phi_i|\,\delta h(\omega)\,|\phi_m\rangle = -\,\langle\phi_i|\,V_{\rm ext}(\omega)\,|\phi_m\rangle$$

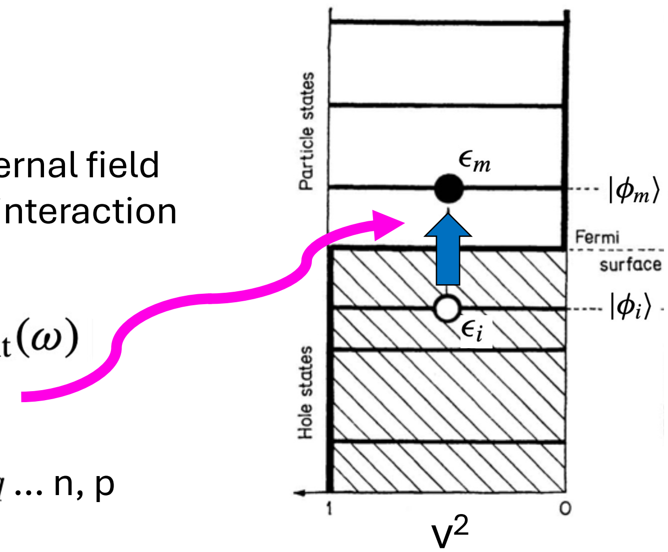
$V_{\rm ext}(\omega)$: Weak external field

$\delta h(\omega)$: Residual interaction

2. Transition strength

$$\frac{dB(E;V_{\rm ext})}{dE} = -\frac{1}{\pi}{\rm Im}\sum_{q}\sum_{m,i\in q}\left(f^{q*}_{mi}X^{q}_{mi} + f^{q*}_{im}Y^{q}_{mi}\right)$$

$V_{\rm ext}(\omega)$



$$f^{q}_{mi} = \int d^3r\,\phi^{q*}_{m}V_{\rm ext}\phi^{q}_{i} \qquad q \ldots \text{n, p}$$

3. Cross sections

- Giant dipole resonance:

$$\sigma_{\rm abs}(E;{\rm E1}) = \frac{16\pi^3}{9\hbar c}E\sum_{K=0,\pm1}\frac{dB(E;D_K)}{dE}$$

External field

$$V_{\rm ext}(\omega) = D_K = \sum_{i=1}^{A} e^{(i)}_{\rm eff}r_iY_{1K}(\theta_i,\varphi_i)$$

- Neutron-induced inelastic scattering:

$$\frac{{\rm d}^2\sigma}{{\rm d}E_x{\rm d}\Omega_\alpha} = \frac{\mu_\alpha\mu_\beta}{(2\pi\hbar^2)^2}\frac{k_\alpha}{k_\beta}\frac{1}{2}\sum_{\Sigma_\alpha\Sigma_\beta}\sum_{J\Pi M}\frac{{\rm d}B(\omega;F^{M}_{\rm inl}(J^{\Pi}))}{{\rm d}E_x}$$

$$V_{\rm ext}(\omega) = \sum_{JM\Pi}F^{M}_{\rm inl}(J^{\Pi})$$

= Nuclear force between the projectile neutron and nucleons inside the target

Finite amplitude method (FAM)

FAM is an effective calculation method to solve the linear response

$$\omega|X_i(\omega)\rangle = (h_0 - \epsilon_i)|X_i(\omega)\rangle + \hat{Q}\{V_{\mathrm{ext}}(\omega) + \delta h(\omega)\}|\phi_i\rangle$$

$$\omega\langle Y_i(\omega)| = -\langle Y_i(\omega)|(h_0 - \epsilon_i) - \langle\phi_i|\{V_{\mathrm{ext}}(\omega) + \delta h(\omega)\}\hat{Q}$$

η : Small parameter

$|\psi_i\rangle$ $\langle\psi_i'|$ Feedback

$$\langle\psi_i'| = \langle\phi_i| + \eta\langle Y_i(\omega)|$$

$$|\psi_i\rangle = |\phi_i\rangle + \eta|X_i(\omega)\rangle$$

$$\delta h(\omega) = \frac{1}{\eta}(h[\langle\psi'|, |\psi\rangle] - h[\langle\phi|, |\phi\rangle])$$

T. Nakatsukasa et al., PRC76, 024318(2007)

Application

- Photoabsorptions

M. Kortelainen et al., PRC92, 051302(R)(2015),
T. Oishi et al., PRC93, 034329(2016),
T. Li, N. Schunck, and M. Grosskopf, PRC110, 034317(2024)

- β decays

E.M. Ney et al., PRC102, 034326(2020),
N. Hinohara and J. Engel, PRC105, 044314(2022)

- Nuclear level density

A. Bjekčić and N. Schunck,
Comp. Phys. Comm. 306 (2025) 109387

- Spontaneous fission

K. Washiyama et al., PRC103, 014306(2021)

RPA and QRPA equations derived from noniterative FAM

Linear response equations for FAM

$$(\epsilon_m - \epsilon_i - \omega)X_{mi}(\omega) + \langle\phi_m|\,\delta h(\omega)\,|\phi_i\rangle = -\langle\phi_m|\,V_{\mathrm{ext}}(\omega)\,|\phi_i\rangle$$

$$(\epsilon_m - \epsilon_i + \omega)Y_{mi}(\omega) + \langle\phi_i|\,\delta h(\omega)\,|\phi_m\rangle = -\langle\phi_i|\,V_{\mathrm{ext}}(\omega)\,|\phi_m\rangle$$

Explicit linearization

$$\lim_{\eta\to 0}\delta h = \sum_{q'}\sum_{nj\in q'} X^{q'}_{nj}\left.\frac{\partial h}{\partial(\eta X^{q'}_{nj})}\right|_{\eta=0} + \sum_{q'}\sum_{nj\in q'} Y^{q'}_{nj}\left.\frac{\partial h}{\partial(\eta Y^{q'}_{nj})}\right|_{\eta=0}.$$

- Avoid the iteration in conventional FAM
- Rederive the RPA and QRPA equations

RPA equation

$$\left\{\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right\}\begin{pmatrix} X^{q'}_{nj} \\ Y^{q'}_{nj} \end{pmatrix} = -\begin{pmatrix} f^q_{mi} \\ f^q_{im} \end{pmatrix}$$

$$A^{q,q'}_{mi,nj} = (\epsilon_m - \epsilon_i)\delta_{mn}\delta_{ij} + \int d^3r\,\phi^{q*}_m\left(\frac{\partial h_q}{\partial(\eta X^{q'}_{nj})}\right)_{\eta=0}\phi^q_i$$

$$B^{q,q'}_{mi,nj} = \int d^3r\,\phi^{q*}_m\left(\frac{\partial h_q}{\partial(\eta Y^{q'}_{nj})}\right)_{\eta=0}\phi^q_i$$

$$f^q_{mi} = \int d^3r\,\phi^{q*}_m V_{\mathrm{ext}}\phi^q_i$$

H. Sasaki, T. Kawano and I. Stetcu, PRC105, 044311(2022)

QRPA equation (HF+BCS)

$$\begin{pmatrix} A-\omega & B \\ B^* & A^*+\omega \end{pmatrix}\begin{pmatrix} X^{q'}_{\alpha\beta} \\ Y^{q'}_{\alpha\beta} \end{pmatrix} = -\zeta^{\tau}_{\mu\nu}\begin{pmatrix} f^q_{\mu\nu} \\ f^q_{\nu\mu} \end{pmatrix}$$

$$A^{q,q'}_{\mu\nu,\alpha\beta} = (E_\mu + E_\nu)\delta_{\mu\alpha}\delta_{\nu\beta} + \zeta^+_{\mu\nu}\zeta^+_{\alpha\beta}\int \mathrm{d}^3r\,\phi^{q*}_\mu\left.\frac{\partial h^{\mathrm{even}}_q}{\partial(\eta\zeta^+_{\alpha\beta}X^{q'}_{\alpha\beta})}\right|_{\eta=0}\phi^q_\nu + \zeta^-_{\mu\nu}\zeta^-_{\alpha\beta}\int \mathrm{d}^3r\,\phi^{q*}_\mu\left.\frac{\partial h^{\mathrm{odd}}_q}{\partial(\eta\zeta^-_{\alpha\beta}X^{q'}_{\alpha\beta})}\right|_{\eta=0}\phi^q_\nu,$$

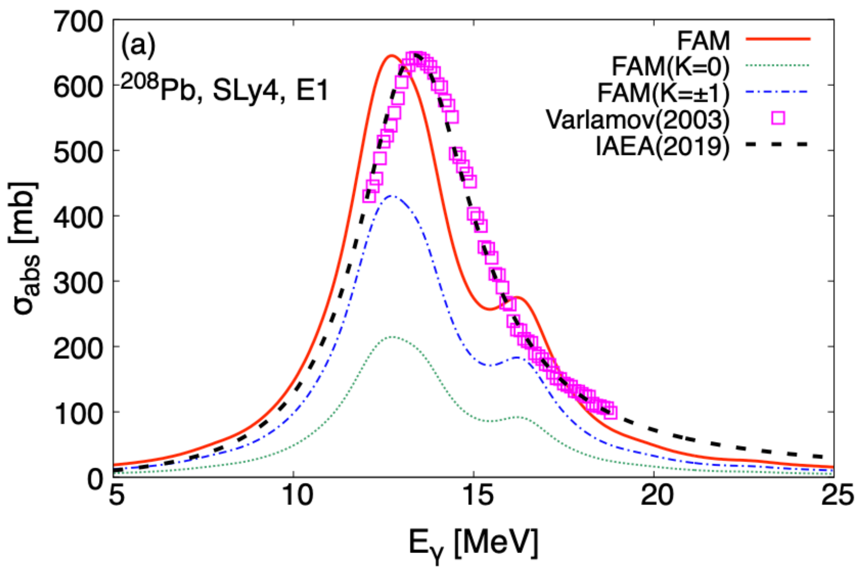
$$B^{q,q'}_{\mu\nu,\alpha\beta} = \zeta^+_{\mu\nu}\zeta^+_{\alpha\beta}\int \mathrm{d}^3r\,\phi^{q*}_\mu\left.\frac{\partial h^{\mathrm{even}}_q}{\partial(\eta\zeta^+_{\alpha\beta}Y^{q'}_{\alpha\beta})}\right|_{\eta=0}\phi^q_\nu + \zeta^-_{\mu\nu}\zeta^-_{\alpha\beta}\int \mathrm{d}^3r\,\phi^{q*}_\mu\left.\frac{\partial h^{\mathrm{odd}}_q}{\partial(\eta\zeta^-_{\alpha\beta}Y^{q'}_{\alpha\beta})}\right|_{\eta=0}\phi^q_\nu,$$

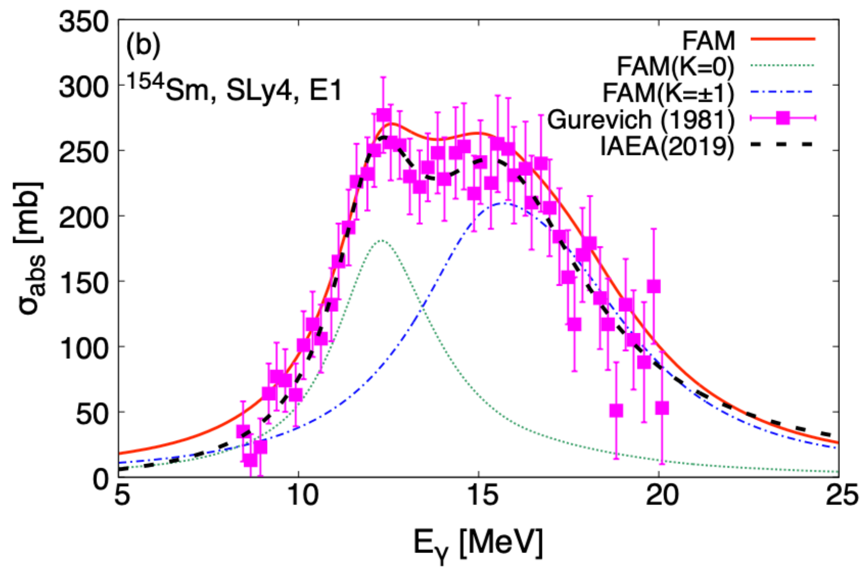
$$\zeta^{\tau}_{\mu\nu} = u_\mu v_\nu + \tau u_\nu v_\mu \quad \text{with} \quad \tau = \pm 1$$

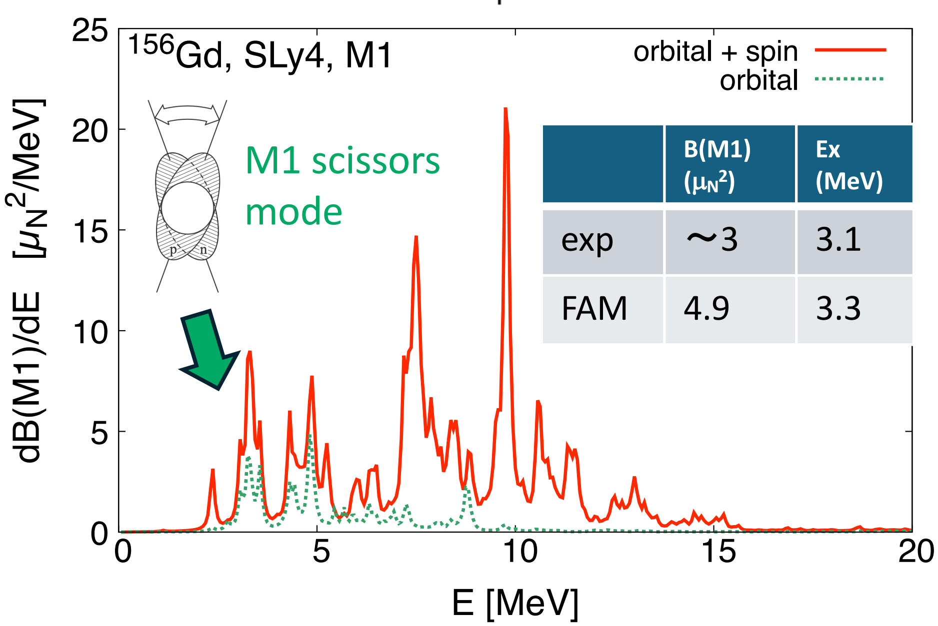
H. Sasaki, T. Kawano, and I. Stetcu, PRC107, 054312(2023)

Noniterative FAM for giant resonances (E1,M1)

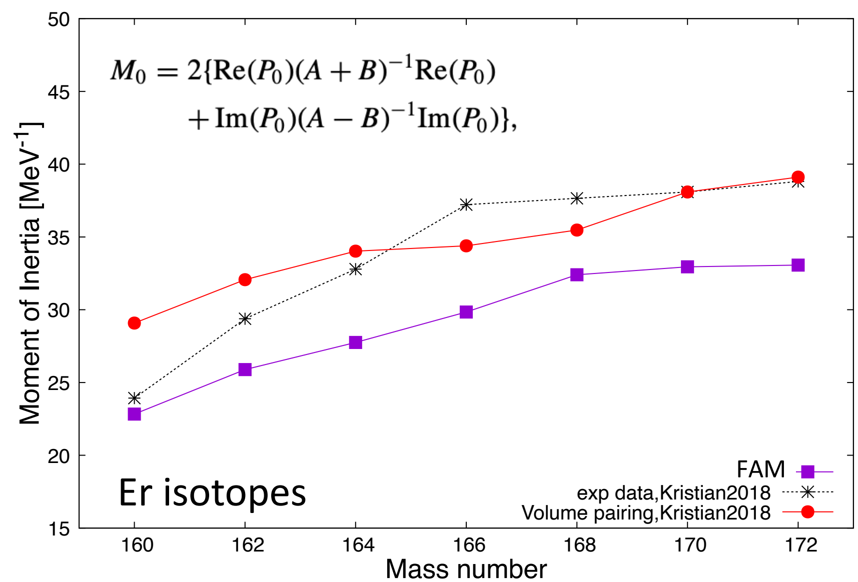
H. Sasaki, T. Kawano, and I. Stetcu, PRC105, 044311(2022)
H. Sasaki, T. Kawano, and I. Stetcu, PRC107, 054312(2023)







	B(M1) (μ_N^2)	Ex (MeV)
exp	～3	3.1
FAM	4.9	3.3



External field for the neutron-induced inelastic scattering

The QRPA equation used for giant resonance calculations are also applicable for the neutron-induced inelastic scattering by replacing the external field

QRPA equation

$$\begin{pmatrix} A-\omega & B \\ B^* & A^*+\omega \end{pmatrix} \begin{pmatrix} X^{q'}_{\alpha\beta} \\ Y^{q'}_{\alpha\beta} \end{pmatrix} = -\zeta^{\tau}_{\mu\nu} \begin{pmatrix} f^{q}_{\mu\nu} \\ f^{q}_{\nu\mu} \end{pmatrix}$$

Matrix components of external field

$$f^q_{mi} = \int d^3r\, \phi^{q*}_m V_{\rm ext} \phi^q_i$$

q ... n, p

The external field is calculated from the distorted-wave Born approximation (DWBA)

External field

$$V_{\rm ext}(\omega) = \int \mathrm{d}^3 r_2 \chi^{(-)*}_{\alpha} v_{12}(r_{12})(1 - P_r P_\sigma P_\tau)\chi^{(+)}_{\beta}$$

Index1 … nucleons inside the target

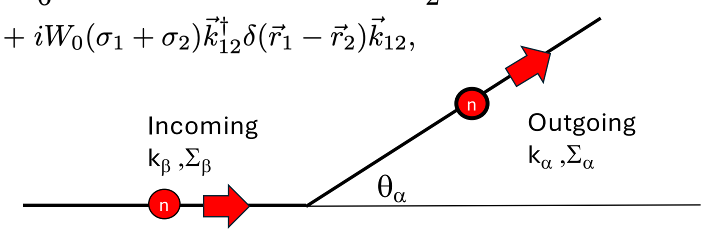
Index2 … projectile or scattered neutrons

$\chi^{(+)}_{\Sigma_\beta}$ … Incoming neutron distorted wave

$\chi^{(-)}_{\Sigma_\alpha}$ … Outgoing neutron distorted wave

Nuclear force (Skyrme force)

$$\begin{aligned} v_{12} = {} & t_0(1+x_0P_\sigma)\delta(\vec{r}_1-\vec{r}_2) \\ & + \frac{1}{2}t_1(1+x_1P_\sigma)[\vec{k}^{\dagger 2}_{12}\delta(\vec{r}_1-\vec{r}_2)+\delta(\vec{r}_1-\vec{r}_2)\vec{k}^{2}_{12}] \\ & + t_2(1+x_2P_\sigma)\vec{k}^{\dagger}_{12}\delta(\vec{r}_1-\vec{r}_2)\vec{k}_{12} \\ & + \frac{1}{6}t_3(1+x_3P_\sigma)\delta(\vec{r}_1-\vec{r}_2)\rho^\alpha(\frac{\vec{r}_1+\vec{r}_2}{2}) \\ & + iW_0(\sigma_1+\sigma_2)\vec{k}^{\dagger}_{12}\delta(\vec{r}_1-\vec{r}_2)\vec{k}_{12}, \end{aligned}$$



We employ the Skyrme force (SLy4) for the nuclear force between the incoming neutron and nucleons inside the target. This Skyrme force (SLy4) is also used for calculations of QRPA matrices

Multipole expansion in the external field

External field for the neutron scattering

$$f^q_{\mu\nu} = (b_0 - \delta_{nq} b'_0) \int \mathrm{d}^3 r \; \phi^{q*}_\mu \phi^q_\nu \chi^{(-)*}_\alpha \chi^{(+)}_\beta + \left(b_1 - \delta_{nq} b'_1\right) \int \mathrm{d}^3 r \; \left(\phi^{q*}_\mu \phi^q_\nu \nabla \chi^{(-)*}_\alpha \cdot \nabla \chi^{(+)}_\beta + \chi^{(-)*}_\alpha \chi^{(+)}_\beta \nabla \phi^{q*}_\mu \cdot \nabla \phi^q_\nu\right)$$

$$- (b_2 - \delta_{nq} b'_2) \int \mathrm{d}^3 r \; \nabla^2 \left(\phi^{q*}_\mu \phi^q_\nu\right) \chi^{(-)*}_\alpha \chi^{(+)}_\beta + c_\alpha (b_3 - \delta_{nq} b'_3) \int \mathrm{d}^3 r \; \frac{2}{3} (\rho_0)^\alpha \phi^{q*}_\mu \phi^q_\nu \chi^{(-)*}_\alpha \chi^{(+)}_\beta$$

$$- (b_4 + \delta_{nq} b'_4) \int \mathrm{d}^3 r \; \{\phi^{q*}_\mu \phi^q_\nu \nabla \chi^{(-)*}_\alpha \cdot (-i)(\nabla \times \vec{\sigma}) \chi^{(+)}_\beta + \chi^{(-)*}_\alpha \chi^{(+)}_\beta \nabla \phi^{q*}_\mu \cdot (-i)(\nabla \times \vec{\sigma}) \phi^q_\nu\}$$

$$- 2(b_1 - \delta_{nq} b'_1) \int \mathrm{d}^3 r \left\{ \frac{1}{2i} \left(\phi^{q*}_\mu \nabla \phi^q_\nu - \phi^q_\nu \nabla \phi^{q*}_\mu\right) \cdot \frac{1}{2i} \left(\chi^{(-)*}_\alpha \nabla \chi^{(+)}_\beta - \chi^{(+)}_\beta \nabla \chi^{(-)*}_\alpha\right) \right\}$$

$+ \ldots.$

Multipole expansion

Natural parity transition ($J = 0^+, 1^-, 2^+, ..$)

$$\chi^{(-)*}_\alpha \chi^{(+)}_\beta = \sum_{LM} \lambda^0_{LM}(r) Y_{LM}(\theta, \phi),$$

$$\lambda^0_{LM}(r) = \int \mathrm{d}\Omega Y^*_{LM}(\theta, \phi) \chi^{(-)*}_\alpha \chi^{(+)}_\beta$$

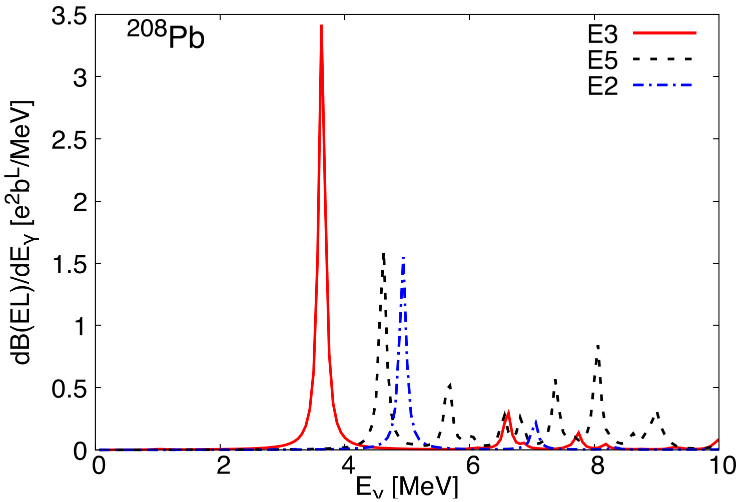
Unnatural parity transition ($J = 1^+, 2^-, ..$)

$$\chi^{(-)*}_\alpha \vec{\sigma} \chi^{(+)}_\beta \equiv \sum_{LM} Y_{LM}(\theta, \phi) \left\{ \frac{\vec{e}_x - i\vec{e}_y}{2} \lambda^+_{LM}(r) + \frac{\vec{e}_x + i\vec{e}_y}{2} \lambda^-_{LM}(r) + \vec{e}_z \lambda^z_{LM}(r) \right\},$$

$$\lambda^{m_s}_{LM}(r) = \int \mathrm{d}\Omega Y^*_{LM}(\theta, \phi) \chi^{(-)*}_\alpha \sigma_{m_s} \chi^{(+)}_\beta \quad (m_s = \pm, z)$$

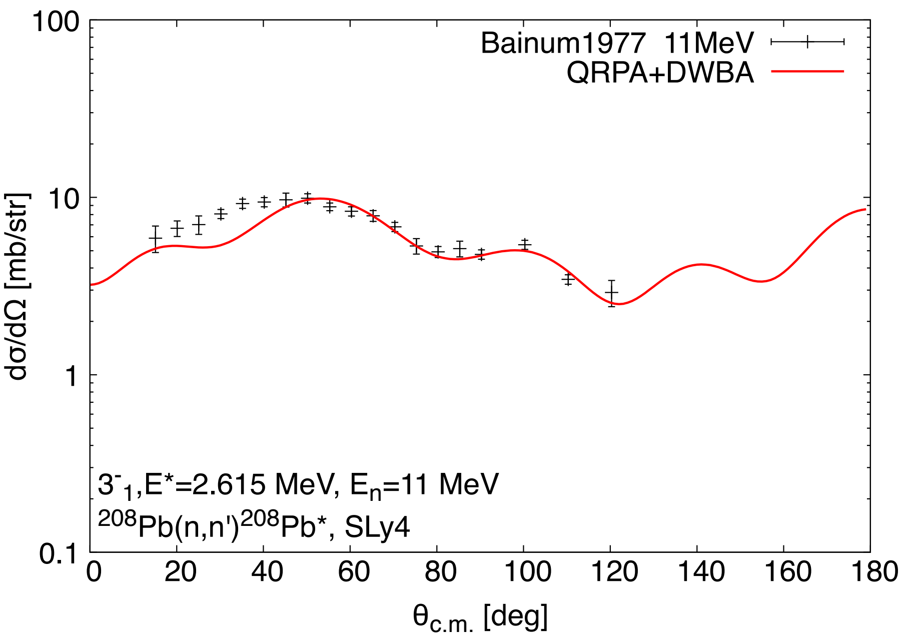
This expansion is used to calculate differential cross sections for excitations to low-lying discrete levels

Strength function and the differential cross section



H. Sasaki, T. Kawano, and M. Dupuis, PRC112, 054607(2025)

Level	$B_{\rm exp}(EL)$	$B_{\rm QRPA}(EL)$	$E_{\rm exp}$	$E_{\rm QRPA}$
3_1^-	0.611	0.656	2.615	3.625
5_1^-	0.0447	0.0415	3.198	4.625
2_1^+	0.318	0.298	4.086	4.938

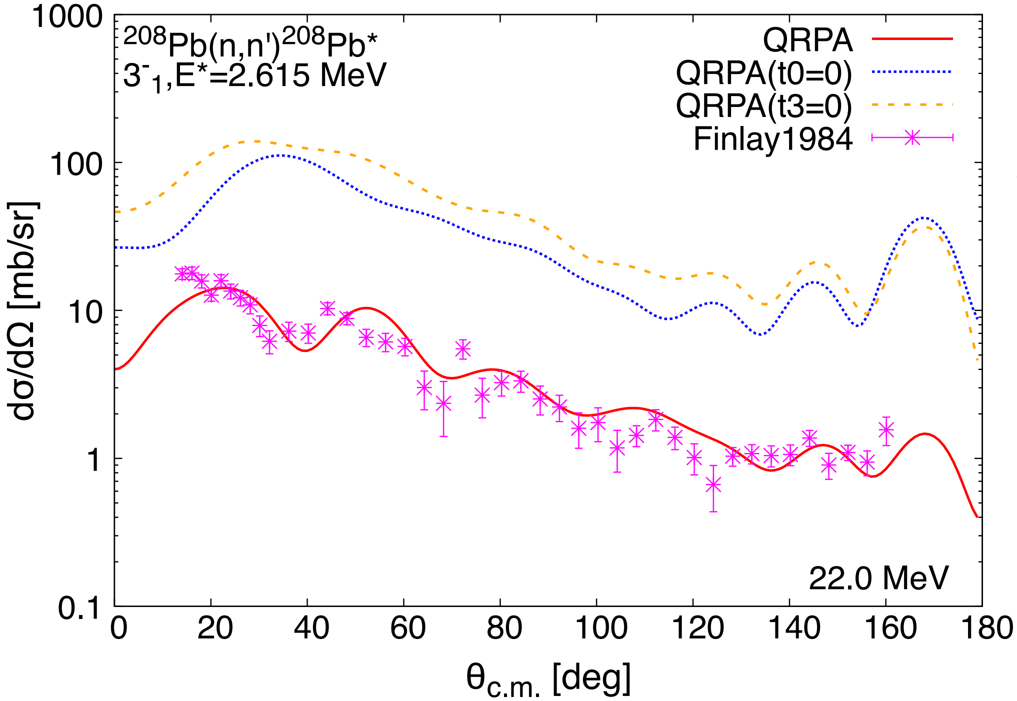


Differential cross section for the discrete level excitation

$$\frac{d\sigma}{d\Omega_\alpha} = \frac{\mu_\alpha \mu_\beta}{(2\pi\hbar^2)^2} \frac{k_\alpha}{k_\beta} \frac{1}{2} \sum_{\Sigma_\alpha \Sigma_\beta M} \int_{E_x-\Delta}^{E_x+\Delta} dE'_x \frac{dB\left(\omega; F_{\rm inl}^M(J^\Pi)\right)}{dE'_x}$$

Energy integration is carried out around the resonance of the discrete level

Contribution from two- and three-body Skyrme forces



Skyrme force for the neutron scattering

$$
\begin{aligned}
v_{12} &= t_0(1+x_0P_\sigma)\delta(\vec{r}_1-\vec{r}_2) \\
&+ \frac{1}{2}t_1(1+x_1P_\sigma)[\vec{k}^{\dagger 2}_{12}\delta(\vec{r}_1-\vec{r}_2)+\delta(\vec{r}_1-\vec{r}_2)\vec{k}^2_{12}] \\
&+ t_2(1+x_2P_\sigma)\vec{k}^{\dagger}_{12}\delta(\vec{r}_1-\vec{r}_2)\vec{k}_{12} \\
&+ \frac{1}{6}t_3(1+x_3P_\sigma)\delta(\vec{r}_1-\vec{r}_2)\rho^\alpha(\frac{\vec{r}_1+\vec{r}_2}{2})\ c_\alpha \\
&+ iW_0(\sigma_1+\sigma_2)\vec{k}^{\dagger}_{12}\delta(\vec{r}_1-\vec{r}_2)\vec{k}_{12},
\end{aligned}
$$

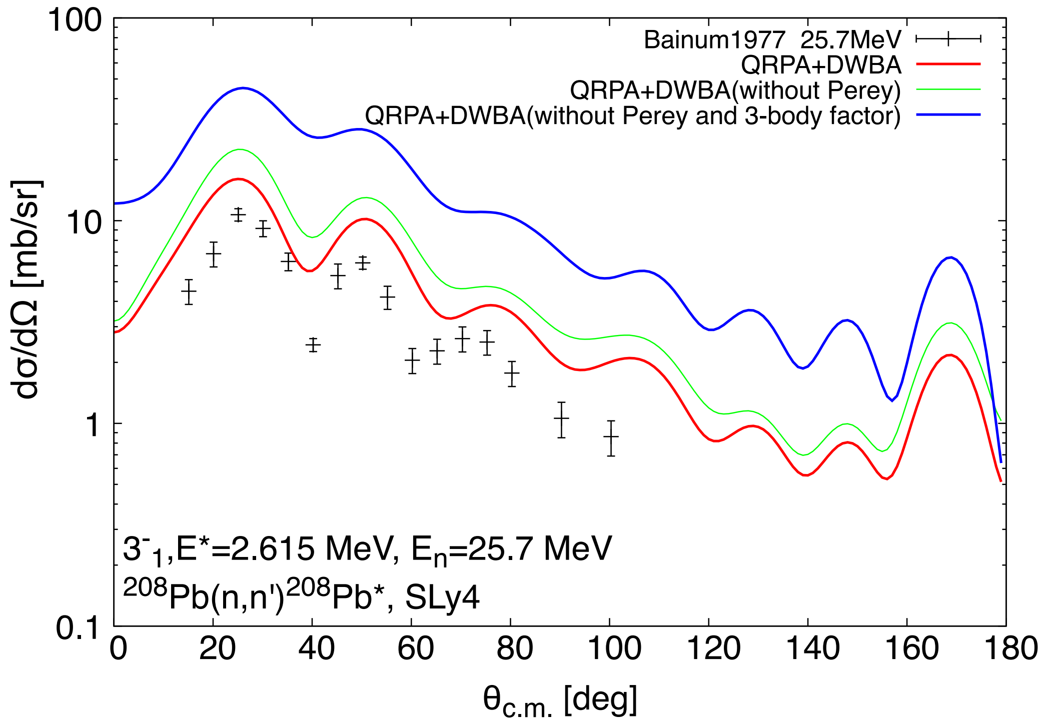
Two-body

Three-body

The QRPA result is more consistent with experimental data when both two- and three-body contributions are included

This cancellation between the two– and three-body forces was found in a previous study (K. T. R. Davies and G. R. Satchler, Nucl. Phys. A 222, 13 (1974))

Three-body factor and nonlocal Perey effect



We multiply a factor c_α by the three-body terms in the Skyrme force for the neutron scattering

$$c_\alpha = \frac{(\alpha+2)(\alpha+1)}{2}$$

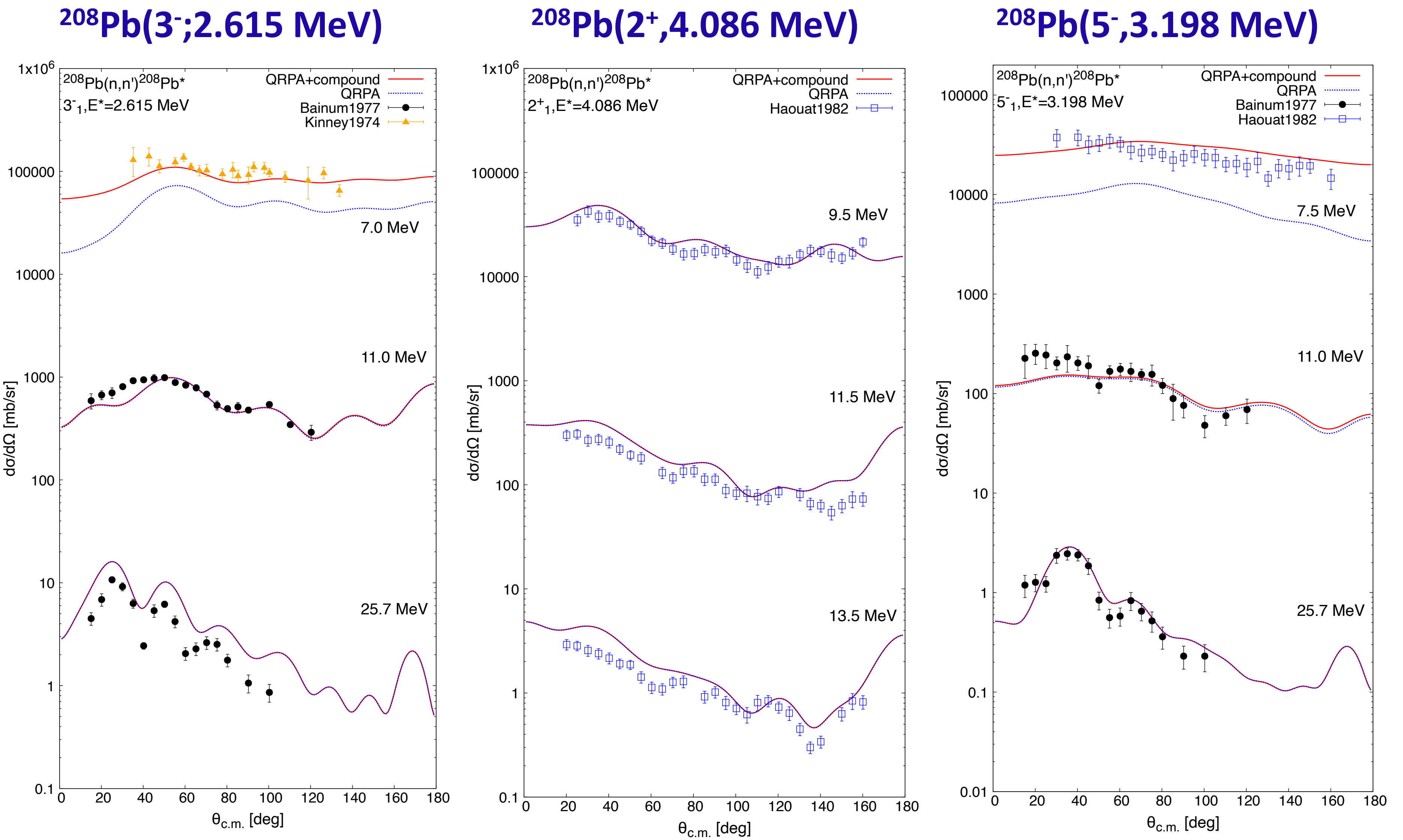
R. Sharp and L. Zamick, Nucl. Phys. A 208, 130 (1973)

K. T. R. Davies and G. R. Satchler, Nucl. Phys. A 222, 13 (1974)

We also consider the nonlocal Perey effect (β=0.85) on the distorted waves

The QRPA result is more consistent with experimental data when both three-body factor and nonlocal Perey effect are taken into account

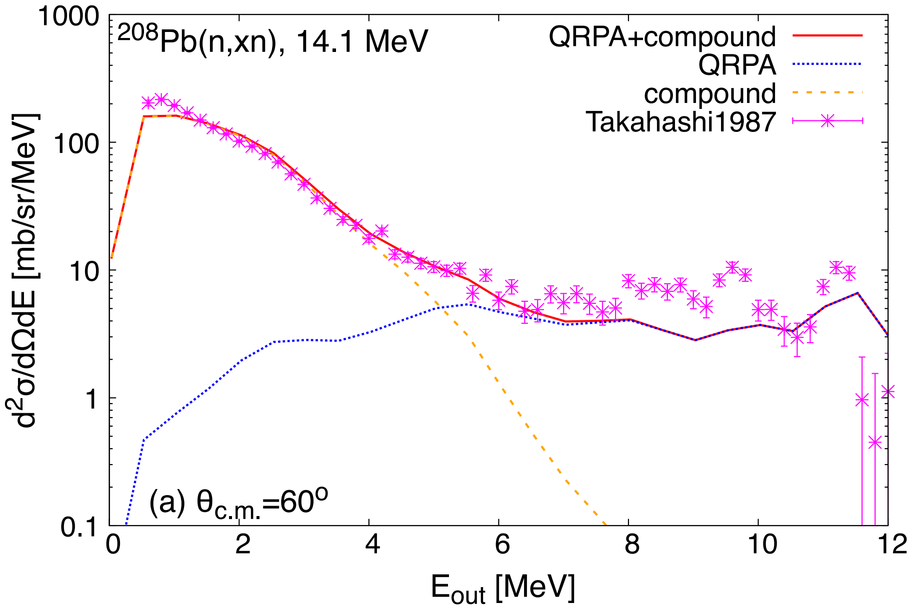
Results of excitations to the low-lying states in ^{208}Pb

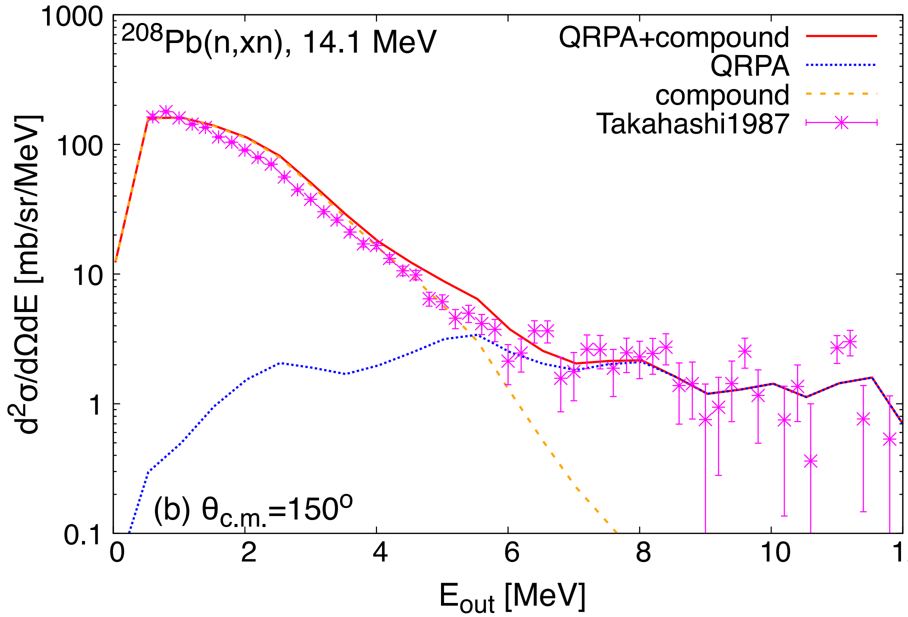


QRPA result can reproduce the shape and strength of the differential cross sections

Results of excitations to continuum states

H. Sasaki, T. Kawano, and M. Dupuis, PRC112, 054607(2025)



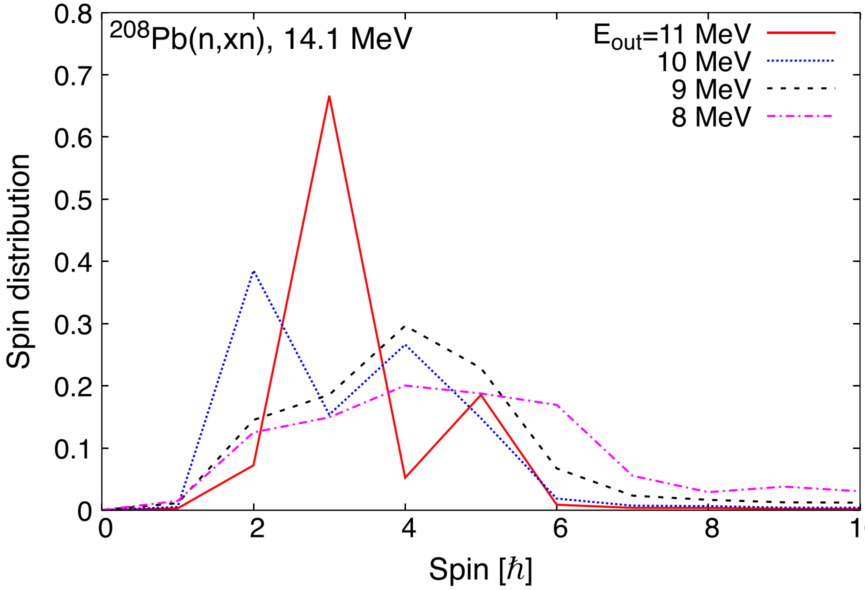


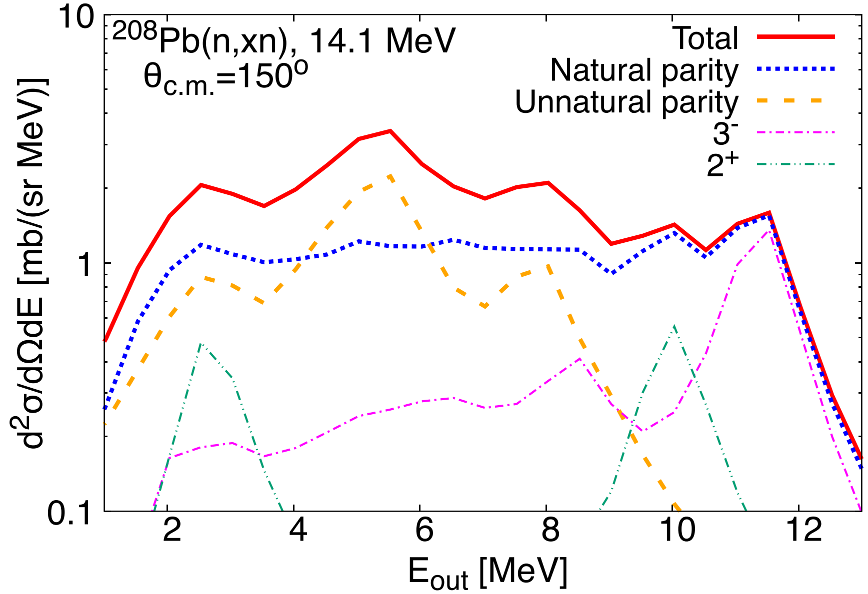
The QRPA result incorporates both contributions from direct and pre-equilibrium processes in a consistent manner

Compoud process is calculated from Coupled-Channels and Hauser-Feshbach Code CoH_3

The QRPA result is more consistent with experimental data in backward direction

Spin distributions of the residual nucleus





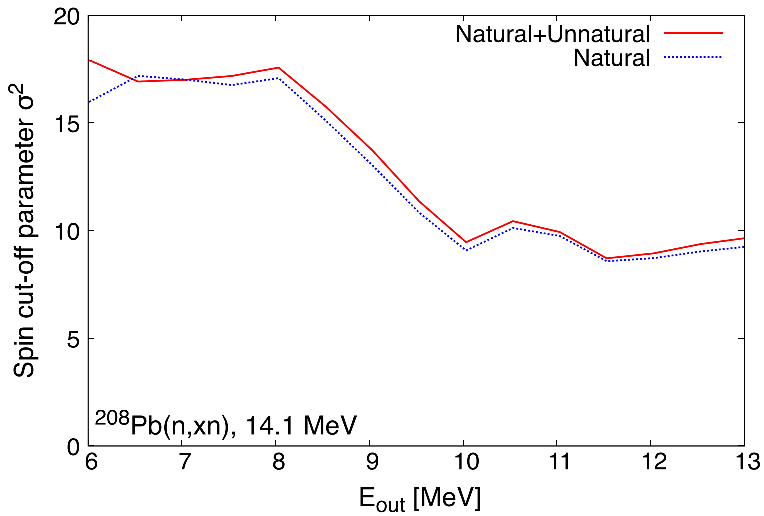
Spin distribution

$$R(E_\alpha, E_x, J) = \frac{\sum_{\Sigma_\alpha \Sigma_\beta M \Pi} \int \mathrm{d}\Omega_\alpha \frac{\mathrm{d}B(\omega; F_{\mathrm{inl}}^M(J^\Pi))}{\mathrm{d}E_x}}{\sum_J \sum_{\Sigma_\alpha \Sigma_\beta M \Pi} \int \mathrm{d}\Omega_\alpha \frac{\mathrm{d}B(\omega; F_{\mathrm{inl}}^M(J^\Pi))}{\mathrm{d}E_x}}$$

The spin distribution reflects the partial contribution from each J^P in the double differential cross section

Spin cutoff parameters

QRPA+DWBA

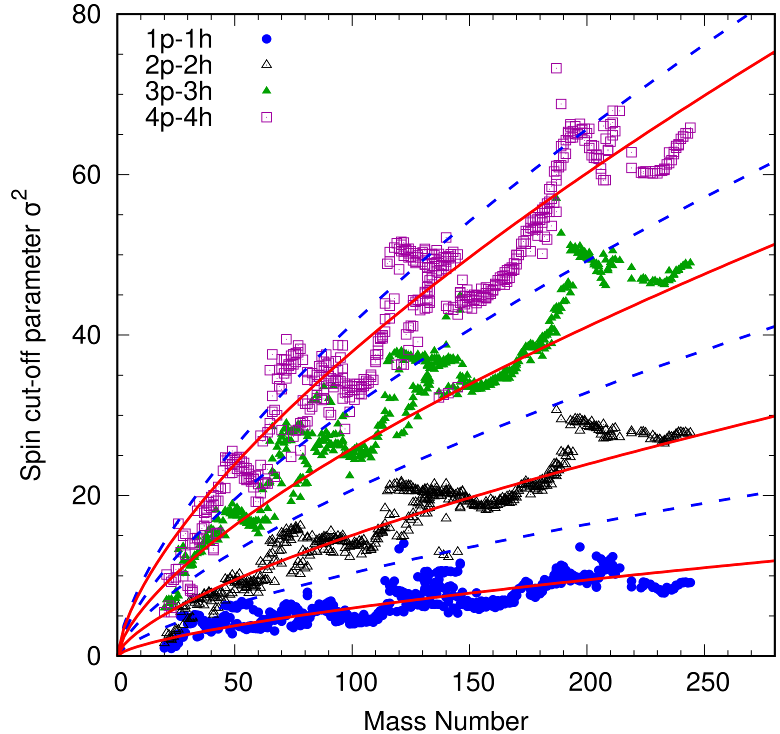


Fitting with analytical Gaussian formula

$$R(J) = \frac{2J+1}{2\sigma^2} \exp\left\{-\frac{(J+\frac{1}{2})^2}{2\sigma^2}\right\},$$

Spin cutoff parameter

Combinatorial calculation with FRDM



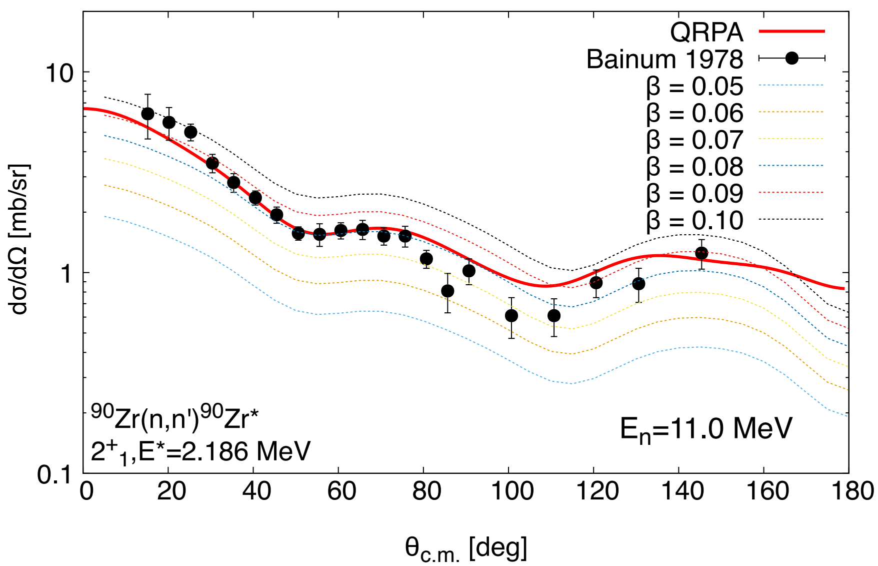
Dashed line: $\sigma^2(n) = 0.24nA^{2/3}$

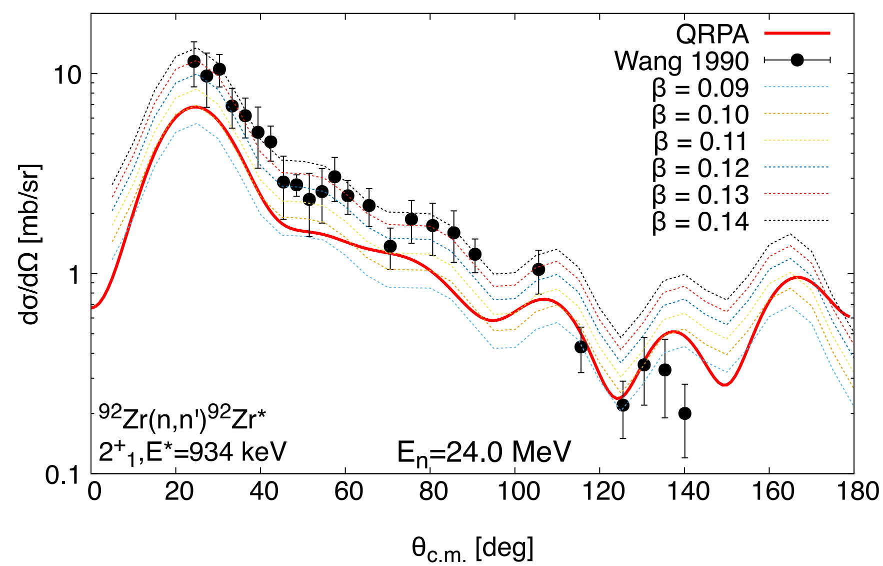
Solid line: $\sigma^2(n) = 0.11(n^2A)^{2/3}$

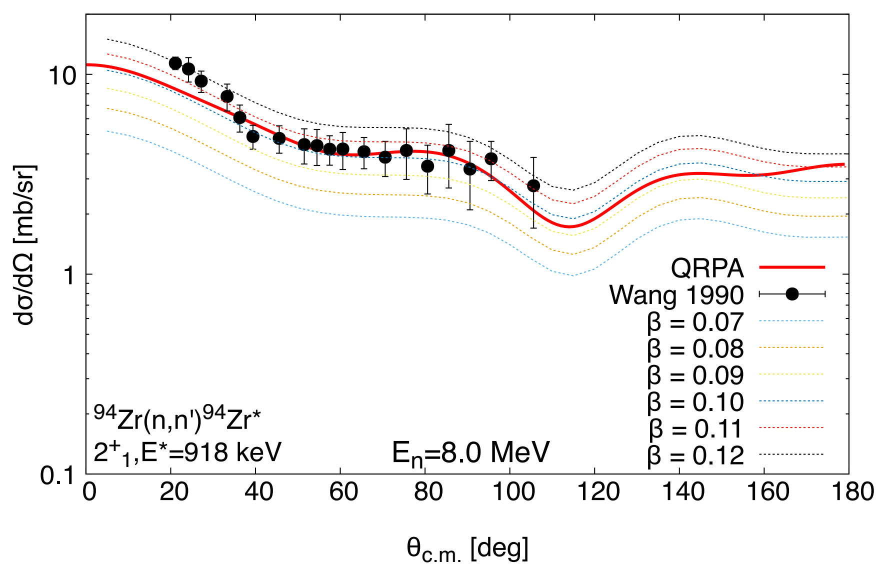
n … The number of particle-hole

The value for QRPA+DWBA is similar to the value of the solid line for 1p-1h, $\sigma^2(2)$=0.973

Zr isotopes







The QRPA model works well for ^{90,92,94}Zr

The deformation parameter β fitted to QRPA results will be transferred to Zr data evaluation

The QRPA model can predict the deformation parameter for nucleus whose experimental data are missing (e.g. ^{88}Zr)

Conclusion

・ We develop a calculation method for direct and pre-equilibrium processes in neutron-induced reactions based on noniterative FAM/QRPA and DWBA

・ We reproduce the shape and strength of differential cross sections for excitations to low-lying states of ^{208}Pb without fitting of deformation parameters for vibrations

・ The calculated double differential cross-section to the continuum state also agrees with the experimental data in the energy region relevant to the direct and pre-equilibrium processes

・ The calculated double differential cross-section are used to investigate the spin distribution of the populated states in the residual nucleus

Future Perspectives

・Application of microscopic calculation framework to nuclear data evaluation

・Unifying both nuclear structure and reaction frameworks

・Challenge to nuclear structure calculations for odd nuclei and the application to reaction calculations (e.g. Y (Z=39), Tl (Z=81))