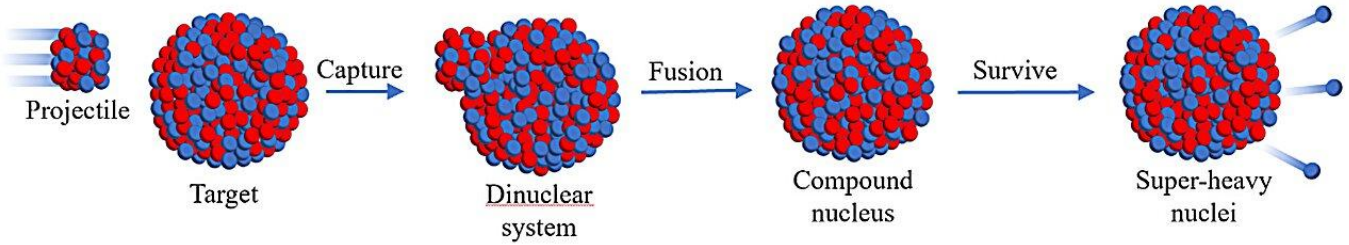
Isoenergetic description of induced fission pathways within energy-density functional theory

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Formation of SHN in fusion reactions



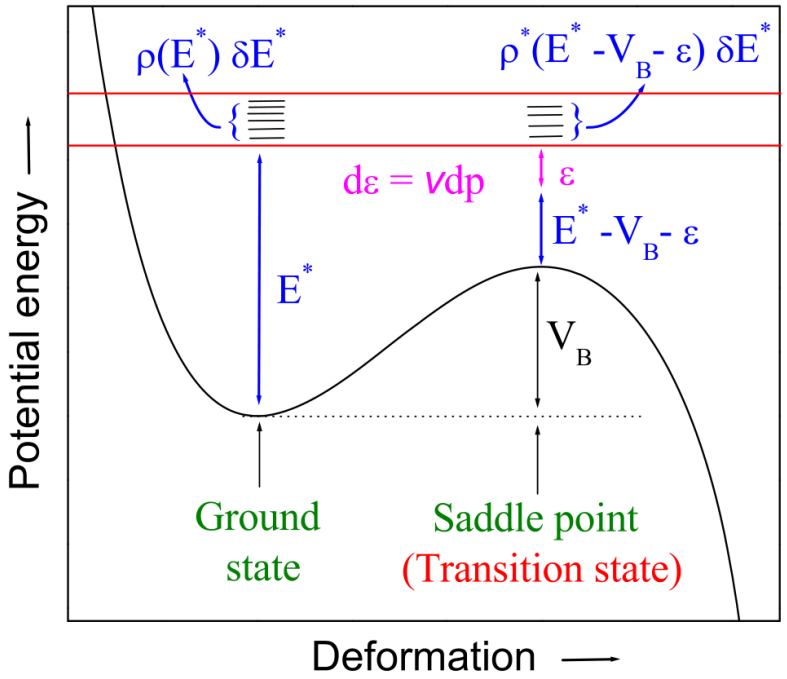
$$\sigma = \sigma_{cap} \times P_{fusion} \times W_{surv}$$

$$W_{surv} = \frac{\Gamma_n}{\Gamma_n + \Gamma_f} = \left(1 + \frac{\Gamma_f}{\Gamma_n}\right)^{-1}$$

$$\Gamma_f \sim \frac{\rho_{\text{saddle}}(E^* - V_B(E^*))}{\rho_{\text{gs}}(E^*)}$$

$$V_B(E^*) \neq V_B(E^* = 0)$$

$$\rho(E) \sim \exp(S(E))$$



How to compute V_B and V_{eff} within EDFT ?

1. $T = \text{const} \Rightarrow V_{\text{eff}}(Q) = F(Q)$
2. $S = \text{const} \Rightarrow V_{\text{eff}}(Q) = E(Q)$
3. $E = \text{const} \Rightarrow V_{\text{eff}}(Q) = \ ?$

In the statistical description of the fission process, the deformation and the energy are given by ensemble average values of the nuclear Hamiltonian, $E = \langle \hat{H} \rangle$, and the respective quadrupole moment operator, $Q = \langle \hat{Q}_{20} \rangle$. Within the grand canonical description, the particle number is also given in the form of an average $N_\tau = \langle \hat{N}_\tau \rangle$ $(\tau = n,\, p)$. To describe local equilibrium properties of a compound nucleus, we are looking for the normalized density operator $\hat{D}$ $(\mathrm{Tr}\hat{D} = 1)$ which satisfies the constraints

$$E = \mathrm{Tr}(\hat{D}\hat{H}),\;\; Q = \mathrm{Tr}(\hat{D}\hat{Q}_{20}),\;\; N_\tau = \mathrm{Tr}(\hat{D}\hat{N}_\tau)$$

Maximization of the entropy $S = -\mathrm{Tr}(\hat{D}\ln\hat{D})$ leads to

$$\hat{D} = \frac{1}{Z} e^{-\beta\hat{H}+\alpha_n\hat{N}_n+\alpha_p\hat{N}_p+\lambda\hat{Q}}, \qquad Z = \mathrm{Tr}(e^{-\beta\hat{H}+\alpha_n\hat{N}_n+\alpha_p\hat{N}_p+\lambda\hat{Q}})$$

where $\beta(E, N_\tau, Q),\;\; \alpha_\tau(E, N_\tau, Q),\;\; \lambda(E, N_\tau, Q)$ are the Lagrange multipliers.

Using the definition of entropy, we get

$$S = \ln Z + \beta E - \alpha_n N_n - \alpha_p N_p - \lambda Q$$

Using the relations

$$\frac{\partial}{\partial\beta}\ln Z = -E, \qquad \frac{\partial}{\partial\alpha_\tau}\ln Z = N_\tau, \qquad \frac{\partial}{\partial\lambda}\ln Z = Q$$

we get

$$dS = \beta\, dE - \alpha_n\, dN_n - \alpha_p\, dN_p - \lambda\, dQ. \qquad (*)$$

This equation expresses how the local equilibrium entropy changes in response to infinitesimal variations in the parameters $E,\ N_\tau,\ Q$, which fully characterize the local equilibrium state of the nucleus.

In the following, we assume that the average number of particles in the nucleus remains constant during the deformation process. By introducing $T = \beta^{-1}$ and $\kappa = \lambda/\beta$ we can write (*) in a form analogous to the first law of thermodynamics

$$dE = T\, dS + \kappa\, dQ \qquad (**)$$

Here, T and κ acquire the physical interpretations of temperature and collective driving force, respectively - quantities that determine the conditions necessary to maintain nuclear equilibrium at given values of total energy and deformation. However, since the nucleus is an isolated quantum system, Eq. (**) should not be interpreted in terms of heat exchange or mechanical work. Rather, this equation expresses how the total energy change dE is distributed between the thermal component TdS and the energy κdQ associated with the evolution of the collective coordinate.

Using the definition of the Helmholtz free energy, $F = E - TS$, the driving force κ is expressed in terms of partial derivatives of three distinct thermodynamic quantities:

$$\kappa(Q,T) = \frac{\partial F(Q,T)}{\partial Q} \qquad \kappa(Q,S) = \frac{\partial E(Q,S)}{\partial Q} \qquad \kappa(Q,E) = -T(Q,E)\frac{\partial S(Q,E)}{\partial Q}$$

Effective potential $V_X(Q), \quad X = T, S, E$

$$V_X(Q+dQ) - V_X(Q) = \kappa(Q,X)dQ \quad \Leftrightarrow \quad \frac{dV_X(Q)}{dQ} = \kappa(Q,X)$$

Isothermal process (T=const)

$$V_T(Q) = F(Q,T) + const$$
$$\text{for} \quad T = 0$$
$$V_T(Q) = E(Q,T=0) = V(Q)$$

Isentropic process (S=const)

$$V_S(Q) = E(Q,S) + const$$
$$\text{for} \quad S = 0$$
$$V_S(Q) = E(Q,S=0) = V(Q)$$

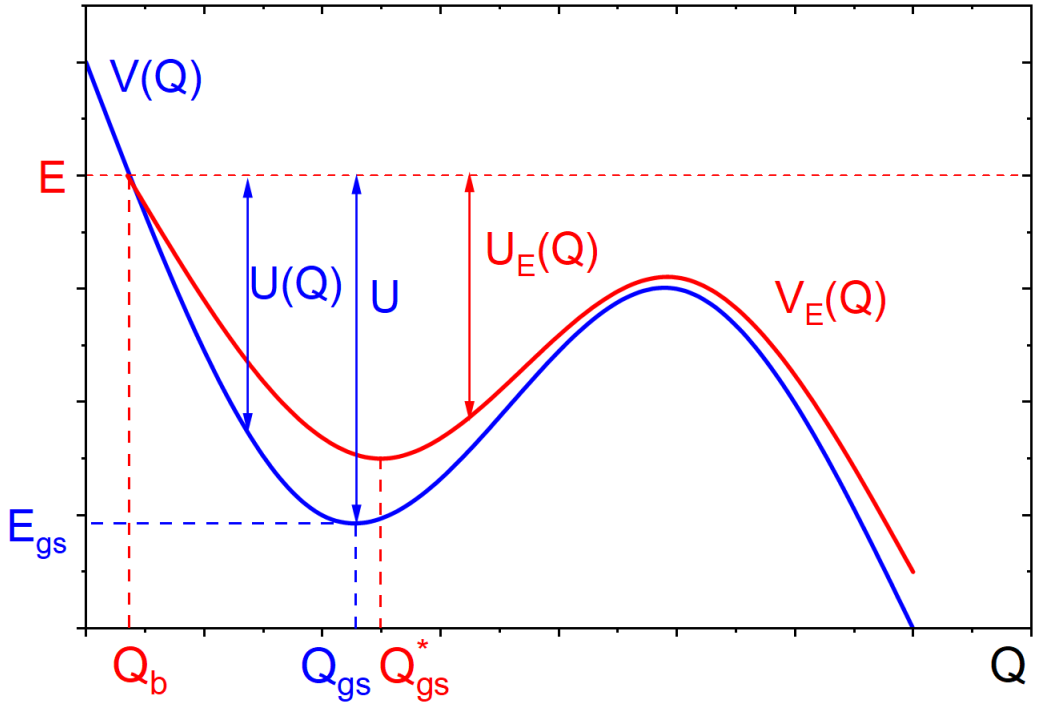
Isoenergetic effective potential (E=const)

$$E_{gs} = V(Q_{gs}) \text{ -ground state energy;}$$

$$U \text{ -excitation energy;}$$

$$E = E_{gs} + U \text{ total energy;}$$

$$E = V(Q) + U(Q), \quad U(Q) \text{ -local excitation energy}$$



For isoenergetic process $V(Q) \le E$ and $V(Q_b) = E$

$$V_E(Q_b) = E$$

$$\frac{dV_E(Q)}{dQ} = \kappa(Q,E)$$

$$\kappa(Q,E) = -T(Q,E)\frac{dS(Q,E)}{dQ}$$

$$V_E(Q) = E - \int_{Q_b}^{Q} T(q,E)\frac{dS(q,E)}{dq}dq$$

$$U_E(Q) = \int_{Q_b}^{Q} T(q,E)\frac{dS(q,E)}{dq}dq$$ - effective local excitation energy

Fermi-gas model

$$U(Q) = E(Q) - V(Q) \text{ - local excitation energy}$$

$$U(Q) = a(Q)T^2(Q)$$

$$S(Q) = 2a(Q)T(Q) = 2\sqrt{a(Q)U(Q)}$$

$a(Q)$ - level density parameter: $\rho(U) \sim \exp\left(2\sqrt{aU}\right)$

$$V_T(Q) = F(Q,T) = V(Q) - a(Q)T^2$$

$$V_S(Q) = E(Q,S) = V(Q) + a(Q)T^2(Q), \quad \left(T(Q) = S/2a(Q)\right)$$

$$V_E(Q) = V(Q) - \int_{Q_b}^{Q} T^2(q)\frac{da(q)}{dq}dq$$

If the level density parameter a(Q) is independent of deformation, the effective potentials differ from the deformation energy V(Q) only by a constant shift. As a result, the three thermodynamic descriptions (isothermal, isentropic, and isoenergetic) become physically equivalent in this case.

FT-HFB approximation

Exact density matrix $\hat{D} = \dfrac{e^{-(\hat{H}-\mu\hat{N}-\kappa\hat{Q})/T}}{Z}$

FT-HFB density matrix $\hat{D}_{HFB} = \dfrac{e^{-(\hat{K}-\mu\hat{N}-\kappa\hat{Q})/T}}{Z_{HFB}}$, where $\hat{K} = \sum_{ij}\left(K_{ij}^{11}c_i^+c_j + K_{ij}^{22}c_ic_j^+ + K_{ij}^{20}c_i^+c_j^+ + K_{ij}^{02}c_ic_j\right)$

and K_{ij}^{ab} are variational parameters . $\max[S] \Rightarrow \delta(E - \mu N - TS - \lambda Q) = 0$

$$\hat{K} = \hat{H}_{HFB} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}$$

$$h_{ij} = t_{ij} + \frac{1}{2}\sum_{lk} v_{ikjl}\rho_{lk}, \quad \rho_{lk} = \mathrm{Tr}(\hat{D}_{HFB}c_k^+c_l)$$

$$\Delta_{ij} = \frac{1}{2}\sum_{lk} v_{ijlkl}\kappa_{lk}, \quad \kappa_{lk} = \mathrm{Tr}(\hat{D}_{HFB}c_kc_l)$$

Thermodynamic consistency of the FT-HFB approximation:

$$E = -\frac{\partial \ln Z_{HFB}}{\partial \beta}$$
$$N_\tau = \frac{\partial \ln Z_{HFB}}{\partial \alpha_\tau}$$
$$Q = \frac{\partial \ln Z_{HFB}}{\partial \lambda}$$

$\Rightarrow$ $dE = T\,dS + \kappa\,dQ$

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Axially deformed solution of the Skyrme-Hartree–Fock–Bogoliubov equations using the transformed harmonic oscillator basis (II) HFBTHO v2.00d: A new version of the program☆

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Calculations are performed for ^{296}Lv with SkM* using 1100 oscillator basis states with N≤30

Density-dependent contact paring interaction with mixed volume-surface character

$$V_{\text{pair}}^{(\text{n,p})}(\boldsymbol{r}) = V_0^{(\text{n,p})}\left(1 - \frac{1}{2}\frac{\rho_0(\boldsymbol{r})}{\rho_c}\right)\delta(\boldsymbol{r}-\boldsymbol{r}'),$$

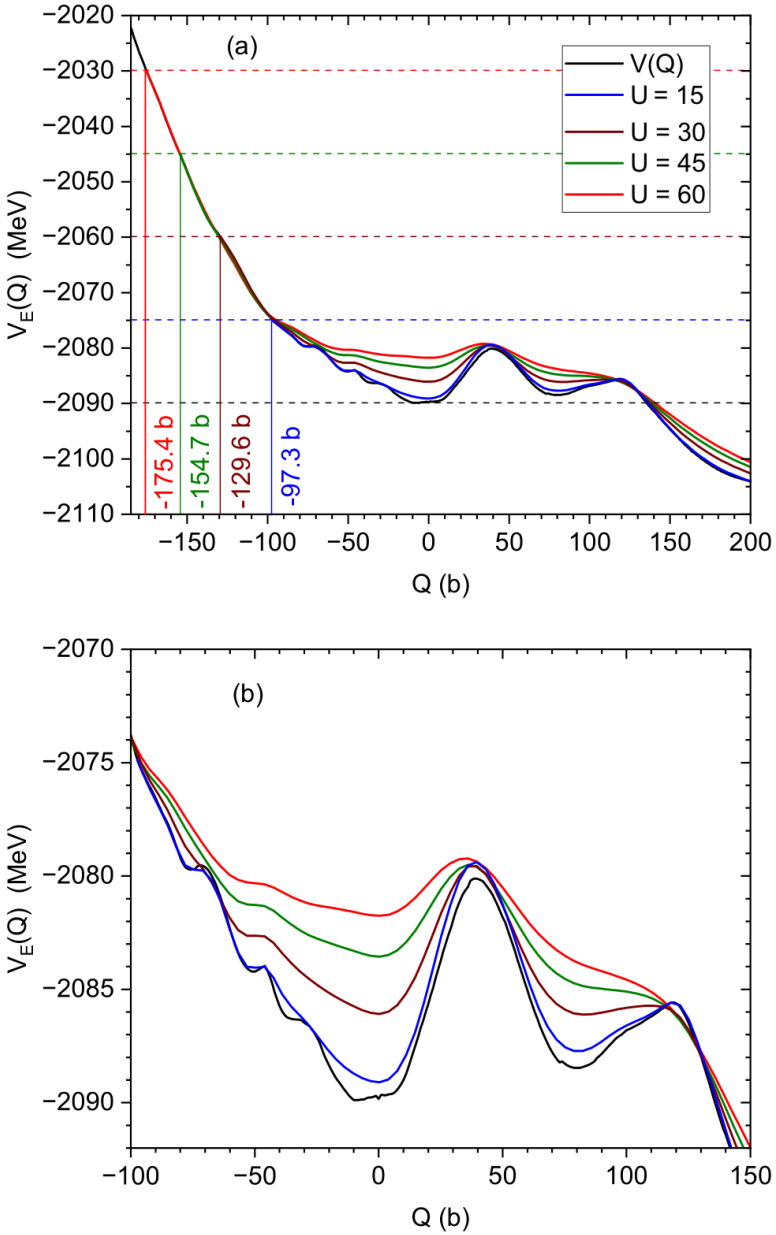
The pairing strengths and energy cutoff were fitted to reproduce the odd-even mass difference for ^{240}Pu

By performing constraint FTHFB calculations over a grid of T and Q we obtain $\kappa(Q,T)$, $E(Q,T)$, $S(Q,T)$

The transformation from the (Q,T) grid to (Q,E) and (Q,S) ones is performed using bilinear interpolation.

$$V_T(Q) = E(Q,T) - TS(Q,T), \quad V_S(Q) = E(Q,S), \quad V_E(Q) = E - \int_{Q_b}^{Q} \kappa(q,E)dQ$$

Isoenergetic effective potential for ^{296}Lv



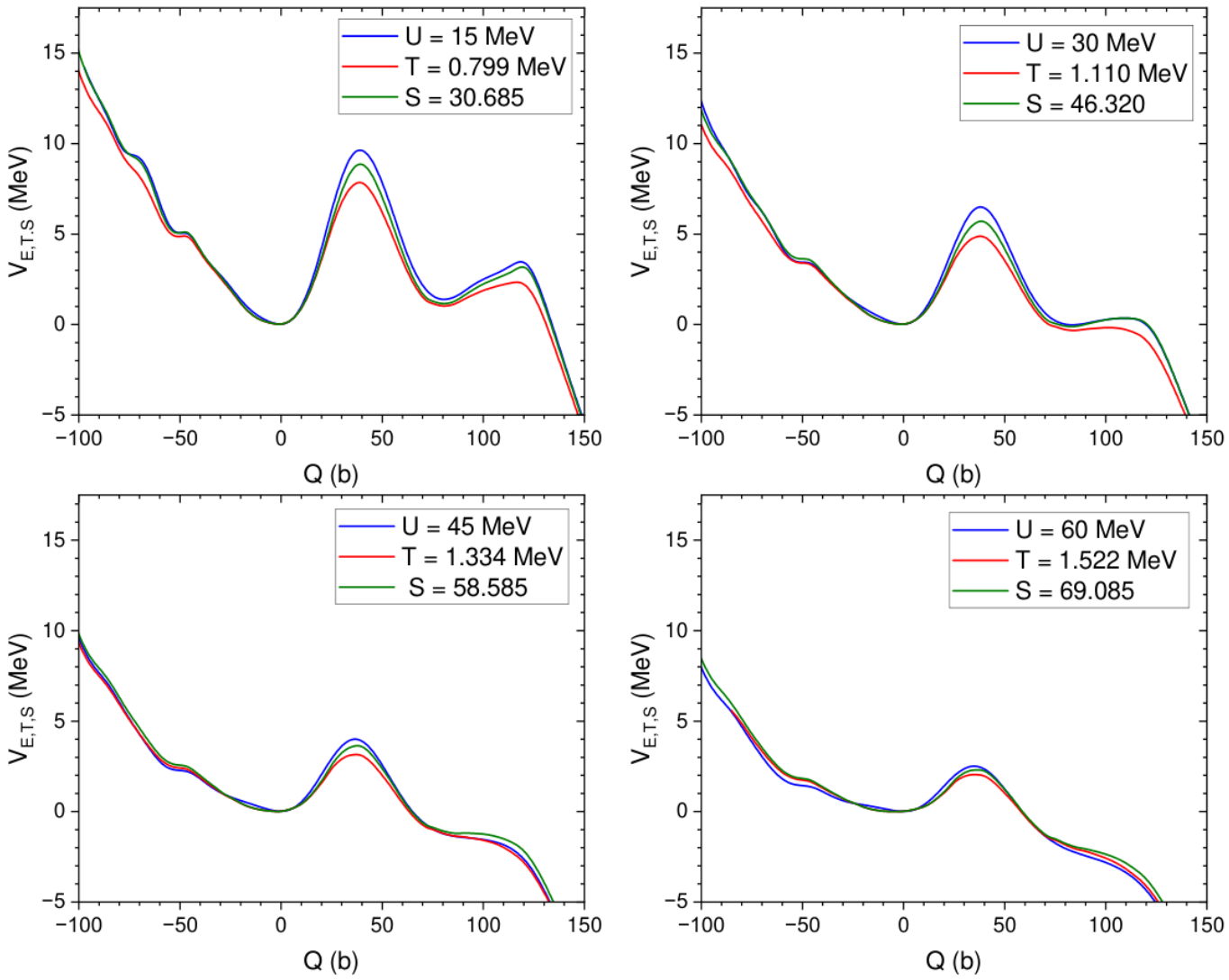
$$V_E(Q) = E + \int_{Q_b}^{Q} \kappa(q, E)\, dq$$

FIG. 1. (a) The deformation energy $V(Q)$ is compared with the isoenergetic effective potentials $V_E(Q)$ at selected excitation energies U (in MeV). The dashed lines indicate the total internal energy $E = E_{gs} + U$, where $E_{gs} = -2089.88$ MeV is the Hartree-Fock-Bogoliubov ground-state binding energy obtained using the SkM* energy density functional. It is worth recalling that for a fixed excitation energy U, the boundary Q_b of the isoenergetic potential is determined by the condition $V(Q_b) = E$. The vertical lines mark the values of Q_b corresponding to the selected excitation energies U. (b) A close-up view of the upper panel, focusing on the fission barrier region.

Micro-macro model

$$E(\beta_2, \beta_4) = E_{LDM}(\beta_2, \beta_4) + \delta E_{mic}(\beta_2, \beta_4) \exp\left(-\frac{U^*}{E_D}\right)$$

Isoenergetic, isentropic and isothermal effective potentials for ^{296}Lv



$$B_f(X) \approx \int_{Q^*_{gs}}^{Q_{sp}} \kappa(Q,X)dQ \quad (X = E,T,S)$$

$$\begin{aligned}\Delta B_f &= B_f(E' = \text{const}) - B_f(S' = \text{const}) \\ &= \int_{Q^*_{gs}}^{Q_{sp}} \left[\kappa(Q,E') - \kappa(Q,S')\right] dQ\end{aligned}$$

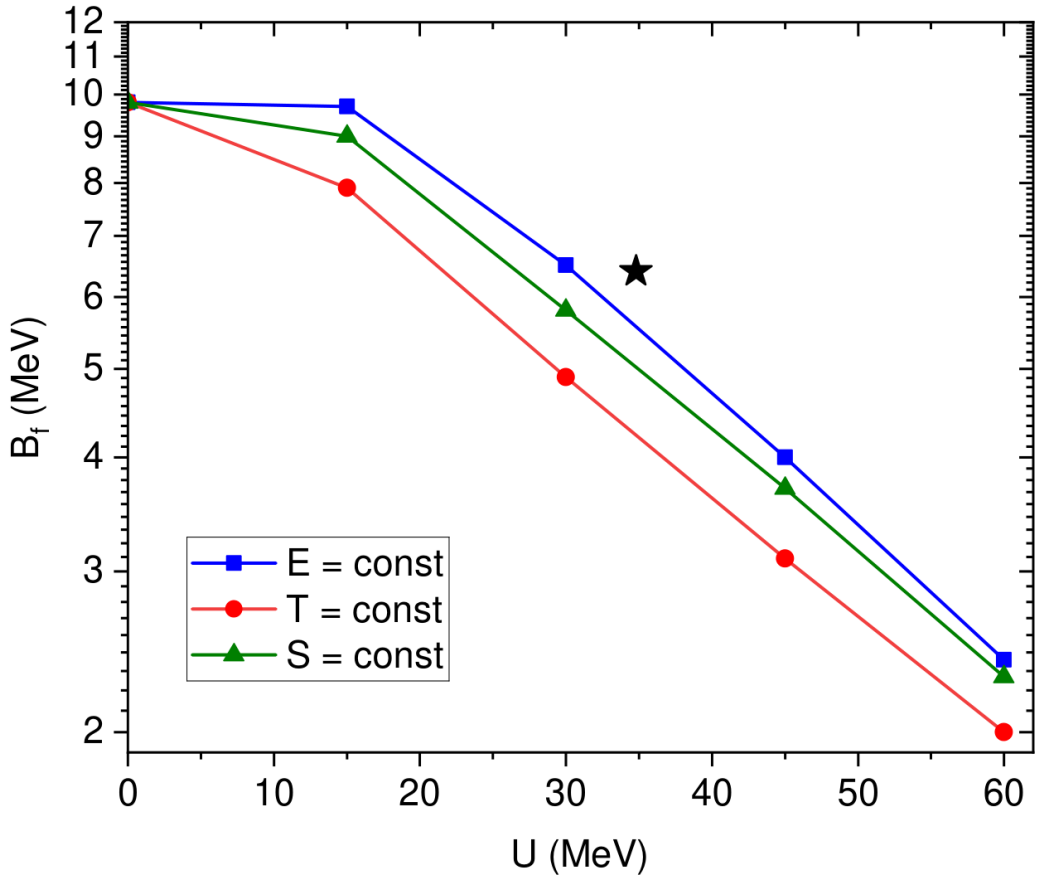
Using $\kappa(Q,S') = \kappa(Q,E(Q,S'))$ we get

$$\Delta B_f \approx \int_{Q^*_{gs}}^{Qsp} \frac{\partial \kappa(Q,E)}{\partial E}\Big|_{E=E'} \left[E' - E(Q,S')\right] dQ$$

Since $E' \le E(Q,S')$ and $\dfrac{\partial \kappa(Q,E)}{\partial E} < 0$

we obtain $B_f(E') > B_f(S')$

Damping of fission barrier height



$$B_f \propto e^{-\gamma_D U}$$

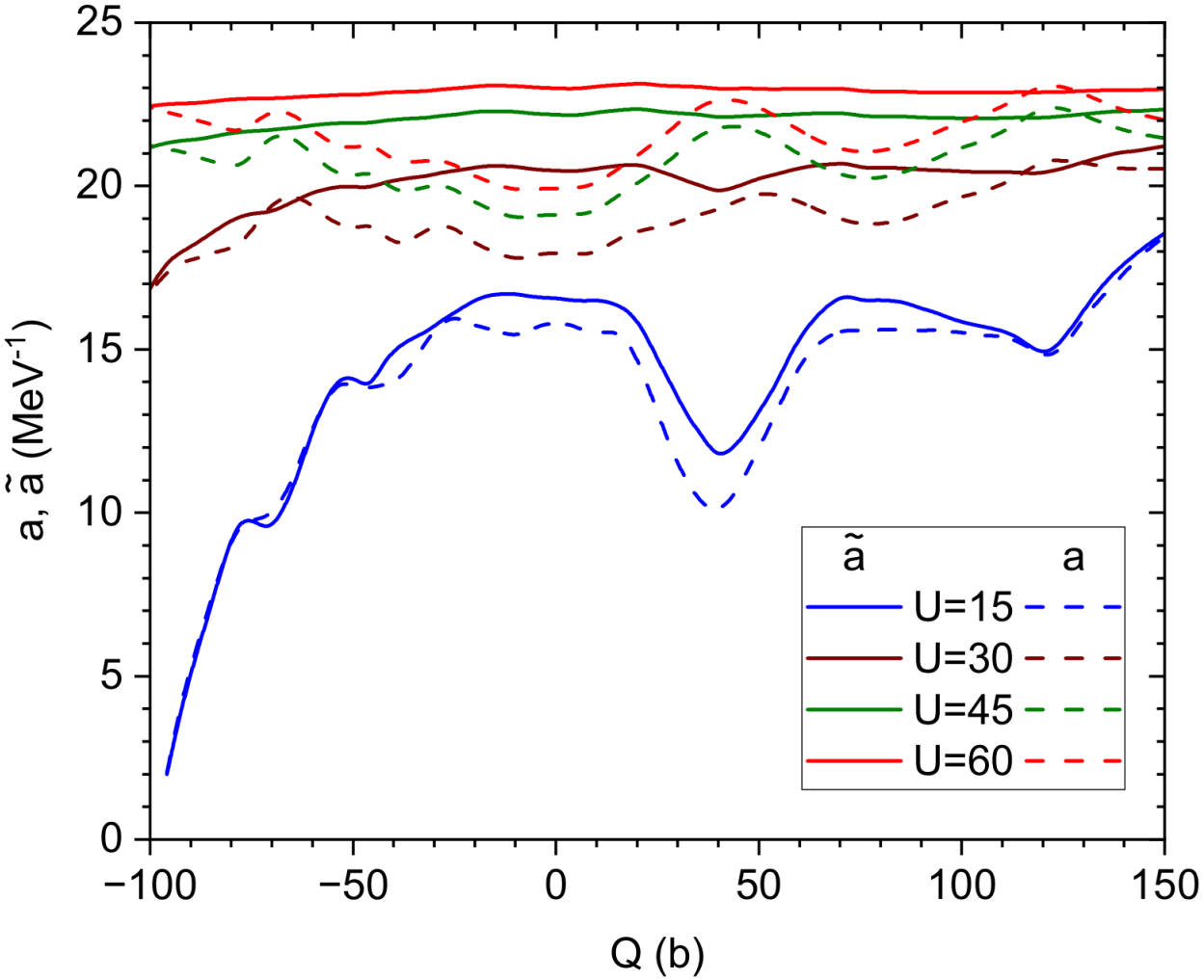
$$\gamma_D^{-1}(E) = 30.1 \text{ MeV}$$

$$\gamma_D^{-1}(T) = 33.5 \text{ MeV}$$

$$\gamma_D^{-1}(S) = 32.4 \text{ MeV}$$

The star denotes the lower limit of the fission barrier deduced from experimental data on $^{48}Ca+^{248}Cm$ at excitation energy of 38.4 MeV [PRC65(2002)044602, M.G. Itkis et al]

Level-density parameter



$$a(Q,E) = \frac{S^2(Q,E)}{4U(Q)}, \quad U(Q) = E - V(Q)$$

$$\tilde{a}(Q,E) = \frac{S^2(Q,E)}{4U_E(Q)}, \quad U_E(Q) = E - V_E(Q)$$

Conclusions

1. Within energy-density functional theory, we can construct an effective potential for an excited compound nucleus while keeping **the total energy constant along the fission pathway;**

2. For ^{296}Lv, the isoenergetic approach predicts a significant damping of the fission barrier with increasing excitation energy. Among the three thermodynamic descriptions considered here, it gives **the largest barrier and the strongest damping**.

3. These calculations can help improve the description of survival probabilities and, ultimately, the formation cross sections of heavy and superheavy nuclei in fusion reactions.