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Shannon Entropy for Ground State of Harmonium in Spherically Confined Plasma

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Harmonium is a system of two electrons whose Coulomb interaction with the nucleus is replaced with harmonic potential. Such a theoretical system is widely used for studying density functional theory, electron correlation, entanglement and black body entropy. It is of great importance to examine spherically confined harmonium in plasma environment, since the results can be useful for nanoelectronics as this system is similar to quantum dots under different confinements. It is well known that plasma environment provides screening effect, and it can be described using two potentials, Debye and Exponentially Cosine Screened Coulomb (ECSC) potential. Debye potential has the form $V(r) = \frac{1}{r}\ exp(-\frac{r}{\lambda})$, while ECSC potential has the form $V(r) = \frac{1}{r}\ exp(-\frac{r}{\lambda})\ cos(\frac{r}{\lambda})$, where λ is Debye radius and r is distance.

Shannon entropy is often used to quantify the degree of electron localization, structural characteristics, electron correlations, to name but a few. Shannon entropy is an information theory measure, and is defined as $S = -\int \rho(\mathbf{r})\ \ ln\rho(\mathbf{r})\ \ d\mathbf{r}$, where $\rho(\mathbf{r})$ is probability density for many-electron system. The smaller Shannon entropy is, the more concentrated the wave function of the state is and the accuracy in predicting the localization of electron is higher.

The goal of this study is to calculate Shannon entropy for the ground state of harmonium in spherically confined plasma and examine how it depends on relevant parameters. The relevant parameters that are varied are - Debye radius (λ), confinement radius of sphere (a) and force constant (ω). Shannon entropy is calculated for both potentials and the results are compared. In order to better examine the system, Shannon entropy is calculated for relative and center of mass motion separately, as well as the total entropy, for the ground state. All numerical calculations are performed by using the 2^{nd} order finite difference method.

It is shown that Shannon entropy for both potentials monotonically decreases to the value for the corresponding free system. It can be also noted that Shannon entropy for ECSC potential has slightly smaller values. On the contrary, it is observed that Shannon entropy increases with an increase of the radius of spherically confined plasma. Finally, it is demonstrated that Shannon entropy for both potentials gradually decreases with an increase of the force parameter (ω).

Primary author: SIMIĆ, Milena (Department of Physics, Faculty of Sciences and Mathematics, University of Niš)

Co-authors: STEVANOVIĆ, Ljiljana (Department of Physics, Faculty of Sciences and Mathematics, University of Niš); FILIPOVIĆ, Nikola (Department of Physics, Faculty of Sciences and Mathematics, University of Niš); PAVLOVIĆ, Vladan (Department of Physics, Faculty of Sciences and Mathematics, University of Niš); ANDREJIĆ, Nikola (Department of Physics, Faculty of Sciences and Mathematics, University of Niš)

Presenter: SIMIĆ, Milena (Department of Physics, Faculty of Sciences and Mathematics, University of Niš)

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