Temperature and Entropy in the Nuclear Shell Model

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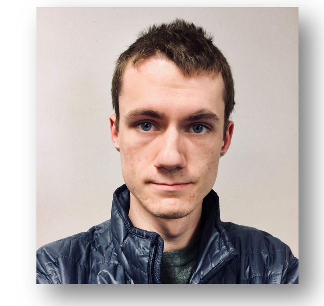
THE DEPARTMENT OF PHYSICS



Big Picture: Statistical physics in nuclear structure is a lesser known area of research in nuclear physics, yet it has the potential for revealing important properties of such systems. This is especially true in the modern reincarnation of statistical physics, quantum information theory (QIT). This intersection of information theory and quantum mechanics, which has applications to quantum computing and black holes, easily transfers to general quantum systems. In this work, I extent a statistical physics analysis of the nuclear shell model to include QIT.

Specific Question: Temperature and entropy have both quantum and statistical (classical) counterparts. We propose to compute the entropy and temperature of nuclear systems in the shell model framework using (1) The statistical distribution of energy levels in the nucleus (2) The quantum information entropy of the nuclear wave functions, and (3) the relatively novel proton-neutron entanglement entropy. We predict that (1) and (2) will show good agreement, being derived from the same statistical formalism, but that (3), a strictly quantum concept, will have different properties.

Interpretations of Entropy

Quantum Physics
A measure of missing information in our description of a system.
$$S = -\mathrm{tr}(\rho \log \rho)$$

Statistical Physics*
A measure of disorder, or complexity, of a system.
$$S = \log \Delta\Gamma$$

Extension to Entanglement Entropy

Quantum Physics
A measure of missing information in our restricted-to-a –subspace description of a system.

-equivalently-

A measure of mutual information dependence of subsystems.
$$S = -\mathrm{tr}(\rho_r \log \rho_r)$$

Statistical Physics
No immediate analog.

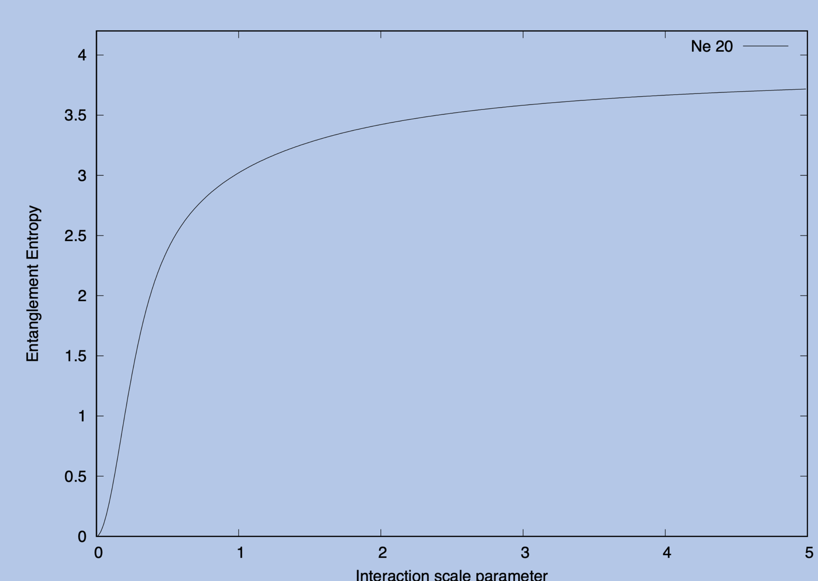


Fig 1. Proton-Neutron Entanglement Entropy study: Scaling the interaction between two subspaces.

$$\mathcal{H}_{total} = \mathcal{H}_p \oplus \mathcal{H}_n$$
$$\hat{H}_p \text{ on } \mathcal{H}_p; \hat{H}_n \text{ on } \mathcal{H}_n$$
$$\hat{H} = \hat{H}_p + \hat{H}_n + \lambda \hat{H}_{pn}$$
λ: Interaction scaling parameter

As expected, increasing the interaction strength increases the entanglement entropy! Mutual information dependence of the subsystems increases, and ignoring one subspace results in greater information loss.

Quantum Mechanics

Quantum mechanics deals with Hermitian operators $\hat{H}$ on a Hilbert space $\mathcal{H}$ (a vector space with additional features). The Schrodinger Equation
$$\hat{H}\Psi = E\Psi$$
is a description of the physical system in terms of a wave function $\Psi \in \mathcal{H}$, which represents a physical object like the nucleus. Solving the Schrodinger equation yields the wave function Ψ.

*Classical Statistical Physics

Temperature and Entropy

Temperature in thermodynamics is defined by a partial derivative:
$$\frac{1}{T} = \frac{\partial S}{\partial E}$$
I assume that the level density has a Gaussian form:
$$\Delta\Gamma(E) = \frac{N \exp\left[-\frac{(E-E_0)^2}{2k^2}\right]}{\sqrt{2\pi k^2}}$$
I then can write a form for the entropy:
$$S(E) = \log(N) - \log\left(\sqrt{2\pi k^2}\right) - \frac{(E-E_0)^2}{2k^2}$$
Finally, a form for the temperature:
$$T = \left(\frac{\partial S}{\partial E}\right)^{-1} = -\frac{k^2}{E-E_0}$$
I compute a temperature parameter k using three different methods: from the level density (statistical method), from the entropy, and from the proton-neutron entanglement entropy. In each case, I fit the corresponding functional form to the calculated data and extract the parameter k.

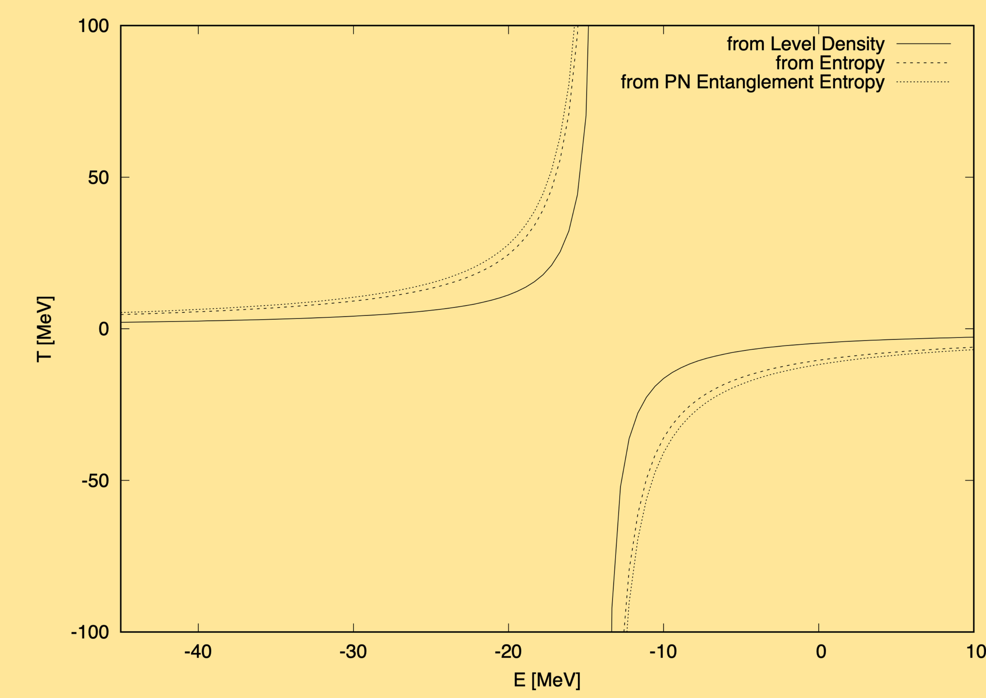


Fig. 2 Temperature for ^{20}Ne based on fits to the Level Density (Fig. 4), the wavefunction entropy (Fig. 2), and the proton-neutron entanglement entropy (Fig. 3). We see that the two quantum temperature calculations are in better agreement with each other than the statistical one.

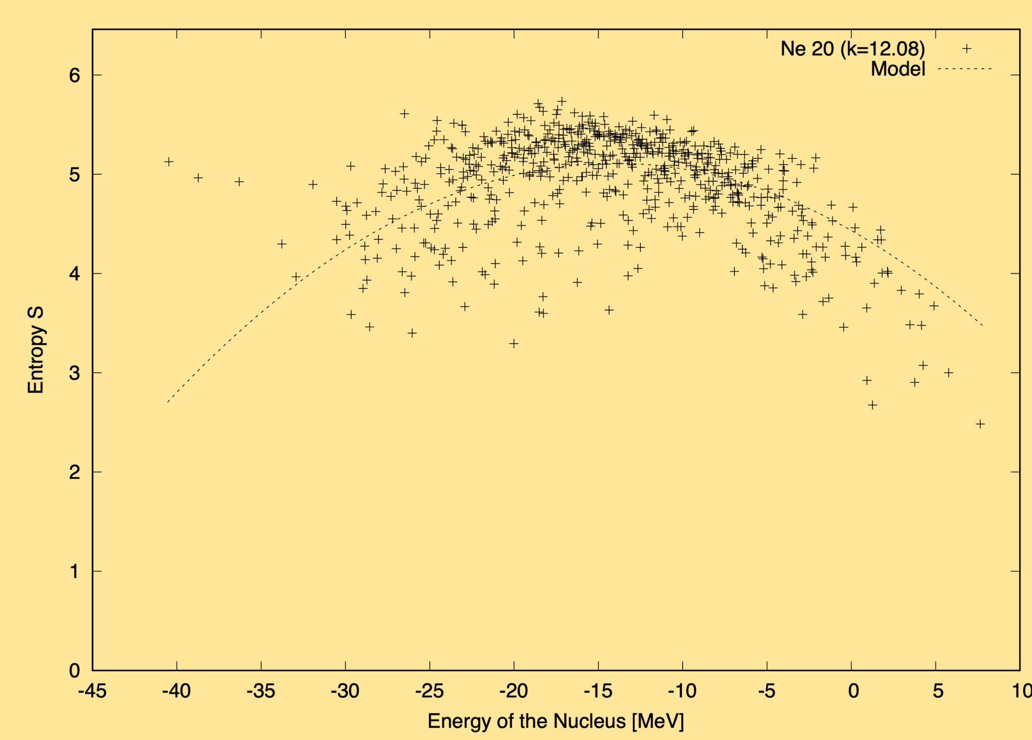


Fig. 3 Entropy computed for each excitation state's wave function. Temperature parameter k=12.1±0.4.

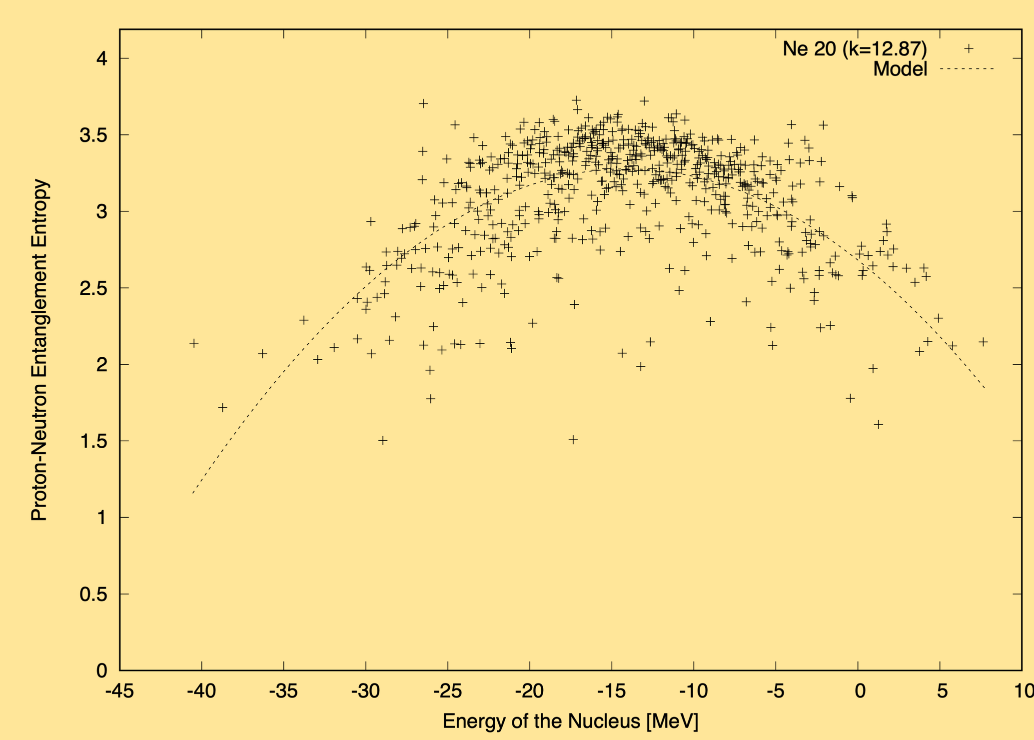


Fig. 4 Proton-Neutron Entanglement Entropy computed for each excitation state's wave function. Temperature parameter k=12.9±0.3.

Conclusions

The hypothesis was incorrect! I find that the proton-neutron entanglement entropy (3) has similar properties to the entropy computed using the nuclear wave functions (2). In particular, they both start out with low energy at low excitation energies, increase to some maximum value near the middle of the spectrum, and fall back down in a relatively symmetric way. Surprisingly, these two entropies also produce similar temperature constants. This is in contrast to the temperature constant computed using the level density (1), which is significantly smaller.

Level Density

Level density is the number of states that the system may occupy in a given energy interval ΔE:
$$\Delta\Gamma(E) = Number\ of\ levels\ between\ E \pm \Delta E$$

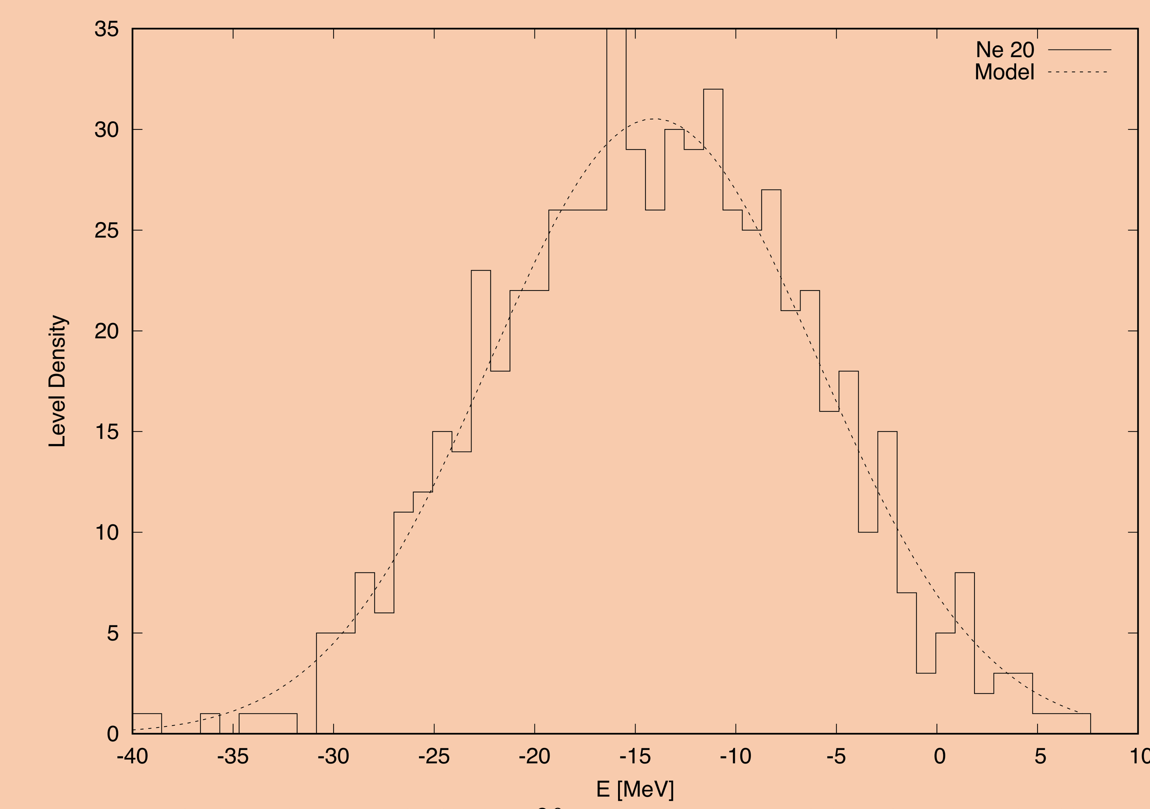


Fig. 5 Level density $\Delta\Gamma(E)$ for ^{20}Ne, computed in the *sd*-shell model space: number of levels at a given excitation energy. Distribution is roughly Gaussian and is fitted with a Gaussian model (dotted curve). Temperature parameter k=8.1±0.2.

Analysis

It turns out that there are some underlying problems in comparing the quantum definition of entropy and temperature to the statistical one.

Both entropy calculations shown in figures 3 and 4 have non-zero entropy for the ground state and nearby excited states. This means that the ground states do not have simple representations in the shell model basis. Figure 5, on the other hand shows that the level density falls off rapidly at the tails. Computing $S = \log \Delta\Gamma$ of this plot would therefore generate an entropy curve that falls off to zero at the boundaries. This is at odds with the previous observation. Furthermore, level density is independent of the choice of shell model basis, unlike for the quantum entropy.

The wider, larger k-parameter entropy curves from the quantum theory are indicative of the fact that the entropy, and therefore a level density computed from that entropy, does not go to zero at the boundaries.

It is interesting that the temperature computed from the proton-neutron entanglement entropy is close to the wave function entropy S. Future studies will investigate other entanglement entropies in the nuclear shell model and toy model systems.

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Oliver Gorton is a doctoral student with CSRC. His advisor is Dr. Calvin Johnson from the department of physics.

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