LA-UR-16-26905

Advances in nuclear reaction calculations by incorporating information from nuclear mean-field theories

T. Kawano

Theoretical Division, Nuclear Physics
Los Alamos National Laboratory

ND2016, Bruges, Belgium, 9/12 – 16, 2016

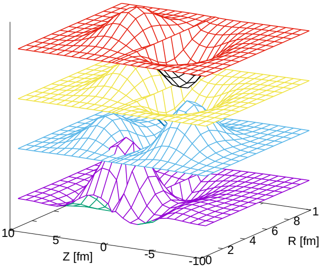
Introduction

Cross section calculations in the keV to a few tens MeV range with the Hauser-Feshbach codes

- Optical and statistical Hauser-Feshbach models with width fluctuation and pre-equilibrium emission play a central role.
- Many phenomenological or empirical treatments of model parameters are involved,
  - level densities, optical potential, strength functions, pre-equilibrium parameters, fission barriers
  - They are often provided in a tabulated form, such as RIPL
- When a mean-field theory is combined with the HF code, we will be able to access nuclear structure information directly.

Mean-field Output as Reaction Calculation Input

By solving Schrödiner equation for one-body potential, we will have



- Single particle energy spectrum
  - level density calculation
- Single particle wave-functions and occupation probabilities
  - direct reaction to the bound states
  - DWBA
  - quantum mechanical pre-equilibrium process
- where, the residual interaction plays an important role

$$H' = \frac{1}{2} \sum \mathcal{V}_{\alpha\beta\gamma\delta} c^{\dagger}_{\alpha} c^{\dagger}_{\beta} c_{\delta} c_{\gamma}$$

Objectives

- Incorporate (reasonably fast) mean-field theories into the Hauser-Feshbach calculations for better prediction of experimentally unknown reaction cross sections.
- The mean-field theories considered here are:
  - Microscopic-macroscopic approach by Möller et al.
  - Hartree-Fock BCS
- Combining nuclear reaction and structure leads to the shell model approach to the nuclear reaction

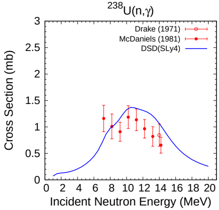
Example: S.P States for Reaction Calculations

Direct/Semidirect Capture Amplitudes

$$T_d \propto \sqrt{S_{ljK}} \langle R_{ljK}(r) | r | \chi^{(+)}_{LJ}(r) \rangle$$

$$T_s \propto \sqrt{S_{ljK}} \langle R_{ljK}(r) | h(r) | \chi^{(+)}(r) \rangle$$

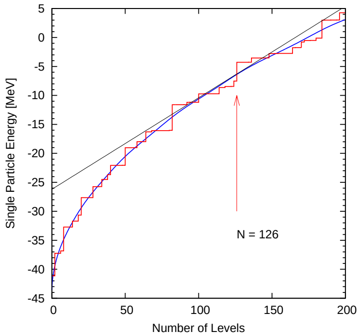
where the spectroscopic factor S_{ljK} can be related with $v^2 = 1 - u^2$



Bonneau, TK, et al. PRC **75**, 054618 (2007)

Strutinsky Method for S.P. State Density

^{208}Pb single-particle levels



$$\omega = \frac{g^n (E - A_{ph})^{n-1}}{p!h!(n-1)!}$$

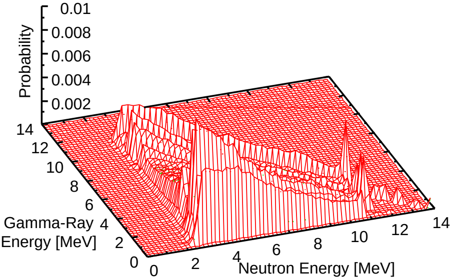
g is given by the tangent at E_F

LANL Coupled-Channels Hauser-Feshbach Code, CoH_3

Hauser-Feshbach-Moldauer theory for Compound Nuclear Reaction

- 44,000 lines C++ code,

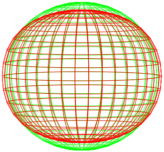
  including very modest comment lines
- rotational and vibrational excitation with the coupled-channels theory
- compound nucleus decay by a deterministic method or Monte Calro technique
  - MC allows to study particle and photon correlation
- Engelbrecht-Weidenmüller transformation for compound reaction with direct channels



TK et al., J. Nucl. Sci. Technol., **47**, 462 (2010)

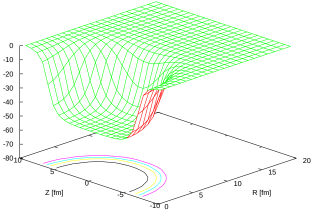
TK et al., Phys. Rev. C **94**, 014612 (2016)

Mean-Field Models Added to CoH_3

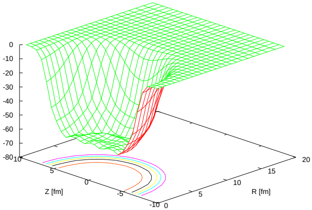


^{197}Au

- FRDM95 Finite-Range Droplet Model
- HF-BCS Skyrme Hartree-Fock BCS Model
  - clone of L. Bonneau's HF-BCS code
  - rewritten in C++ from scratch
- Two models share the Hamiltonian diagonalization part



FRDM



HF-BCS

Folded-Yukawa Potential for Independent Particle Model

- Axially-symmetric potentials in HF-BCS and FRDM yield comparable single-particle wave-functions
- We prefer FRDM because
  - calculation is very fast,
  - optimized potential shape parameters by Möller et al. available,
  - better prediction for single particle energies in general, and
  - we are Los Alamos!

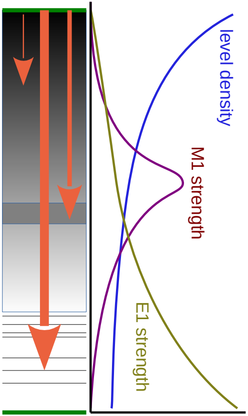
We solve the Schrödinger equation for

$$V = V_1 + V_{\mathrm{s.o}} + V_{\mathrm{Coul}}$$

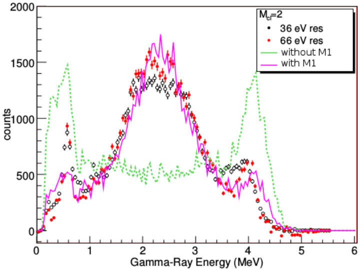
where the central part is calculated in terms of the folded Yukawa potential

$$V_1(\mathbf{r}) = -\frac{V_0}{4\pi a^3} \int \frac{\exp(-|\mathbf{r} - \mathbf{r}'|/a)}{|\mathbf{r} - \mathbf{r}'|/a} d^3 r'$$

Level Density Beyond Gilbert-Cameron



DANCE γ-ray spectrum for multiplicity two



- an additional strength in the low energy region needed
- we assume this is an M1 scissors mode

J. Ullmann, TK, et al. PRC **89**, 034603 (2014)

Different multipolarity of strength functions yields additional sensitivities to spin and parity distributions in the final states.

Realistic spin and parity distribution crucial.

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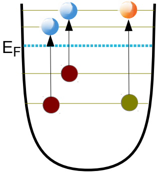
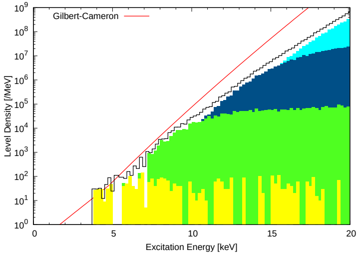
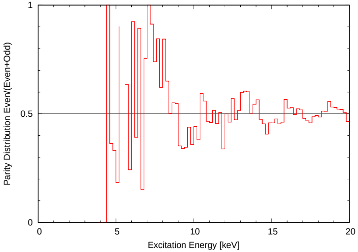
Combinatorial Level Density on Single Particle Spectrum

- Microscopic level density by counting particle-hole configurations yields spin and parity distributions
- By creating the single-particle spectrum, calculation of the combinatorial level density is very fast







However, such calculation does not include particle-hole interactions.

Random Matrix Approach to Level Density

Approximation to shell model level density based on the random matrix theory

Z. Pluhař, H. A. Weidenmüller, Phys. Rev. C **36**, 1046 (1988).

Sato, Takahashi, Yoshida, Z. Phys. A, **339**, 129 (1991).

TK, Yoshida, Phys. Rev. C, **63**, 024603 (2001).

- Hamiltonian for the nuclear system $H = H_0 + V$
  - H_0 independent particle model

$$(H_0 - \epsilon_{m\mu})|m\mu\rangle = 0$$

  - $\rho_m^{(0)J\pi}$ unperturbed state density, or combinatorial level density

$$\rho_m^{(0)J\pi}(E) = \sum_\mu \delta(E - \epsilon_{m\mu})$$

  - V residual interaction, is assumed to form a Gaussian Orthogonal Ensemble, and calculate second moment $\mathcal{M}_{mn}$

Second Moments of Residual Interaction

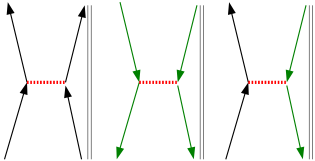
We assume the delta interaction for calculating matrix elements

$$\langle \alpha\beta | V | \gamma\delta \rangle_a = \frac{V_0}{4\pi} \int \phi_\alpha(r)\phi_\beta(r)\phi_\gamma(r)\phi_\delta(r) \frac{1}{r^2} dr$$

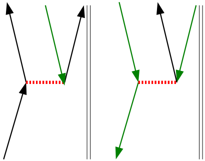
Convolution of active 4 quasi-particles and a spectator

$$S_m(J) = \left\{ \sum |\langle \alpha\beta | V | \gamma\delta \rangle_a|^2 \otimes N_s \right\}_J$$

$$S_{m+2}(J) = \left\{ \sum |\langle \alpha | V | \beta\gamma\delta \rangle_a|^2 \otimes N_s \right\}_J$$



particle-hole collision



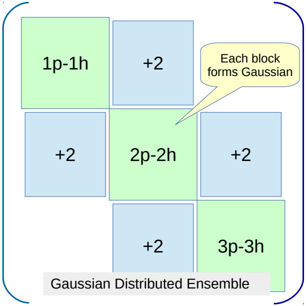
particle-hole creation

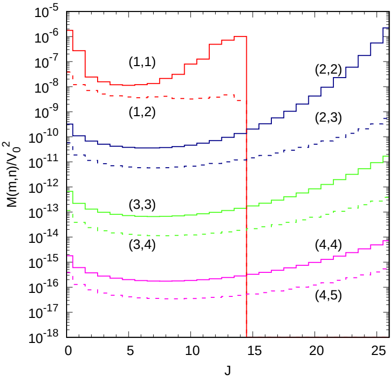
$$\mathcal{M}_{m,m}(J) = S_m(J)/N_m(J)^2$$

$$\mathcal{M}_{m,m+2}(J) = S_{m+2}(J)/[N_m(J)N_{m+2}(J)]$$

Calculated Second Moments

- Calculated for ^{208}Pb with δ-interaction
- $\mathcal{M}_{mm}$ for diagonal elements, $\mathcal{M}_{m,m+2}$ for off-diagonal ones
- Single-particle states and wave-functions generated with FRDM





Saddle Point Equation and Level Density

Saddle point equation solved for $\sigma_n(E)$

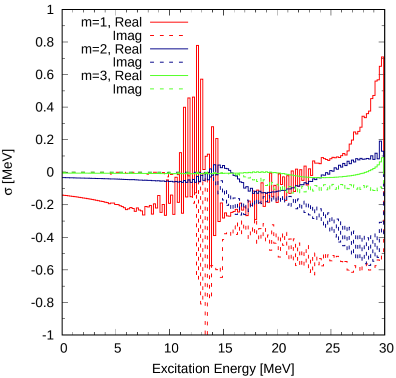
$$\sigma_m^{J\pi}(E) = \sum_n \mathcal{M}_{mn} \int \rho_n^{(0)J\pi}(\epsilon) \frac{1}{E - \epsilon - \sigma_n^{J\pi}(E)} d\epsilon$$

Partial level density for fixed $J\pi$ and $m$particle-$m$hole states

$$\rho_m^{J\pi}(E) = -\sum_\mu \frac{1}{\pi} \Im \frac{1}{E - \epsilon_{m\mu} - \sigma_m^{J\pi}(E)}$$

where $\Re\sigma$ energy shift, and $\Im\sigma$ energy spread of p-h state

The magnitude of σ depends on the calculated $\mathcal{M}_{mm}$



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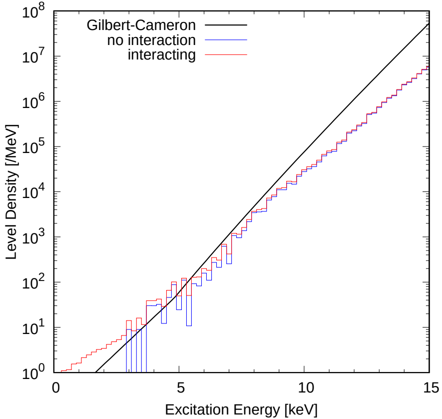
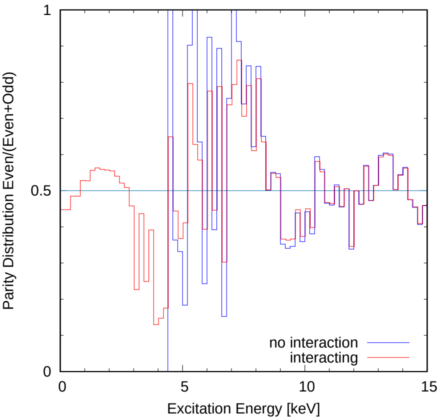
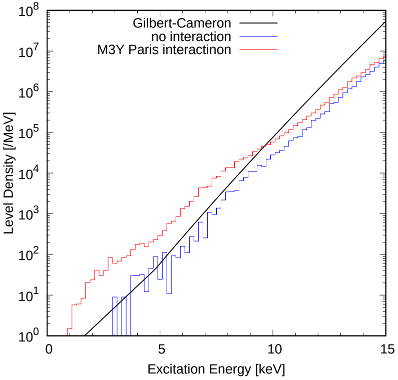
Combinatorial and GOE Level Densities for ^{208}Pb





Random Matrix Level Density with Realistic Interaction



- M3Y-Paris potential
- Too strong enhancement seen
- We might need more careful optimization
- Since calculation takes long time, we used spherical Woods-Saxon wave-functions
  - Monte Carlo sampling technique under development
- Skyrme interaction might be a reasonable choice

Future Extension and Feasibility

We envision many nuclear reaction model inputs, currently provided by an external database or phenomenological parameterization, could be replaced by the shell model approach to nuclear reaction.

- β-decay strength function and β-delayed γ and neutron emissions, and fission with Hauser-Feshbach theory

M. Mumpower et al, http://arxiv.org/abs/1608.01956

- Internal calculation of GDR for neutron radiative capture
- Multi-step direct reactions by calculating matrix elements of

$$\sum_{\mu} |\langle \chi_b^{(-)} u_{m\mu} | \mathcal{V} | \chi_a^{(+)} u_0 \rangle|^2 \rho_{m\mu}(E_x)$$

- Folding optical potential
- Dynamical calculation of fission along the fission path

Concluding Remarks

- For better prediction of experimentally unknown nuclear reaction cross sections, we incorporated the mean-field theories into the Hauser-Feshbach code, CoH_3.
- two cases already implemented:
  - single-particle wave-functions for direct/semidirect capture by Bonneau et al.
  - single-particle level density from Strutinsky method
- Microscopic level density based on the random matrix theory
  - combinatorial calculation including quasi-particle interaction
  - this calculation is much faster and less memory space than diagonalization of full shell mode Hamiltonian

Collaborators: P. Talou, I. Stetcu, M. Mumpower, P. Möller, J. Ullmann, L. Bonneau, H. A. Weidenmüller, T. Ichikawa, S. Yoshida (deceased)