Uncertainty quantification in the Gamow Shell Model

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Nuclei near the drip lines are excellent examples of Open Quantum Systems. The development and implementation of new theoretical models to describe these systems have produced many interesting insights into underlying nuclear phenomena. This work outlines the general strategy for performing a full Bayesian uncertainty quantification for one such model - the Gamow Shell Model.

I. INTRODUCTION

Nuclear structure problems can be roughly classified into two groups, Closed Quantum Systems (CQS) and Open Quantum Systems (OQS). CQS-type problems treat an object as a completely isolated system from which no external factors can influence its properties. OQS are featured across physics from macroscopic, molecular, systems to mesoscopic, nuclear, systems and have shared phenomena in the form of resonances and scattering states.

In the nuclear context, the primary focus is to study weakly-bound states or resonances which are inherent to OQS. Resonances are particularly interesting as they are thought to be a result of coupling between bound and scattering states in nuclei and are typically found in the "Correlation dominated" region of Figure 1. For a more approachable definition of a resonance, we could say that it is associated with a specific energy which produces a substantial increase in the cross section of a nucleus (the probability of an interaction occurring). In other words, a resonance is a local band of an energy region where a projectile can alter the structure of a nucleus without ever being bound or knocking another particle from the target. Essentially, a resonance is a feature in a nucleus where the lifetime of exotic states is extended beyond what one might typically assume to be short lived in the CQS picture.

One framework which has been implemented to explore nuclear resonances and, more generally, continuum coupling is the Gamow Shell Model (GSM). Fundamentally, it is similar to the traditional nuclear shell model (SM) which is built on the assumption that nucleons (protons or neutrons) prefer to order themselves in a particular order. In the case of the ground state of a nucleus this ordering would be the configurations which minimize the total energy of the nucleus. Although this concept was proposed very early (1932) and has been refined over the decades (and GSM is one such refinement of the SM); there has been little effort taken in performing a full Bayesian study to quantify the uncertainties in these models. This paper will propose the general strategy one might take when performing uncertainty quantification (UQ) for GSM.

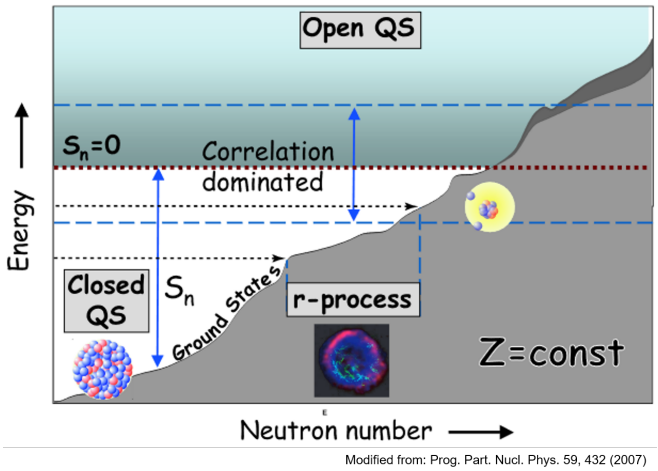

FIG. 1: Illustration of openness in nuclear systems and the emergence of exotic phenomena at energies closer to threshold ($S_n = 0$).

II. GSM FRAMEWORK

This section provides a brief overview of the important components to GSM which will be of interest when performing UQ, but a full description can be found in Ref. [1]. Fundamentally, since GSM is a SM extension, we are solving the Schrödinger equation

$$H\left|\Psi\right\rangle = \tilde{E}\left|\Psi\right\rangle, \quad \text{with} \quad \tilde{E} = E - \frac{i\Gamma}{2} \tag{1}$$

for a many-body system whose wave functions $|\Psi\rangle$ are represented by Slater Determinants, built from single particle states, and the complex energy eigenstate $\tilde{E}$ which contains a real energy (E) and the decay width of the system (Γ). The GSM Hamiltonian can be expressed as

$$H = \sum_{i}^{N_{\rm val}} \left[\frac{\vec{p}_i^{\,2}}{2\mu_i} + U_c(i)\right] + \sum_{i=1,j>i}^{N_{\rm val}} \left[V_{i,j} + \frac{\vec{p}_i\vec{p}_j}{M_c}\right] \tag{2}$$

with $N_{\rm val}$ denoting the number of valence nucleons and μ_i, M_c being the reduced mass of the nucleon and core respectively. U_c represents the core-nucleon potential (which contains Woods-Saxon (WS), spin-orbit, and

Coulomb terms)

$$U_c(r) = V_0 f(r) - 4V_{\ell s}\frac{1}{r}\frac{df(r)}{dr}\vec{\ell}\cdot\vec{s} + U_{\rm Coulomb}(r)$$
$$\text{where} \quad f(r) = \frac{-1}{1+\exp\left[r-R_0\right]/a}. \tag{3}$$

and $V_{i,j}$ being the valence nucleon-nucleon interaction. This Hamiltonian is written in terms of cluster-orbital shell model coordinates with respect to the core's center of mass. The valence nucleon-nucleon interaction is also written as

$$V = V_c + V_{\rm LS} + V_T + V_{\rm Coulomb} \tag{4}$$

with the central, spin-orbit, and tensor terms being based on the Furutani-Horiuchi-Tamagaki (FHT) force. These are written based on spin-isospin projectors (Π_{ST})

$$\begin{aligned} V_c(r) &= V_c^{11} f_c^{11}(r)\Pi_{11} + V_c^{10} f_c^{10}(r)\Pi_{10} \\ &\quad + V_c^{00} f_c^{00}(r)\Pi_{00} + V_c^{01} f_c^{01}(r)\Pi_{01} \\ V_{LS} &= \left(\vec{L}\cdot\vec{S}\right) V_{LS}^{11} f_{LS}^{11}(r)\Pi_{11} \\ V_T(r) &= S_{ij}\left[V_T 11 f_t^{11}(r)\Pi_{11} + V_T^{10} f_t^{10}(r)\Pi_{10}\right] \end{aligned} \tag{5}$$

where $\vec{L}$ is the relative orbital angular momentum, $\vec{S} = (\vec{\sigma_i} + \vec{\sigma_j})/2$, and $S_{ij} = 3(\vec{\sigma_i}\cdot\hat{r})(\vec{\sigma_j}\cdot\hat{r}) - \vec{\sigma_i}\cdot\vec{\sigma_j}$. The distance between nucleons i and j is represented by r_{ij} and $\hat{r} = \vec{r}_{ij}/r_{ij}$. It should be noted that there are a number of nucleon-nucleon interactions one could pick for V and this is just one possible case.

III. OBSERVABLES AND PRIORS

As we saw in Sec. II, there are a number of different parameters we can adjust in the Hamiltonian but the primary parameters which tend to be adjusted are the core-nucleon terms V_0 and $V_{\ell s}$ (for protons and neutrons) and the nucleon-nucleon FHT terms ($V_{\rm type}^{ij}$) in Eq. 5 (7 total). In total there could be 11 model parameters which would be contained in θ; however, the parameters were all optimized for light nuclei and are presented in Table I. These will serve as the starting point for our initial calculations and we note that only 4 of the nucleon-nucleon interaction parameters were nonzero. In other words, we will use these parameters for our priors $P(\theta)$ where $\theta = (V_0^p, V_{\ell s}^p, V_0^n, V_{\ell s}^n, V_c^{01}, V_c^{10}, V_c^{00}, V_T^{10})$ with 8 parameters.

In order to provide experimental insight into our calculations, we will choose to study the following nuclei (and their two lowest energy states): ^{6}Be$(0^+, 2^+)$, ^{6}Li$(1^+, 3^+)$, ^{6}He$(0^+, 2^+)$, ^{7}B$(3/2^-)$, ^{7}Be$(3/2^-, 1/2^-)$, ^{7}Li$(3/2^-, 1/2^-)$, and ^{7}He$(3/2^-)$. Due to instability in GSM calculations we will also only calculate ^{8}C(0^+) and ^{8}He(0^+). We will compare the state energies and decay widths (shown in Table II). Note, there are no experimental values reported for $1/2^-$ in ^{7}B and ^{7}He, so we did not include those observables.

TABLE I: Parameters optimized in Ref. [2] and their errors. When applicable, for the core-nucleon interactions only, we present the different parameters for protons and neutrons; otherwise, the parameters are shared for all nucleon types. Those parameters not listed are set to 0.

Parameter	Neutrons	Protons
V_0 (MeV)	39.5 (2)	42.1 (4)
$V_{\ell s}$ (MeV fm^2)	10.7 (2)	11.1 (5)
V_c^{01} (MeV)	-9.425 (70)	
V_c^{10} (MeV)	-8.309 (90)	
V_c^{00} (MeV)	-8.895 (1130)	
V_T^{10} (MeV)	-22.418 (970)	

Since GSM uses a complex energy formalism (Eq. 1) we will take the real and imaginary parts of the GSM complex energies to compare to the experimental energies and decay widths. This separation is justified as the two experimental observables are subject to different experimental error values. Also, this prevents us from having complex values in our likelihood function - keeping the formalism simple. This gives us 14 energies and 14 decay widths (28 observables total). Ideally, we would pick another quantity which is available across most nuclei to serve as another observable check (like RMS radius).

TABLE II: Experimental data for each nucleus. Energy is relative to α core i.e. $E = (4\times{}^4\text{He(BE/A)}) - (A\times{}^A_Z\text{X(BE/A)})$ and are taken from [3].

Nucleus	State	$E^{\rm exp}$ (MeV)	$\Gamma^{\rm exp}$ (keV)
^{6}Be	0^+	1.372 (9)	92 (6)
^{6}Be	2^+	3.042 (50)	1160 (60)
^{6}He	0^+	-0.975 (9)	0 ($\sim$ 0)
^{6}He	2^+	0.822 (5)	113 (20)
^{6}Li	1^+	-3.698 (3)	0 ($\sim$ 0)
^{6}Li	3^+	-1.512 (2)	24 (2)
^{7}He	$3/2^-$	-0.566 (11)	150 (20)
^{7}Be	$3/2^-$	-9.305 (10)	0 ($\sim$ 0)
^{7}Be	$1/2^-$	-8.876 (10)	0 ($\sim$ 0)
^{7}Li	$3/2^-$	-10.949 (6)	0 ($\sim$ 0)
^{7}Li	$1/2^-$	-10.472 (3)	0 ($\sim$ 0)
^{7}B	$3/2^-$	3.383 (10)	810 (20)
^{8}He	0^+	-3.101 (11)	0 ($\sim$0)
^{8}C	0^+	3.483 (23)	130 (50)

IV. CHOOSING OUR LIKELIHOOD FUNCTION

Now that we have data to compare to and have identified our priors we can begin to try to identify the form of our likelihood function. If we consider applying our model using the prior parameters identified in Table I, we can get an initial estimate of how our model might deviate from experiment. Assuming our model (y_i^{model}) is fixed and the deviation from experiment is

$$y_i^{\text{exp}} = y_i^{\text{model}} + \delta_i + \epsilon_i \tag{6}$$

where the experimental error for each measurement is ϵ_i, then the difference between experimental and model results when including said error is

$$\delta_i = y_i^{\text{exp}} - y_i^{\text{model}} - \epsilon_i. \tag{7}$$

Now, we can think of δ_i as a random variable because - assuming we find a reasonable form - it can be reproduced in such a way that any generated pseudo-data would be indistinguishable from the true data set. This concept is illustrated in Figure 2.

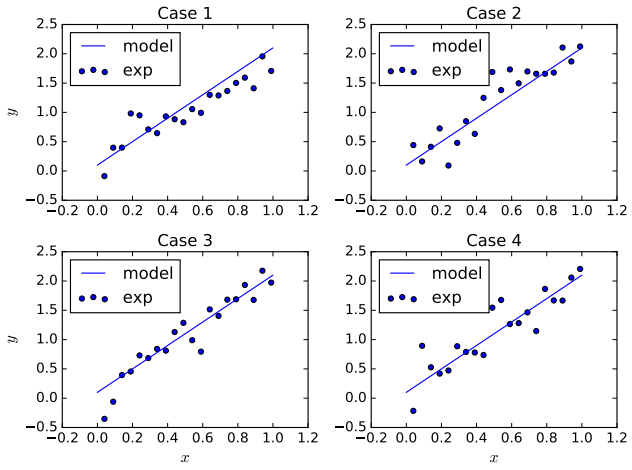

FIG. 2: Simple depiction of δ contribution to a system which is described as $y_i^{\text{exp}} = y_i^{\text{model}}(x) + \delta_i + \epsilon_i$ where $y_i^{\text{model}}(x) = \theta_1 x + \theta_2$. We see that if δ is treated as randomly distributed, we can generate data which is indistinguishable from the original dataset (set 1).

Since we're treating δ as a random variable, we can attempt to assign it to a distribution. Considering the difference between the model results (calculated with our parameters in Table I) and experiment we see in Figure 3 that the difference between the decay widths is centered about zero and would appear Gaussian. Unfortunately, it is harder to identify a reasonable distribution to assign the energies; however, as this paper is a preliminary discussion of the methods used, we can assign this as a Gaussian for simplicity at this point. Additionally, we will assume the experimental errors ϵ_i are all normally distributed.

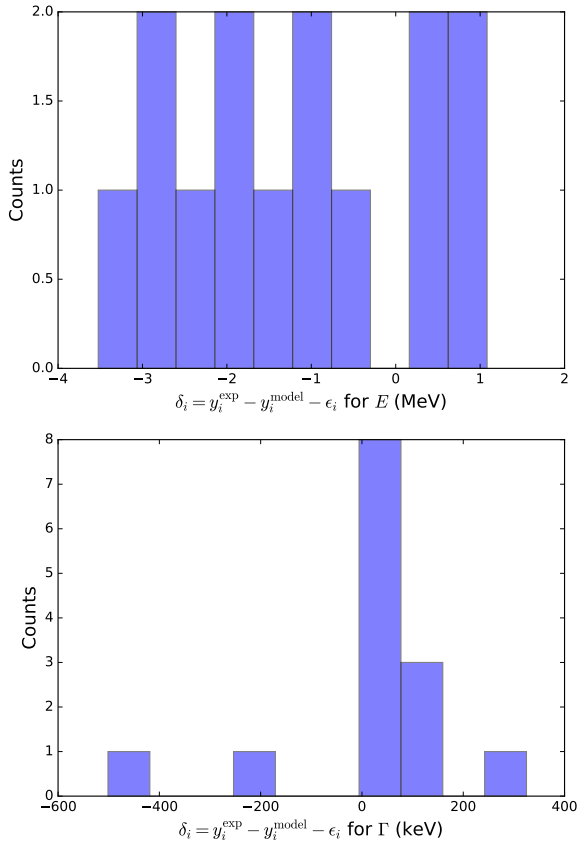

FIG. 3: Histograms of values of δ_i which were obtained with Eq. 7 using the initial GSM calculations and experimental data. Since we only have 14 experimental data points for each observable (28 total), we do not have enough points to generate a good Gaussian shape.

From this point, we have identified that both $\epsilon_i \sim \mathcal{N}\left(0, \left(\sigma_i^{\text{exp}}\right)^2\right)$ and $\delta_i \sim \mathcal{N}\left(0, \left(\sigma_i^{\text{model}}\right)^2\right)$. This makes the construction of our likelihood function easier as if we assume each measurement is independent of one-another then,

$$\begin{aligned} P(\boldsymbol{Y}|\theta) &= P(y_1|\theta)P(y_2|\theta)...P(y_N|\theta) \qquad (8)\\ &= \frac{1}{\left(2\pi\sigma_{\text{total}}^2\right)^{N/2}} \prod_{i=1}^{N} \exp\left(-\frac{(y_i^{\text{model}} - y_i^{\text{exp}})^2}{2\sigma_{\text{total}}^2}\right) \\ &= \frac{1}{\left(2\pi\sigma_{\text{total}}^2\right)^{N/2}} \exp\left(-\sum_{i=1}^{N} \frac{(y_i^{\text{model}} - y_i^{\text{exp}})^2}{2\sigma_{\text{total}}^2}\right) \qquad (9) \end{aligned}$$

where $\left(\sigma_i^{\text{total}}\right)^2 = \left(\sigma_i^{\text{exp}}\right)^2 + \left(\sigma_i^{\text{model}}\right)^2$. We can justify that these can be represented as a Gaussian as y_i^{model} is fixed while ϵ and δ (for both E and Γ) are both normally distributed - and the sum of two Gaussians is another

Gaussian.

V. CALCULATING THE POSTERIORS

To determine our posteriors, we simply need to follow Bayes theorem

$$P(\theta|\boldsymbol{Y}) \propto P(\boldsymbol{Y}|\theta)P(\theta). \tag{10}$$

and thus can begin our UQ process. It should be stated that the $P(\boldsymbol{Y})$ term will be accounted for when performing the Monte Carlo operations described below. Randomly sampling the parameter space θ from the likelihood allows us to generate a list of θ values for M sample sets, or $\theta_1, \theta_2, ...\theta_M$. When pulling a set of parameters from our likelihood, we will tend to randomly sample the regions centered around our priors. This is shown for V_0^p and $V_c^0 0$ in Figure 4 where we will have a Monte Carlo algorithm to sample the shaded region.

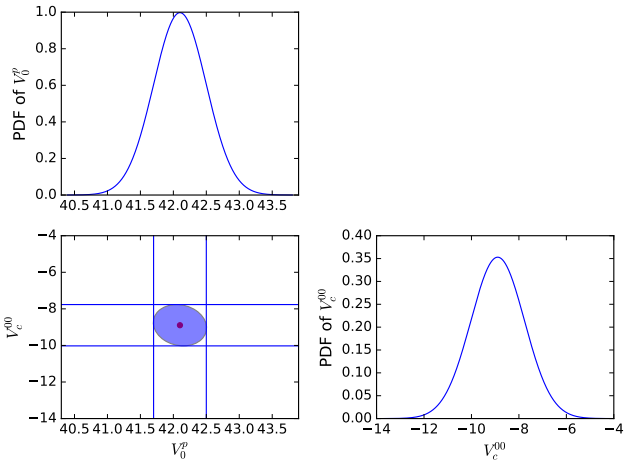

FIG. 4: Simplified depiction of sampling V_0^p and $V_c^0 0$ where the shaded region is centered about their prior value and the shaded area represents 1σ. Their PDFs are presented as well.

Based on other Bayesian studies of nuclear models [4, 5], the optimal approach is to use the Metropolis-Hastings algorithm for our Markov Chain Monte Carlo (MCMC) parameter sampling. This algorithm includes a random walk which has rejection criteria to effectively sample much of the shaded region in Figure 4 and traverse slightly outside it. The minimum required number of samples appears to be on the order of 10^5 samples per parameter [4, 5], but more would improve the fidelity.

This will prove to be a significant bottleneck in UQ of GSM as each calculation for the simplest nuclei will take ∼30 seconds on a personal computer. To speed up calculations, we can transition to large clusters like the High Performance Computing Center at Michigan State University however this will still be insufficient for more complex nuclei like ^{8}C which can take 12 hours per calculation. This could be an area to explore by using emulators as was done in Ref. [4]. In this case, we would introduce an emulator error term η which (like δ) represents the difference between the true model and the emulated version.

After using the Metropolis-Hastings algorithm to traverse our parameter space, we then input each parameter set (our $\theta_1, \theta_2, ...\theta_N$) into our model to compare their distributions to experiment (like was done in Figure 6 in Ref. [4]). This then allows us to give uncertainty values to our model predictions for each observable.

VI. CONCLUSIONS

The description of nuclei near the drip lines requires models which treat bound states, resonant states, and scattering states on equal footing, yet little work has been done to fully quantify their model uncertainties. In such exotic regions, where experimental errors are higher and the underlying physics is not as well understood, assigning uncertainties to our theoretical predictions is essential.

We have illustrated how one might approach full Bayesian UQ in GSM, but more investigation is needed. While the decay widths seem to generally follow a normal distribution, more information to identify the distribution of δ for the energies is required. Additionally, while performing this process for very light nuclei might be feasible with current computational resources, extending this to $A \geq 7$ may require the implementation of emulators to avoid run-time bottlenecks. Overall, there are a few dimensions to this issue which need to be explored further before implementing UQ on GSM.

[1] N. Michel and M. Płoszajczak Gamow Shell Model: The Unified Theory of Structure and Reactions. (Springer, Cham, Switzerland, 2021) https://www.springer.com/gp/book/9783030693558
.

[2] X. Mao, J. Rotureau,W. Nazarewicz, N. Michel, R. M.Id Betan,and Y. Jaganathen, Gamow-shell-model description of Li isotopes and their mirror partners. 2020. Phys. Rev. C **102**, 024309 (2020)
.

[3] http://www.nndc.bnl.gov/ensdf (2015)
.

[4] P. Giuliani, K. Godbey, E. Bonilla, F. Viens, J Piekarewicz, Bayes goes fast: Uncertainty Quantification for a Covariant Energy Density Functional emulated by the Reduced Basis Method. (2022) https://arxiv.org/

abs/2209.13039
.

[5] Habib N. Najm, Twelfth International Workshop on Measurement and Computation of Turbulent Flames: Uncertainty Quantification, Bayesian Inference, and Analysis of Models. (2014) https://www.osti.gov/servlets/purl/1497531
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