# Comparative Analysis of Classical and Quantum Machine Learning Models for Predicting Nuclear Binding Energy and Introduction a GUI


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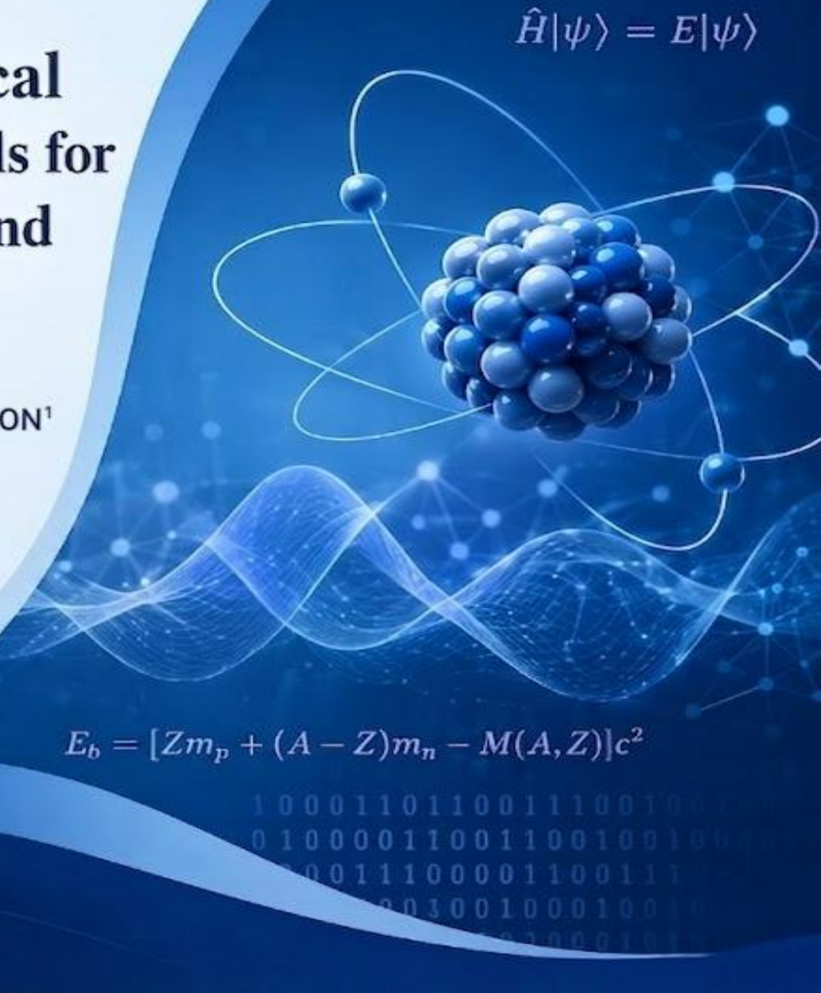
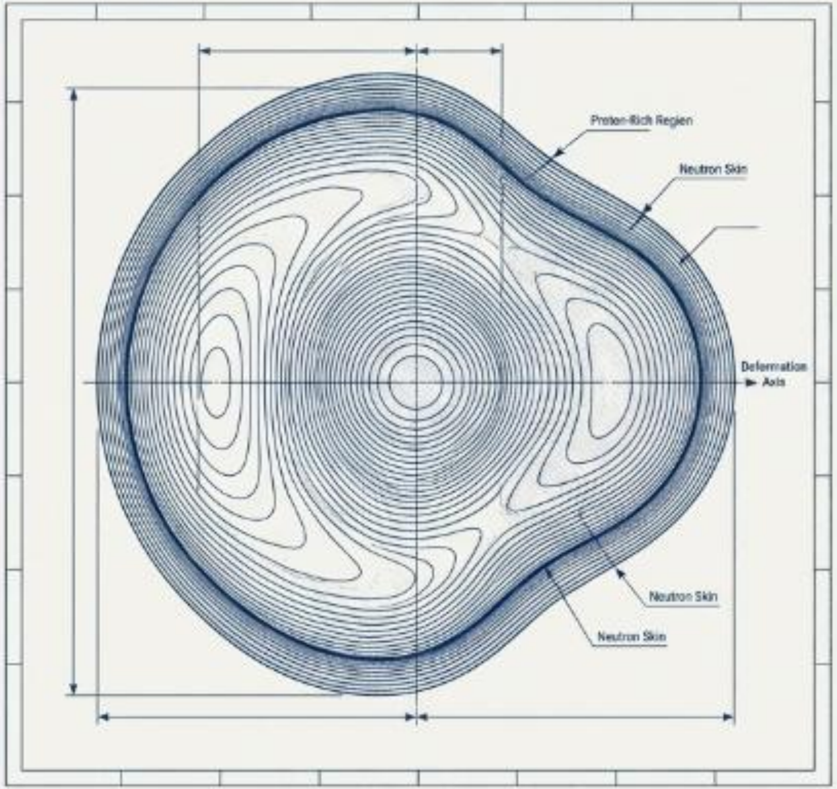


# The Binding Energy

Nuclear binding energy dictates stability, nucleosynthesis, and reactor physics. Yet, predicting it rapidly and accurately remains computationally elusive.




### Macroscopic Models

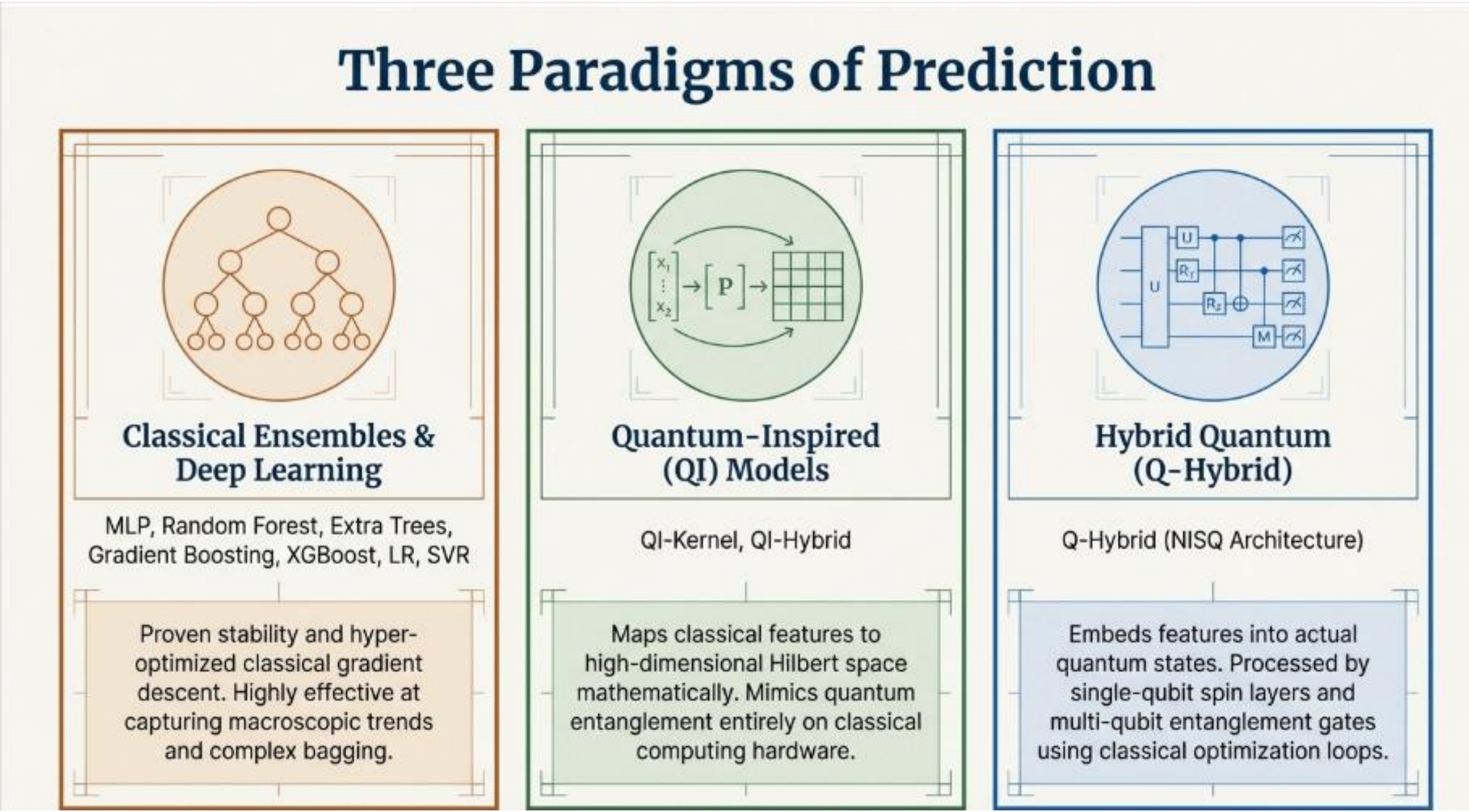
- **Advantage:** Fast, captures global trends.
- **Limitation:** Misses local shell and deformation effects.

### Microscopic Models

- **Advantage:** High structural accuracy.
- **Limitation:** Computationally prohibitive for heavy nuclei.

## The Machine Learning Opportunity

ML bridges this gap by interpolating complex shell effects and deformation-induced nonlinearities, delivering microscopic accuracy at macroscopic speeds.



Three Paradigms of Prediction
Classical Ensembles & Deep Learning
MLP, Random Forest, Extra Trees, Gradient Boosting, XGBoost, LR, SVR
Proven stability and hyper-optimized classical gradient descent. Highly effective at capturing macroscopic trends and complex bagging.
Quantum-Inspired (QI) Models
QI-Kernel, QI-Hybrid
Maps classical features to high-dimensional Hilbert space mathematically. Mimics quantum entanglement entirely on classical computing hardware.
Hybrid Quantum (Q-Hybrid)
Q-Hybrid (NISQ Architecture)
Embeds features into actual quantum states. Processed by single-qubit spin layers and multi-qubit entanglement gates using classical optimization loops.

# Nuclear Binding Energy — The Physics

Nuclear Binding Energy (BE) is the energy required to completely disassemble an atomic nucleus into its constituent protons and neutrons. It is the central quantity governing nuclear stability, reaction Q-values, astrophysical nucleosynthesis, and radioisotope production.

### Bethe-Weizsäcker Formula

- $BE = a_vA - a_sA^{2/3} - a_cZ^2/A^{(1/3)}$

  $- a_aI^2/A \pm \delta$ (pairing)
- Volume + Surface + Coulomb
- Asymmetry + Pairing terms
- Semi-empirical liquid drop model (1935)

### Physical Importance

- Nuclear stability (chart of nuclides)
- Reaction Q-values & thresholds
- r-process nucleosynthesis in stars
- Nuclear reactor fuel cycle design
- Medical radioisotope production
- Constrains nuclear equation of state

### Prediction Challenges

- ~3535 measured nuclei (AME2020)
- Local shell & deformation effects
- Light nuclei (A<40): sparse, noisy
- Heavy nuclei: strong nonlinearity
- Beyond drip line: no experimental data
- Microscopic models: heavy nuclei intractable

# Dataset: AME2020 & Three Mass Regions

| 3,535 | 80% / 20% | 2,828 | 707 | 20 |
|---|---|---|---|---|
| Total Nuclei | Test / Train split | Test set | Training set | Engineered Features |

## LIGHT ZONE

**$A < 40$**

**292 nuclei**

8.3% of dataset

Most challenging region. Sparse data, high noise-to-signal ratio. Strong shell effects dominate. Ideal for testing model robustness.

**Key challenge: Sparse + noisy data**

## MEDIUM ZONE

**$40 \leq A \leq 120$**

**1141 nuclei**

32.3% of dataset

Transition region. Balanced complexity. Near-linear BE/A systematics dominate. Surprising performance of linear models.

**Key challenge: Linear-to-nonlinear transition**

## HEAVY ZONE

**$A > 120$**

**2102 nuclei**

59.5% of dataset

Data-rich, low-noise region. Strong collective nonlinear phenomena (deformation, rotational bands). Best test for quantum ML.

**Key challenge: Rich nonlinear structure**

# Why Machine Learning for Nuclear Physics?

### ✕ Limitations of Traditional Models

- Liquid Drop Model: accurate globally, fails locally near shell closures
- Shell Model: exact for light nuclei; intractable for heavy/deformed
- Energy Density Functionals: computationally heavy, heavy nuclei challenging
- Macroscopic-Microscopic: manual tuning required per nucleus region

### ✓ Machine Learning Advantages

- Data-driven: learns correlations without explicit physics assumptions
- Fast inference after training (microseconds per nucleus)
- Captures shell effects, pairing, deformation automatically
- Uncertainty quantification available (Bayesian, Gaussian Process)

### Prior Work Timeline — ML in Nuclear Physics

| 2014 | 2017 | 2018 | 2021 | 2025 |
|---|---|---|---|---|
| ANN for nuclear charge radii (Bayram, Akkoyun) | Bayesian NN for nuclear masses (Utama) | Bayesian GP extrapolation (Neufcourt) | GP & Deep ML for nuclear mass (Gao) | This Work: QML Comparison + GUI |

# Quantum Computing — Core Principles

## Superposition

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad |\alpha|^2 + |\beta|^2 = 1$$

A qubit exists simultaneously in a combination of $|0\rangle$ and $|1\rangle$ with complex amplitudes. Measurement collapses it probabilistically. This allows quantum processors to explore exponentially many states at once.

*vs Classical: Classical bit: fixed 0 OR 1*

## Entanglement

$$|\Phi+\rangle = (1/\sqrt{2})(|00\rangle + |11\rangle)$$

Two or more qubits can be correlated so that the state of one determines the other, regardless of distance. Entanglement enables non-local feature correlations that classical kernels cannot reproduce.

*vs Classical: No classical analog — purely quantum*

## Interference

$$P(x) = |\langle x|\psi\rangle|^2 = |\alpha_x|^2$$

Quantum algorithms amplify probability amplitudes of correct answers and cancel incorrect ones — exactly like wave interference. This is the core mechanism behind quantum computational speedup.

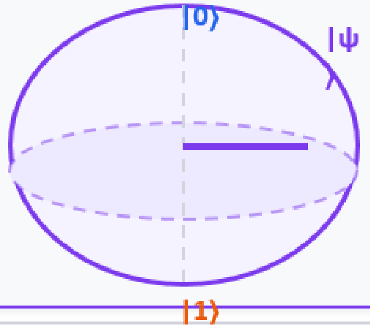
*vs Classical: Analogous to wave optics (constructive/destructive)*

*Quantum advantage emerges when superposition, entanglement & interference combine — exactly the mechanism QML algorithms exploit for nuclear physics regression.*

# Qubits — The Quantum Bit

| | Classical Bit | Qubit |
|---|---|---|
| **State** | 0 or 1 (binary, deterministic) | $\|\psi\rangle = \alpha\|0\rangle + \beta\|1\rangle$ (complex superposition) |
| **Information** | 1 bit | Encodes quantum state of Hilbert space |
| **N units →** | $2^N$ possible states (ONE at a time) | $2^N$ states simultaneously (quantum parallelism) |
| **Measurement** | Reads exact value | Collapses probabilistically: $P(0)=\|\alpha\|^2$, $P(1)=\|\beta\|^2$ |
| **Operations** | NAND, OR, XOR (irreversible) | Unitary gates U (reversible, $U^\dagger U = I$) |

### Bloch Sphere Representation




$|\psi\rangle = \cos(\theta/2)|0\rangle +$
$e^{\wedge}(i\phi)\sin(\theta/2)|1\rangle$
Every point on the sphere = valid qubit state

### Exponential State Space Scaling

| | | |
|---|---|---|
| **1 qubit** | 2 states | — |
| **4 qubits** | 16 states | — |
| **10 qubits** | 1,024 states | — |
| **50 qubits** | $2^{50} \approx 10^{15}$ states | *Exceeds classical RAM* |
| **300 qubits** | $2^{300}$ states | *More than atoms in universe* |

# Quantum Gates — Universal Operations

*Quantum gates are unitary operations ($U^\dagger U = I$) applied to qubits — analogous to classical logic gates but reversible and continuously parameterizable.*

### Pauli-X (NOT)

**X**

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

*Bit flip; state inversion; error correction*

### Pauli-Y

**Y**

$$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

*Combined bit + phase flip*

### Pauli-Z

**Z**

$$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

*Phase flip; used in VQC encoding layers*

### Hadamard (H)

**H**

$$(1/\sqrt{2})\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

*Creates superposition; core of QML feature maps*

### CNOT (CX)

**⊕**

2-qubit gate:

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

*Creates entanglement — essential for QML circuits*

### RX / RY / RZ (Rotation)

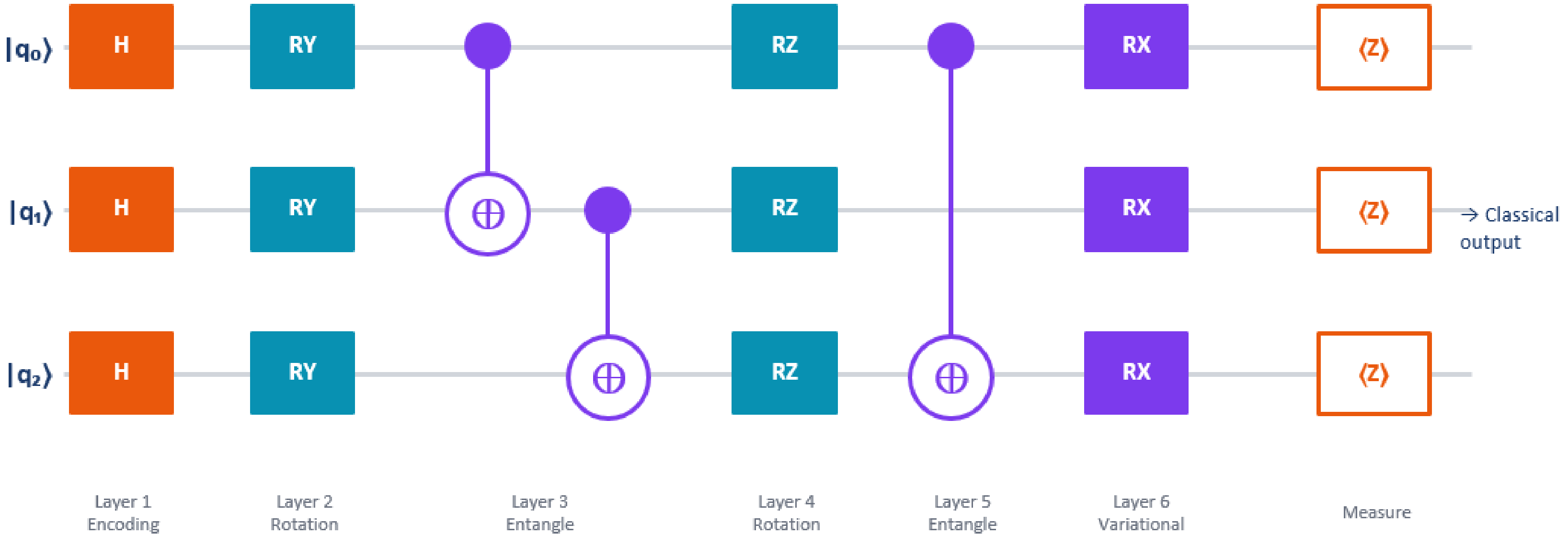
**Rθ**

$$RY(\theta)=\begin{bmatrix} \cos\theta/2 & -\sin\theta/2 \\ \sin\theta/2 & \cos\theta/2 \end{bmatrix}$$

*Encodes classical data as angles (angle encoding)*

# Quantum Circuits — Structure & Anatomy

*A quantum circuit is a sequence of quantum gate layers applied to qubits. Circuit depth = sequential layers; width = qubit count.*

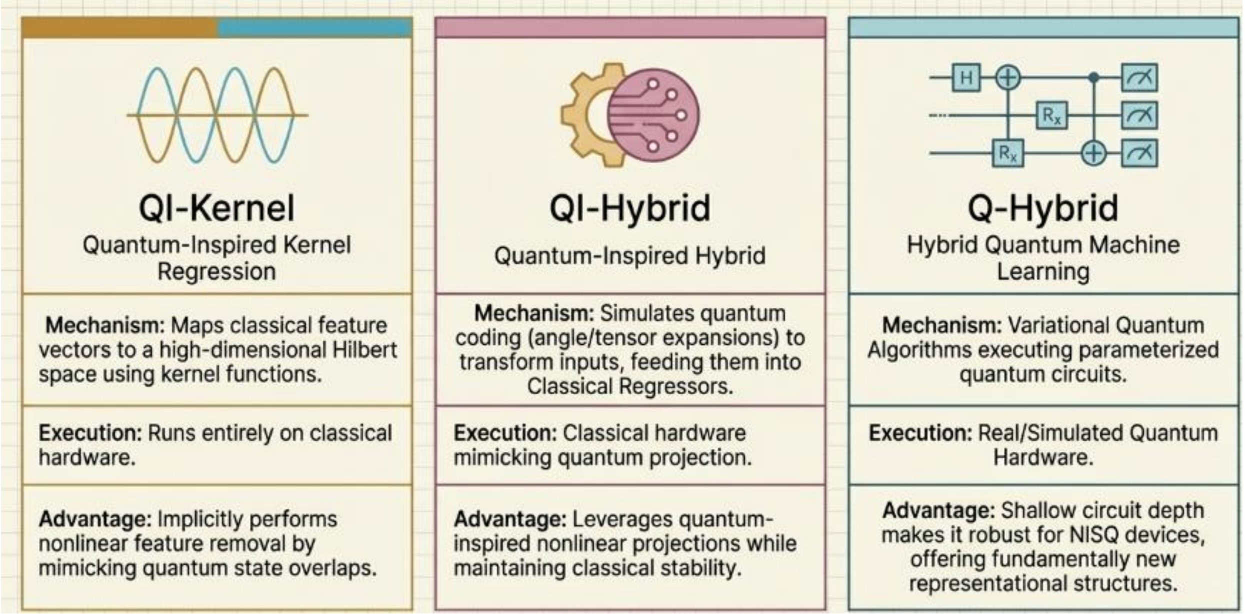



**Circuit Depth:** Number of sequential gate layers — directly impacts noise on real hardware. **NISQ Constraint:** Current devices are noisy; shallow circuits (< ~50 layers) are preferred.

**Parameterized Gates:** Trainable rotation angles θ form the basis of variational quantum algorithms (VQE, QAOA, QNN). **Measurements:** Pauli expectation values ⟨Z⟩ yield continuous real outputs suitable for regression tasks.

# Quantum Machine Learning — Landscape

1. **Classical Data** — Nuclear features A, Z, N/Z, shells
2. **Feature Encoding** — Angle / amplitude encoding to qubits
3. **Quantum Circuit** — Variational layers + entanglement
4. **Measure Output** — Pauli ⟨Z⟩ expectation values → real output
5. **Classical Optimizer** — Adam / COBYLA minimizes loss
6. **Prediction** — BE/A value (keV)



# Variational Quantum Circuits — The Q-Hybrid Model

$f(x; \theta) = \langle 0 | U^\dagger(x,\theta)\, \hat{O}\, U(x,\theta) | 0 \rangle$ where $U$ = encoding(x) · variational(θ) and $\hat{O}$ is a Pauli observable

### Encoding Layer U_enc(x)

- Input: classical feature vector x (nuclear features)
- Operation: apply $RY(x_i)$ to qubit i
- Maps classical data into quantum Hilbert space
- Fixed (not trained) — determined by data
- One qubit per feature required

### Variational Layer U_var(θ)

- Trainable rotation gates: $RX(\theta_i)$, $RY(\theta_i)$, $RZ(\theta_i)$
- Entanglement via CNOT gates between qubits
- L layers (circuit depth) — tunable hyperparameter
- Parameters θ optimized by classical routine
- Gradient: parameter-shift rule $\partial f/\partial\theta_i = f(\theta+\pi/2) - f(\theta-\pi/2)$

### Measurement & Loss

- Measure Pauli-Z expectation value: $\langle Z \rangle_i$
- Yields continuous scalar output for regression
- Loss: MSE = $(1/N)\, \Sigma\, (BE\_pred - BE\_exp)^2$
- Optimizer: Adam or gradient-free COBYLA
- Classical feedback updates θ until convergence

**NISQ-Compatible:** Shallow circuits tolerate decoherence on current quantum hardware. **Novel Feature Geometry:** Hilbert space correlations capture shell-deformation interactions beyond classical kernels. **Status:** Complements, rather than replaces, state-of-the-art classical ML methods under NISQ constraints.

# Results — Overfitting Check & Overall Performance

*Overfitting Gap = Train $R^2$ − Test $R^2$. Green Zone: < 0.005 | Yellow Zone: 0.005–0.02 | Red Zone: > 0.02*

**LIGHT ZONE (A < 40)**

| Model | Gap | Perf. |
|---|---|---|
| QI-Hybrid | +0.0483 | lowest |
| MLP_3×256 | +0.0047 | 1.000 |
| Extra Trees | +0.0049 | 1.000 |
| Linear Reg. | −0.0020 | 0.977 |
| QI-Kernel | −0.0005 | 0.884 |
| Q-Hybrid | +0.0104 | 0.789 |

**MEDIUM ZONE (40–120)**

| Model | Gap | Perf. |
|---|---|---|
| Linear Reg. | +0.0001 | 1.000 |
| MLP_3×256 | −0.0026 | 0.787 |
| Q-Hybrid | +0.0057 | 0.745 |
| QI-Hybrid | +0.0068 | 0.652 |
| Random Forest | +0.0096 | 0.422 |
| QI-Kernel | −0.0034 | 0.356 |

**HEAVY ZONE (A > 120)**

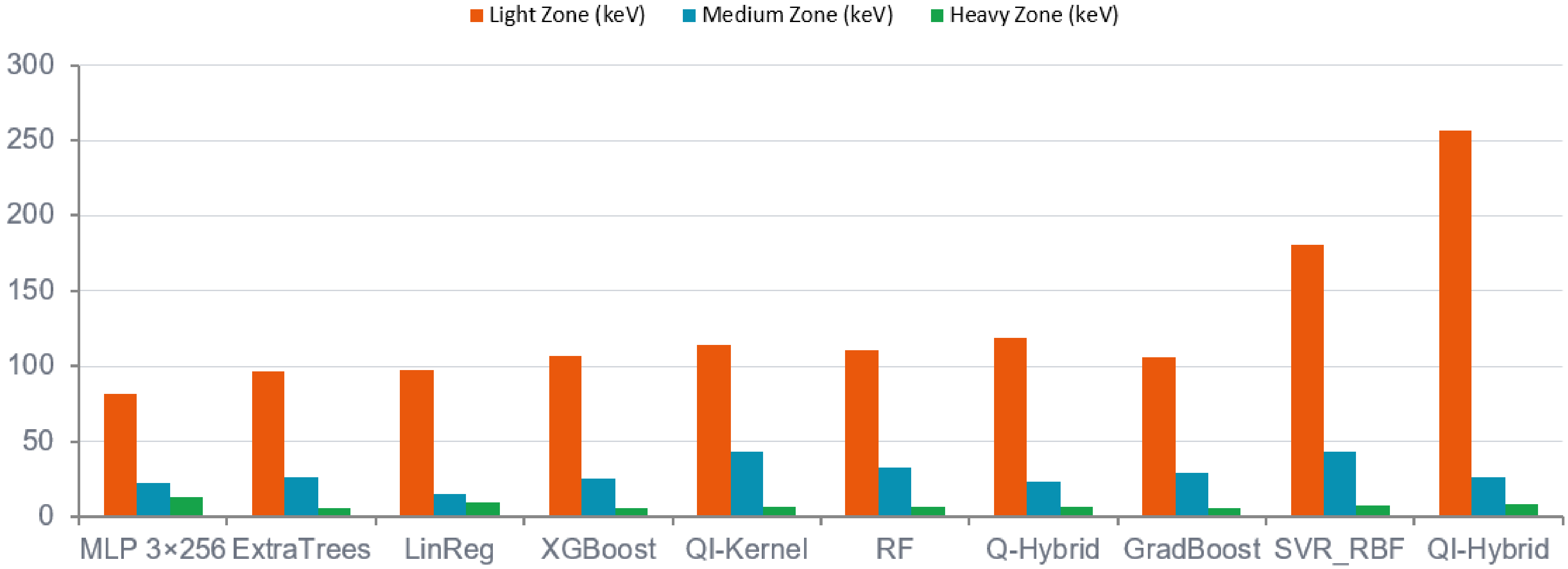
| Model | Gap | Perf. |
|---|---|---|
| Extra Trees | +0.0003 | 1.000 |
| Grad. Boost | +0.0003 | 0.984 |
| Q-Hybrid | +0.0004 | 0.908 |
| XGBoost | +0.0004 | 0.934 |
| Linear Reg. | −0.0001 | 0.470 |
| MLP_3×256 | +0.0005 | 0.281 |

# $R^2$ Heatmap — All Models × All Mass Regions

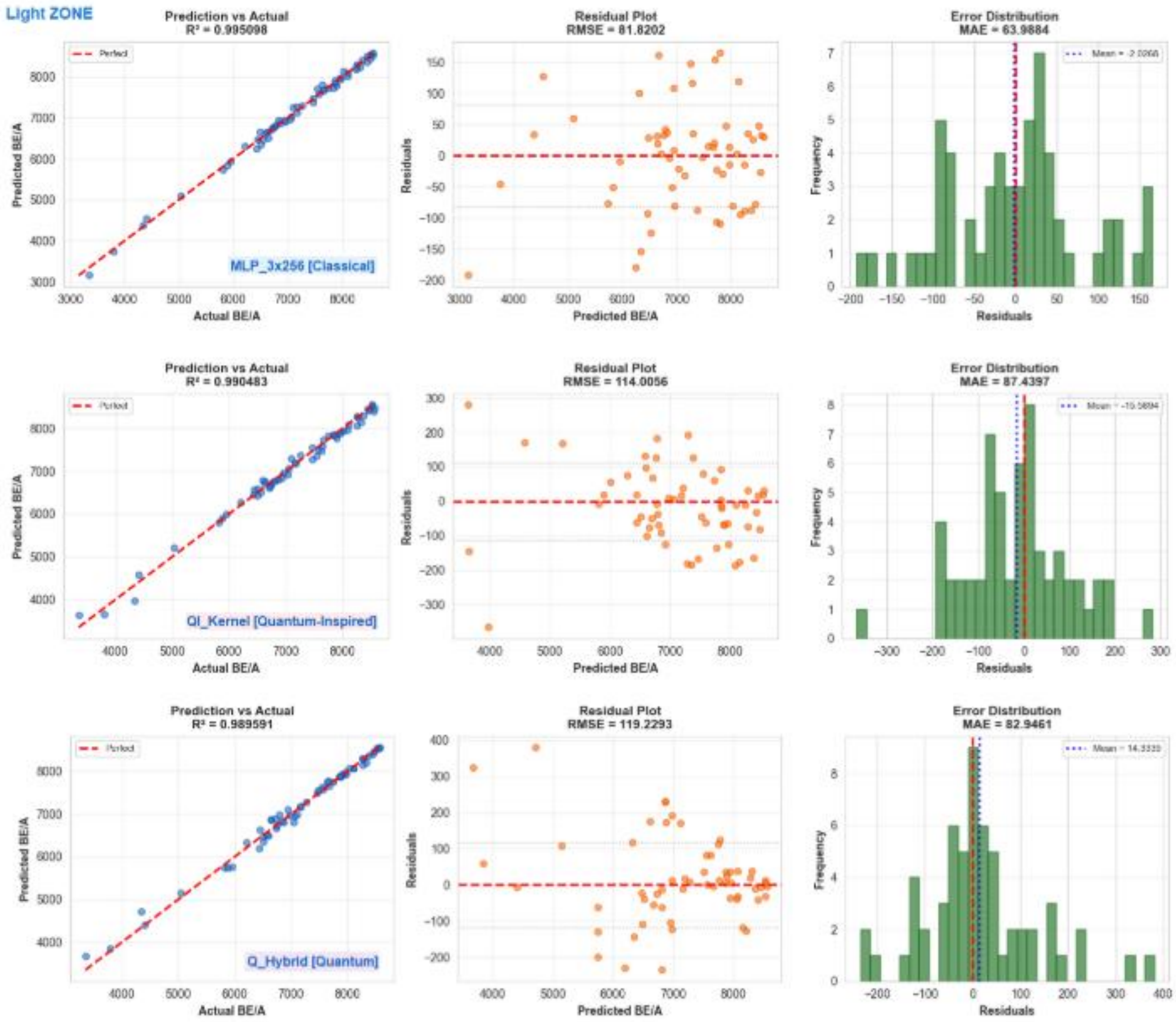
| Model | Light (A<40) | Medium (40-120) | Heavy (A>120) |
|---|---|---|---|
| LinearRegression | 0.99444 | 0.99768 | 0.99915 |
| RandomForest | 0.99002 | 0.98917 | 0.99960 |
| ExtraTrees | 0.99508 | 0.99317 | 0.99971 |
| GradientBoosting | 0.98847 | 0.99292 | 0.99970 |
| XGBoost_strong | 0.99165 | 0.99349 | 0.99965 |
| SVR_RBF_tuned | 0.97597 | 0.98129 | 0.99947 |
| MLP_3×256 | 0.99510 | 0.99495 | 0.99853 |
| QI-Kernel | 0.99048 | 0.98795 | 0.99892 |
| QI-Hybrid | 0.95168 | 0.99293 | 0.99932 |
| Q-Hybrid | 0.98959 | 0.99434 | 0.99963 |

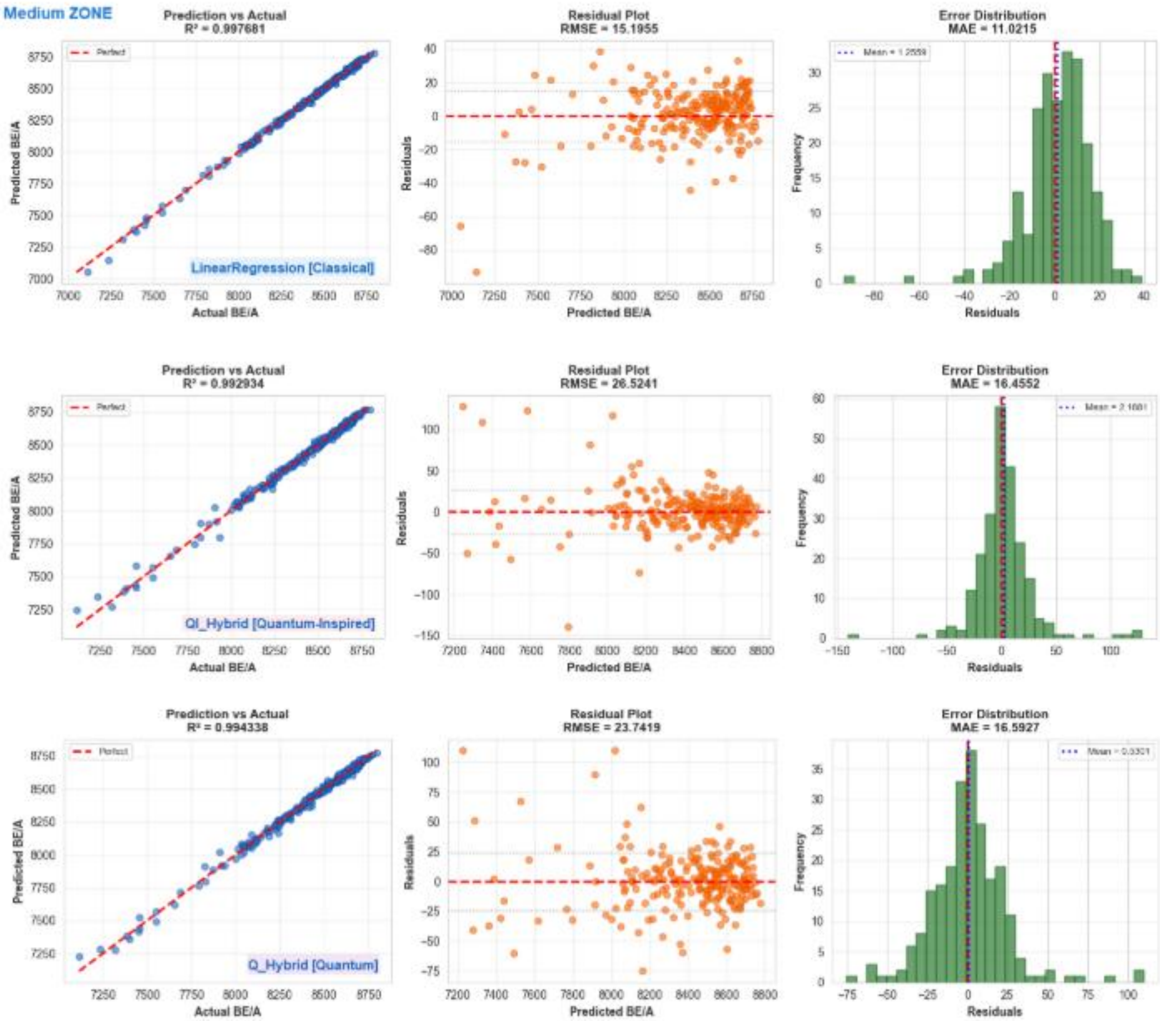
# RMSE Analysis — Error Across Mass Regions

*RMSE drops by ~one order of magnitude from Light → Medium → Heavy. The signal-to-noise ratio improves dramatically with nucleon number.*

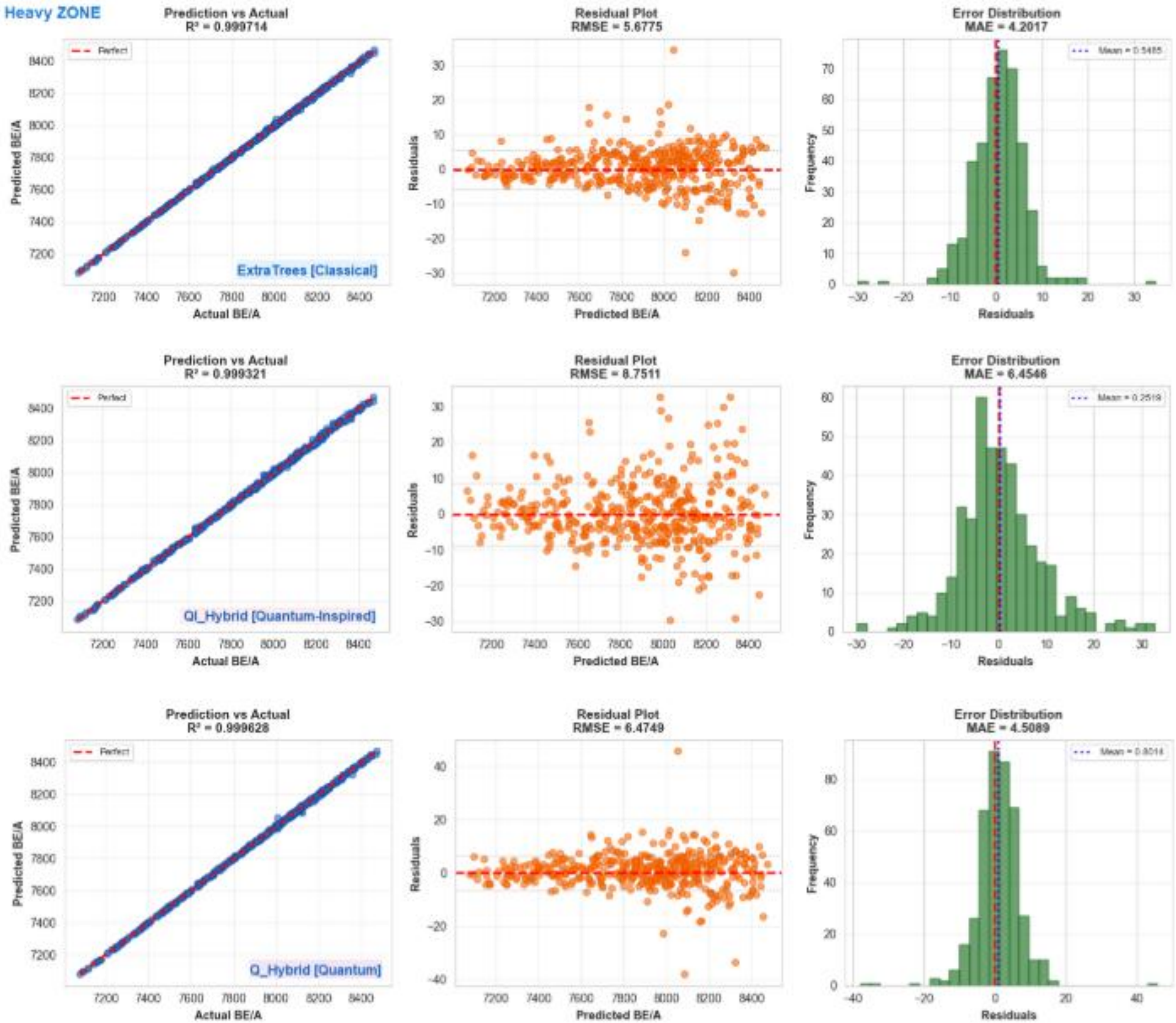



| Best Light Zone | Best Medium Zone | Best Heavy Zone | Worst (Light) | Q-Hybrid Heavy |
|---|---|---|---|---|
| **MLP: 81.8 keV** | **LinReg: 15.2 keV** | **ExtraTrees: 5.68 keV** | **QI-Hybrid: 256.9 keV** | **6.47 keV (≈ classical)** |


Light ZONE
Prediction vs Actual
R² = 0.995098
Perfect
MLP_3x256 [Classical]
Predicted BE/A
Actual BE/A
Residual Plot
RMSE = 81.8202
Residuals
Predicted BE/A
Error Distribution
MAE = 63.9884
Frequency
Residuals
Prediction vs Actual
R² = 0.990483
Perfect
QI_Kernel [Quantum-Inspired]
Predicted BE/A
Actual BE/A
Residual Plot
RMSE = 114.0056
Residuals
Predicted BE/A
Error Distribution
MAE = 87.4397
Frequency
Residuals
Prediction vs Actual
R² = 0.989591
Perfect
Q_Hybrid [Quantum]
Predicted BE/A
Actual BE/A
Residual Plot
RMSE = 119.2293
Residuals
Predicted BE/A
Error Distribution
MAE = 82.9461
Frequency
Residuals



Medium ZONE
Prediction vs Actual
R² = 0.997681
Perfect
LinearRegression [Classical]
Actual BE/A
Predicted BE/A
Residual Plot
RMSE = 15.1955
Residuals
Predicted BE/A
Error Distribution
MAE = 11.0215
Mean = 1.2559
Frequency
Residuals
Prediction vs Actual
R² = 0.992934
Perfect
QI_Hybrid [Quantum-Inspired]
Actual BE/A
Predicted BE/A
Residual Plot
RMSE = 26.5241
Residuals
Predicted BE/A
Error Distribution
MAE = 16.4552
Frequency
Residuals
Prediction vs Actual
R² = 0.994338
Perfect
Q_Hybrid [Quantum]
Actual BE/A
Predicted BE/A
Residual Plot
RMSE = 23.7419
Residuals
Predicted BE/A
Error Distribution
MAE = 16.5927
Frequency
Residuals


Heavy ZONE
Prediction vs Actual
R² = 0.999714
Perfect
Predicted BE/A
Actual BE/A
ExtraTrees [Classical]
Residual Plot
RMSE = 5.6775
Residuals
Predicted BE/A
Error Distribution
MAE = 4.2017
Frequency
Residuals
Prediction vs Actual
R² = 0.999321
Perfect
Predicted BE/A
Actual BE/A
QI_Hybrid [Quantum-Inspired]
Residual Plot
RMSE = 8.7511
Residuals
Predicted BE/A
Error Distribution
MAE = 6.4546
Frequency
Residuals
Prediction vs Actual
R² = 0.999628
Perfect
Predicted BE/A
Actual BE/A
Q_Hybrid [Quantum]
Residual Plot
RMSE = 6.4749
Residuals
Predicted BE/A
Error Distribution
MAE = 4.5089
Frequency
Residuals

# Classical + Quantum ML GUI Platform

**1**

### Data Config

Load AME2020 Excel or generate synthetic data. Select input features, target variable (BE/A). Live data preview. Missing value detection.

**2**

### Feature Eng.

Physics-aware templates: Basic Ratios, Asymmetry, Surface/Volume, Magic Numbers. Add custom algebraic expressions via formula editor.

**3**

### Model Config

Select Classical / Quantum-Inspired / Quantum models. Adjust hyperparameters (n_trees, depth, VQC layers) via sliders. PennyLane toggled here.

**4**

### Training

Choose mass region (All/Light/Medium/Heavy ). Set train-test split. Launch training. Real-time log shows $R^2$, RMSE, training time per model.

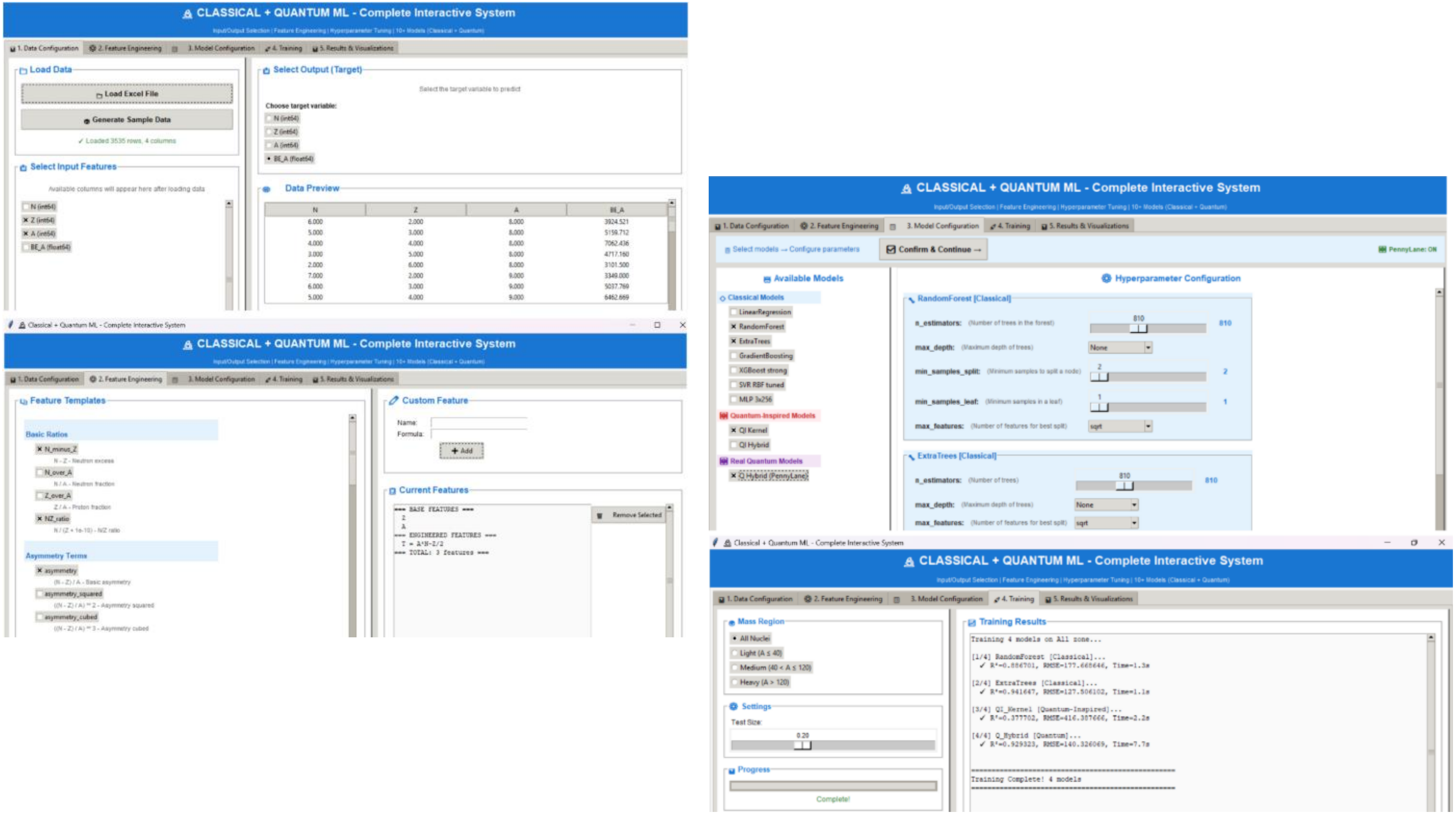
**5**

### Results & Viz

Summary table ($R^2$, $R^2$-gap, RMSE, time). Prediction vs Actual scatter plots. Overfitting & performance bar charts. Export results & figures.

### Platform Highlights

- ✓ 10+ classical + 3 quantum models in a single unified interface
- ✓ PennyLane integration for real variational quantum circuits
- ✓ Physics-aware mass region selection (Light / Medium / Heavy)
- ✓ Real-time overfitting detection and normalized performance scoring
- ✓ Exportable publication-ready plots and numerical results
- ✓ Extendable to any nuclear observable: radii, fission barriers, cross-sections


CLASSICAL + QUANTUM ML - Complete Interactive System
Input/Output Selection | Feature Engineering | Hyperparameter Tuning | 10+ Models (Classical + Quantum)
1. Data Configuration
2. Feature Engineering
3. Model Configuration
4. Training
5. Results & Visualizations
Load Data
Load Excel File
Generate Sample Data
✓ Loaded 3535 rows, 4 columns
Select Input Features
Available columns will appear here after loading data
N (int64)
Z (int64)
A (int64)
BE_A (float64)
Select Output (Target)
Select the target variable to predict
Choose target variable:
N (int64)
Z (int64)
A (int64)
BE_A (float64)
Data Preview
N Z A BE_A
6.000 2.000 8.000 3924.521
5.000 3.000 8.000 5159.712
4.000 4.000 8.000 7062.436
3.000 5.000 8.000 4717.160
2.000 6.000 8.000 3101.500
7.000 2.000 9.000 3349.000
6.000 3.000 9.000 5037.769
5.000 4.000 9.000 6462.669
Classical + Quantum ML - Complete Interactive System
Feature Templates
Basic Ratios
N_minus_Z
N - Z - Neutron excess
N_over_A
N / A - Neutron fraction
Z_over_A
Z / A - Proton fraction
NZ_ratio
N / (Z + 1e-10) - N/Z ratio
Asymmetry Terms
asymmetry
(N - Z) / A - Basic asymmetry
asymmetry_squared
((N - Z) / A) ** 2 - Asymmetry squared
asymmetry_cubed
((N - Z) / A) ** 3 - Asymmetry cubed
Custom Feature
Name:
Formula:
+ Add
Current Features
=== BASE FEATURES ===
Z
A
=== ENGINEERED FEATURES ===
T = A*N-Z/2
=== TOTAL: 3 features ===
Remove Selected
Select models → Configure parameters
Confirm & Continue →
PennyLane: ON
Available Models
Classical Models
LinearRegression
RandomForest
ExtraTrees
GradientBoosting
XGBoost strong
SVR RBF tuned
MLP 3x256
Quantum-Inspired Models
QI Kernel
QI Hybrid
Real Quantum Models
Q Hybrid (PennyLane)
Hyperparameter Configuration
RandomForest [Classical]
n_estimators: (Number of trees in the forest) 810
max_depth: (Maximum depth of trees) None
min_samples_split: (Minimum samples to split a node) 2
min_samples_leaf: (Minimum samples in a leaf) 1
max_features: (Number of features for best split) sqrt
ExtraTrees [Classical]
n_estimators: (Number of trees) 810
max_depth: (Maximum depth of trees) None
max_features: (Number of features for best split) sqrt
Mass Region
All Nuclei
Light (A ≤ 40)
Medium (40 < A ≤ 120)
Heavy (A > 120)
Settings
Test Size:
0.20
Progress
Complete!
Training Results
Training 4 models on All zone...
[1/4] RandomForest [Classical]...
✓ R²=0.886701, RMSE=177.668646, Time=1.3s
[2/4] ExtraTrees [Classical]...
✓ R²=0.941647, RMSE=127.506102, Time=1.1s
[3/4] QI_Kernel [Quantum-Inspired]...
✓ R²=0.377702, RMSE=416.387666, Time=2.2s
[4/4] Q_Hybrid [Quantum]...
✓ R²=0.929323, RMSE=140.326069, Time=7.7s
Training Complete! 4 models

# Conclusions

| | |
|---|---|
| **C1** | Three distinct learning regimes confirmed: Light (sparse/noisy), Medium (near-linear), Heavy (data-rich, nonlinear). No single model dominates all regions — physics-motivated region selection is essential for optimal performance. |
| **C2** | Extra Trees & Gradient Boosting win the Heavy Zone (RMSE ≈ 5.7 keV, $R^2$=0.9997). MLP_3×256 dominates the Light Zone (RMSE=81.8 keV). Linear Regression leads in Medium Zone (RMSE=15.2 keV). Model selection must match the physical learning regime. |
| **C3** | Q-Hybrid (true variational quantum circuit) achieves $R^2$=0.99963 in Heavy Zone — gap from best classical model is less than one ten-thousandth. The classical-quantum accuracy gap essentially closes when data are abundant and structurally rich. |
| **C4** | QI-Hybrid RMSE drops from 256.9 keV (Light) to 8.75 keV (Heavy) — a 30× improvement. Data quality determines quantum model success more than circuit architecture. Quantum-inspired models require dense, clean training data to reveal their potential. |
| **C5** | The developed GUI provides a complete, reproducible research platform: data loading → physics-aware feature engineering → classical+quantum training → diagnostic visualization. Exportable and extendable to any nuclear observable. |
| **C6** | Under realistic NISQ constraints, hybrid quantum architectures complement — rather than replace — state-of-the-art classical ML. This study establishes the first systematic benchmark for QML in nuclear mass modelling, pointing toward a quantum-enhanced future. |

# Thank You

**Prof. Dr. Serkan Akkoyun**

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## Key References

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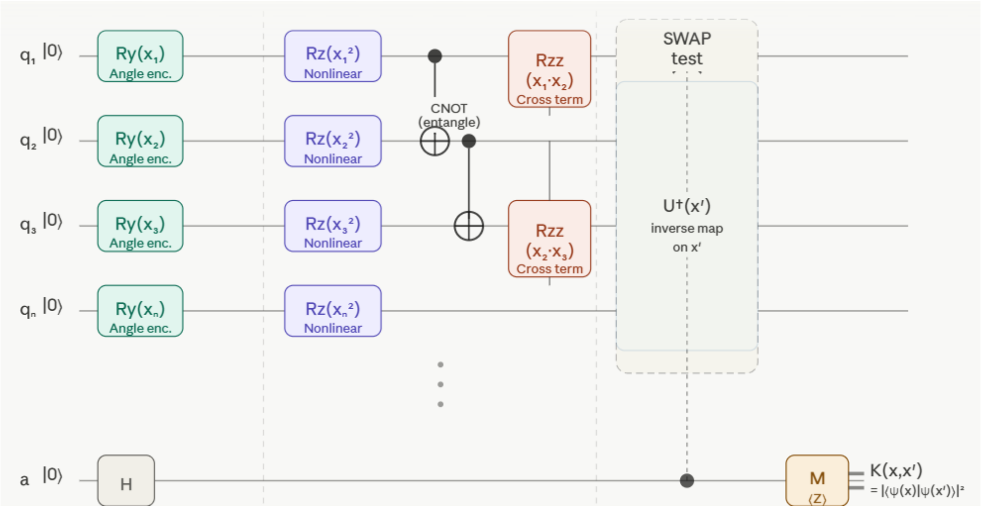
# Quantum-Inspired Kernel Regression (QI-Kernel)

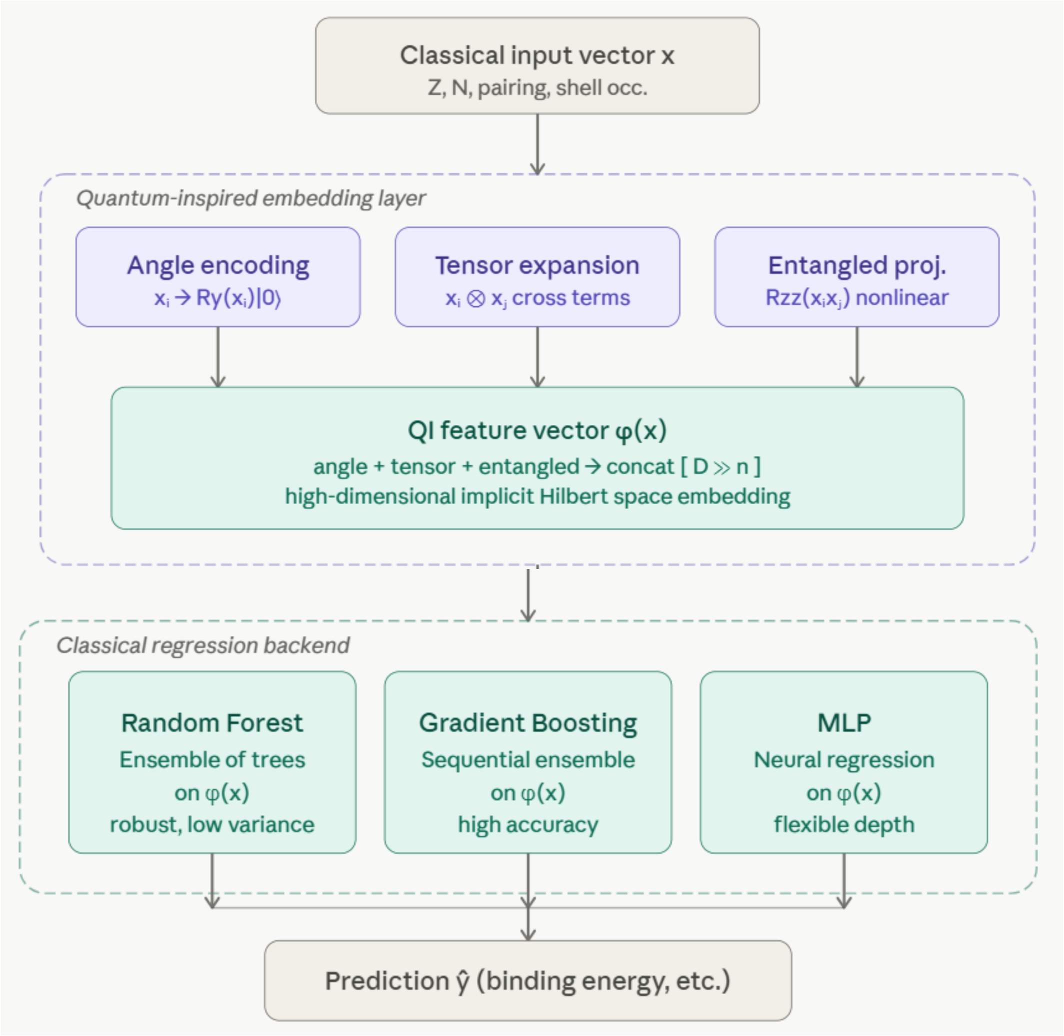
We have the properties of a kernel — numbers like Z=28, N=30. Instead of directly comparing them, we ask: "How 'similar' would these two kernels be in a quantum system?"

Step 1 — Angle encoding: We "write" each property $x_i$ to a qubit. We do this with a Ry($x_i$) gate. The Ry gate spins the qubit on a Bloch sphere.

Step 2 — Entanglement-style cross-terms: In real quantum computing, qubits are connected by CNOT gates, and this connection produces multiplications like $x_i \cdot x_j$. We calculate this mathematically in a classical computer — there are no real qubits, but the math is the same.

Step 3 — Kernel calculation: We calculate the quantum states $|\psi(A)\rangle$ and $|\psi(B)\rangle$ separately for the two kernels A and B. Then we take their inner product: $K(A,B) = |\langle\psi(A)|\psi(B)\rangle|^2$. If this number is close to 1, the two kernels are "very similar," and if it is close to 0, they are "very different."

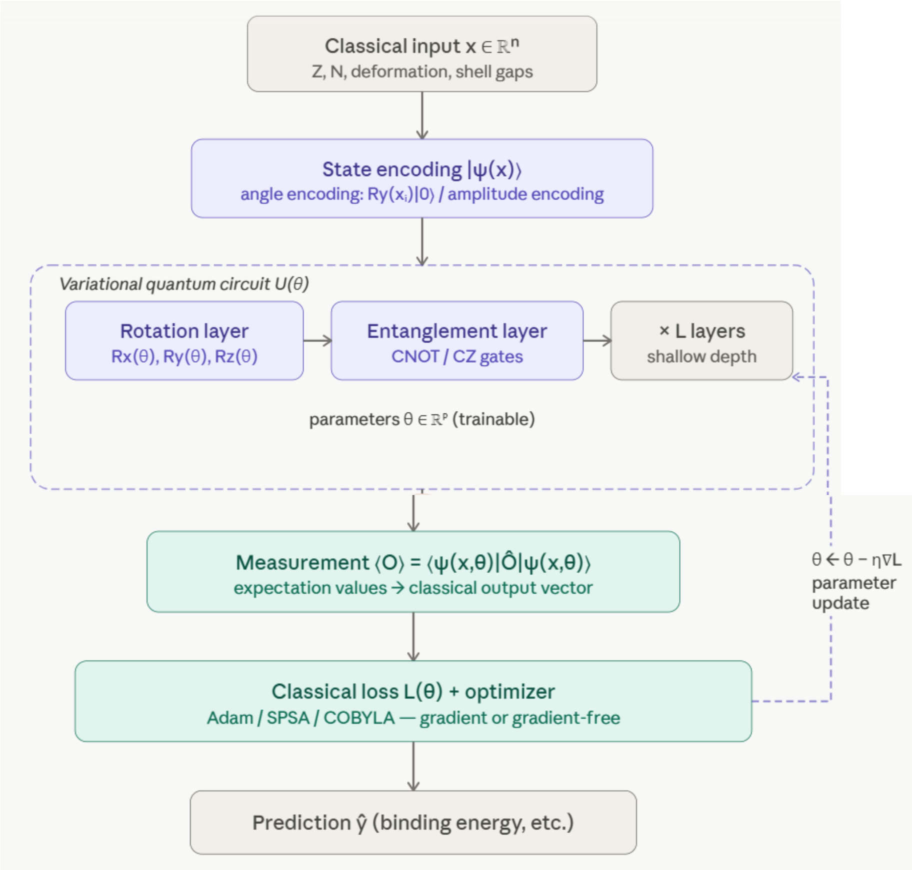





## Quantum-Inspired Hybrid Model (QI-Hybrid)

QI-Kernel calculated the similarity between two points. QI-Hybrid, on the other hand, transforms each point independently, generating a new, enriched feature vector.

They are given 3 numbers: A, Z, N. Instead of using these directly, you first derive 20 new features such as "$A^2$", "Z·N", "sin(N/100)". Then you make predictions using these 20 features. QI-Hybrid does the same thing — but its derivation rules come from quantum mechanics.




# Hybrid Quantum Machine Learning Model (Q-Hybrid)

This model is very different from the other two: the circuit parameters are not fixed, they are learned.

1. Write the data to the qubits: Encode the values $x_1$, $x_2$, $x_3$, $x_4$ to the qubits using $Ry(x_i)|0\rangle$.

2. Apply the variational layer: Three gates for each qubit in sequence: $Rx(\theta_1)$, $Ry(\theta_2)$, $Rz(\theta_3)$. These three gates move a qubit to any desired location on the Bloch sphere.

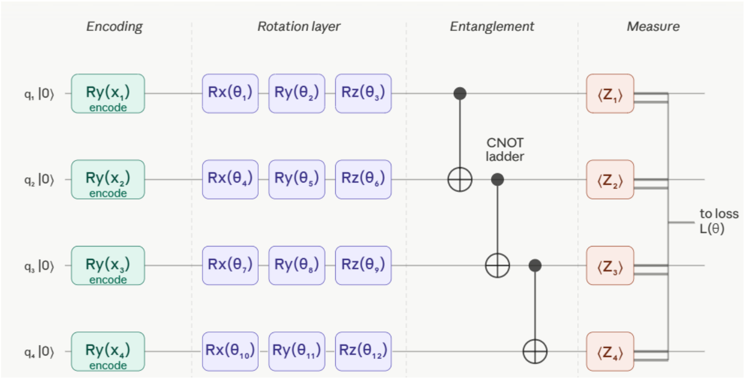
3. Add entanglement: Connect the qubits with CNOT gates: $q_1 \rightarrow q_2$, $q_2 \rightarrow q_3$, $q_3 \rightarrow q_4$. This allows the qubits to "know" each other.

4. Measure: Measure each qubit using the Pauli-Z operator. The result is a number between -1 and +1: $\langle Z_i \rangle$. These numbers are now classical numbers — they form a vector.

5. Calculate the loss: Generate a prediction from this vector, compare it to the actual value, and calculate the error.

6. Update the parameters: Apply a classical optimizer (Adam, SPSA...).

This cycle repeats hundreds of times — each time the circuit learns to make slightly better predictions.



# Physical Interpretation of Results

### Q Why does Linear Regression dominate the Medium Zone?

In the $40 \leq A \leq 120$ region, BE/A is nearly a linear combination of our engineered features ($A^{(2/3)}$, $Z^2/A$, $(N-Z)^2/A$, etc.) — which explicitly encode Bethe-Weizsäcker structure. A linear model therefore naturally captures most variance. Complex nonlinear models add parameters without adding useful signal in this regime.

### Q Why does MLP outperform quantum models in the Light Zone?

Light nuclei ($A<40$) show stochastic shell effects — pairing, clustering, halo phenomena — highly specific to individual nuclei. With only 292 data points, quantum models cannot tune their many parameters effectively. MLP's depth and regularization provide better noise tolerance, while VQCs face the barren plateau problem with sparse gradients.

### Q What makes the Heavy Zone ideal for Quantum ML?

With 2102 heavy nuclei, the dataset is rich enough that quantum-inspired feature geometry can be exploited. Heavy nuclei exhibit smooth collective phenomena (deformation, rotational bands) where nonlinear correlations across many features are systematic rather than random — exactly the pattern Hilbert space feature maps capture naturally.

### Q What does QI-Hybrid's 30× RMSE improvement tell us?

QI-Hybrid's RMSE drops from 256.9 keV (Light) to 8.75 keV (Heavy) — a 30-fold improvement. This is not hardware noise but data noise: tensor product expansions amplify measurement variance in sparse regions. In the Heavy Zone, the same expansions capture genuine physical feature interactions. Data quality matters more than circuit architecture for QML.

# Future Directions & Open Challenges

### Real Quantum Hardware

Execute Q-Hybrid circuits on IBM Quantum, IonQ, or Rigetti devices. Quantify decoherence and shot noise effects on nuclear regression accuracy. Benchmark simulator vs hardware results.

### Extended Observables

Apply the GUI framework to nuclear charge radii, β-decay half-lives, quadrupole deformation, neutron-capture cross-sections. Platform is observable-agnostic by design.

### Astrophysical R-Process

Predict masses of exotic neutron-rich nuclei beyond AME2020 for r-process nucleosynthesis. QML's Hilbert space extrapolation may reduce uncertainty in unexplored nuclear chart regions.

### Uncertainty Quantification

Integrate Bayesian neural networks and Gaussian processes alongside QML models. Provide prediction uncertainty bands — essential for astrophysical and reactor applications.

### Quantum Kernel Hardware

Implement quantum kernel estimation on real hardware. Bypass classical kernel approximation. Potential quantum advantage when n_features approaches hardware qubit limits.

### Fault-Tolerant QML

Transition from NISQ to fault-tolerant quantum computing will transform QML capabilities. Models developed here are designed to scale naturally onto future quantum processors.

*The transition from NISQ to fault-tolerant QC will be transformative. The hybrid framework developed here is designed to scale naturally onto future quantum processors.*