Shannon Entropy for Ground State of Harmonium in Spherically Confined Plasma

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Abstract

The harmonium embedded in spherically confined plasma is the subject of the present work. The ground state of the harmonium is computed using both Debye potential and exponentially cosine screened Coulomb potential for weak coupled and quantum plasma, respectively. Shannon entropies for center of mass and relative motion, as well as the total entropy are calculated. Dependence of the computed quantities on the parameters defining the screening potentials, confining potential and harmonium is then discussed.

Introduction

Harmonium is a two-electron system in which Coulomb interaction with the nucleus is replaced with harmonic potential. It is also often referred to as a Hooke's atom, due to used potential, or as a harmonic quantum dot [1]. This system is often used to test approximate electron structure methods [2], electron correlations, entanglement and black body entropy [3]. It is important to examine spherically confined harmonium in plasma environment, since the results can be useful for nano-electronics [4]. The study of structural properties, electron localization and electron correlations of two-electron systems embedded in plasma or in quantum dot can be useful for some applications. In the present work Shannon entropy is used to achieve that goal [5].

Theory

Hamiltonian of harmonium embedded in spherically confined plasma environment in atomic units is given by

$$H(\mathbf{r}_1,\mathbf{r}_2) = -\frac{1}{2}\Delta_1 - \frac{1}{2}\Delta_2 + \frac{1}{\omega}^{2}(r_1^2+r_2^2) + V(\mathbf{r}_{1,2}) + V_c(\mathbf{r}_1,\mathbf{r}_2)\,, \qquad (1)$$

where $\mathbf{r}_1$ and $\mathbf{r}_1$ are the radius vectors of electrons, ω is the force constant, V is the screening potential and V_c is the confining potential. For weakly coupled plasma the screening potential is Debye potential

$$V(\mathbf{r}_1,\mathbf{r}_2) = \frac{\exp\left(-|\mathbf{r}_1-\mathbf{r}_2|/\lambda\right)}{|\mathbf{r}_1-\mathbf{r}_2|}\,, \qquad (2)$$

and for dense quantum plasma is given by exponentially cosine screened Coulomb (ECSC) potential

$$V(\mathbf{r}_1,\mathbf{r}_2) = \frac{\exp\left(-|\mathbf{r}_1-\mathbf{r}_2|/\lambda\right)}{|\mathbf{r}_1-\mathbf{r}_2|}\cos\left(|\mathbf{r}_1-\mathbf{r}_2|/\lambda\right)\,. \qquad (3)$$

Parameter λ in (2) and (3) is the screening parameter. It depends on plasma temperature and density in (2), and on on plasma frequency and wave number in (3). It is supposed that the confining potential has the form of impenetrable sphere of radius a implying homogeneous Dirichlet boundary condition on the harmonium wave function.

Eigenvalue problem of Hamiltonian (1) is solved by dividing it in two parts: one describing the center of mass motion and the other part describing the relative motion. Then, energy and wave function of the harmonium take the form

$$E = E_{CM} + E_r \qquad (4)$$
$$\psi(\mathbf{r}_1,\mathbf{r}_2) = \psi_{CM}(\mathbf{R})\psi_r(\mathbf{r})\,, \qquad (5)$$

where $\mathbf{R} = (\mathbf{r}_1+\mathbf{r}_2)/2$ and $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ are the radius vectors of the center of mass and relative position of electrons, respectively.

Using wave functions in (5) Shannon entropies for center of mass and relative motion are calculated

$$S_{CM} = -\int \rho_{CM}(\mathbf{R})\ln\rho_{CM}(\mathbf{R})d\mathbf{R} \qquad (6)$$
$$S_r = -\int \rho_r(\mathbf{r})\ln\rho_r(\mathbf{r})d\mathbf{r}\,, \qquad (7)$$

where $\rho_{CM}(\mathbf{R})$ and $\rho_r(\mathbf{r})$ are the electron densities related with the center of mass and relative motion: $\rho_{CM}(\mathbf{R}) = |\psi_{CM}(\mathbf{R})|^2$ and $\rho_r(\mathbf{r}) = |\psi_r(\mathbf{r})|^2$. The total Shannon entropy, related with the wave function $\psi(\mathbf{r}_1,\mathbf{r}_2)$ is then obtained as

$$S = S_{CM} + S_r\,. \qquad (8)$$

Results

The eigenproblem of Hamiltonian (1) is solved numerically by finite difference method of the second order. The wave functions (5) are generated for the corresponding ground states of both center of mass and relative motion. The Shannon entropies (6) - (8) are calculated for both potentials (2) and (3) at different values of the radius of confining potential a, inverse values of the screening parameter λ and force constant ω.

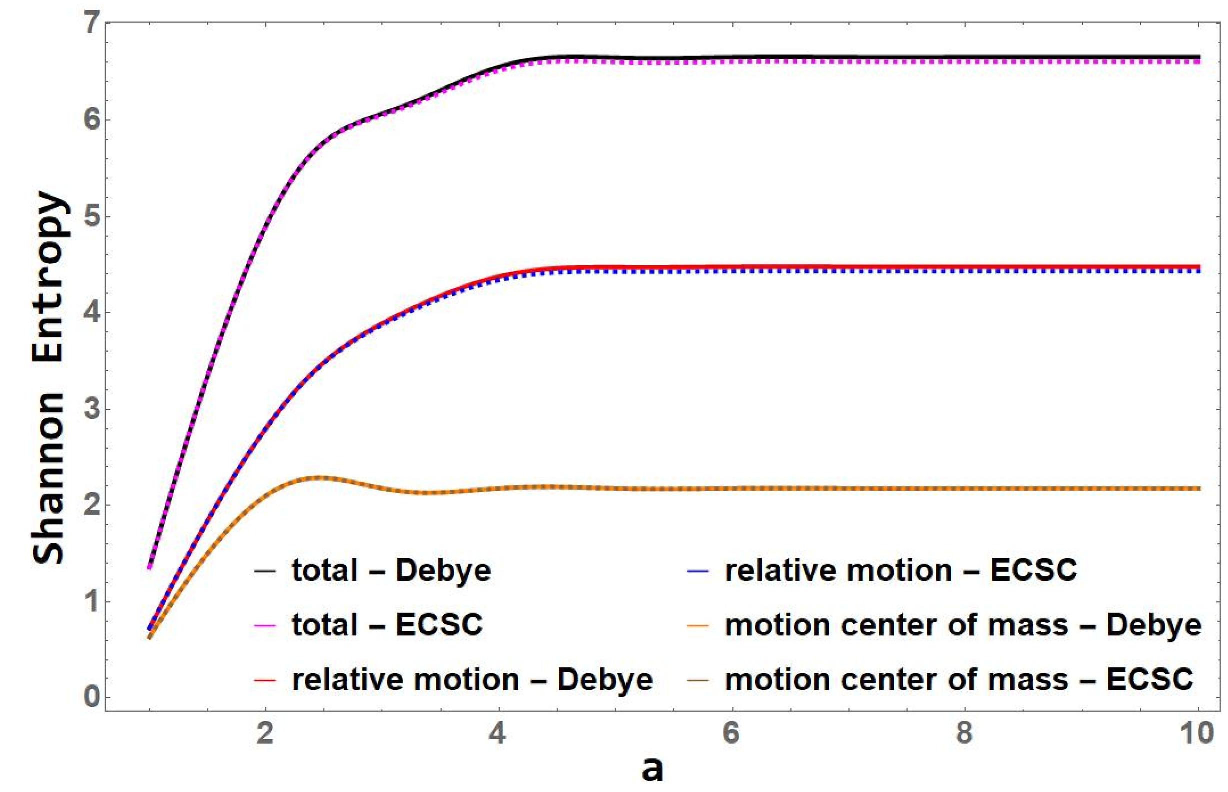

Figure 1: Variation of Shannon entropy with confinement radius, while $1/\lambda_d = 1$ and ω=1

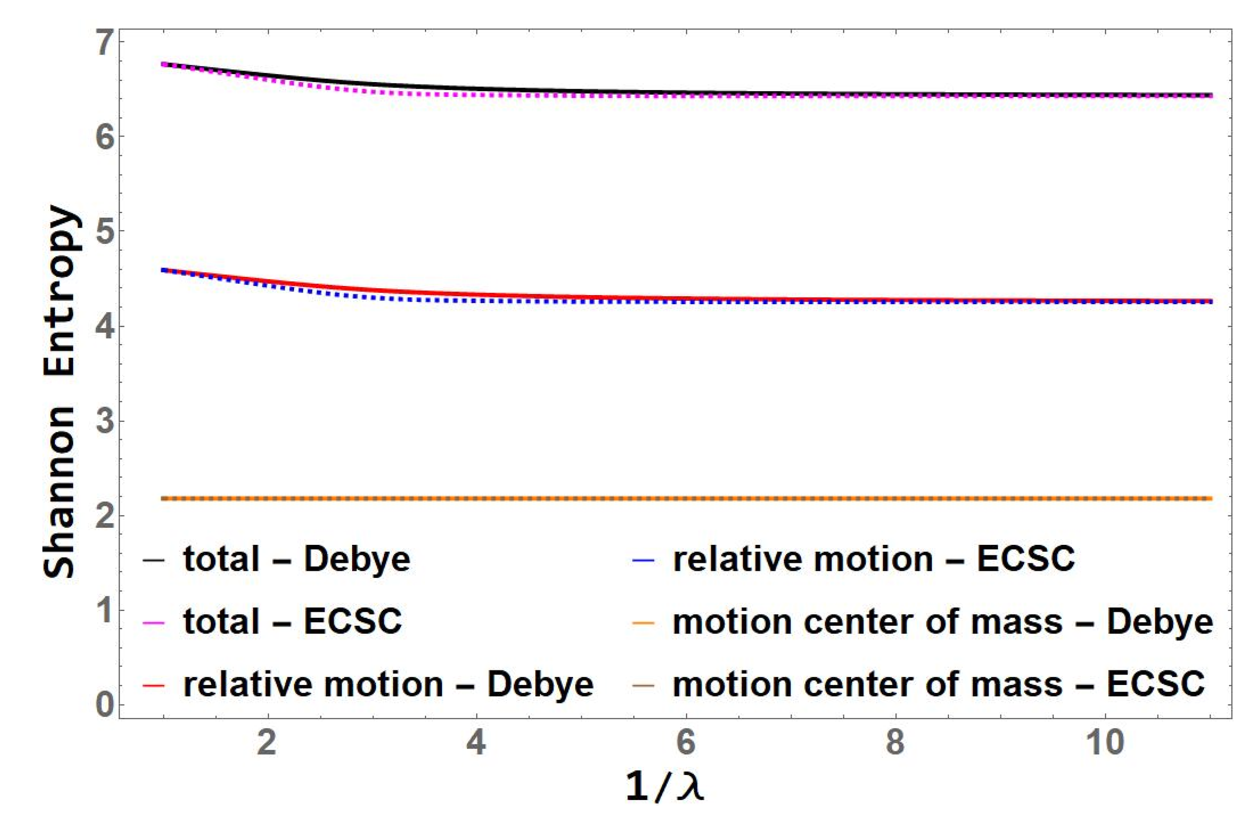

Figure 2: Variation of Shannon entropy with inverse of Debye radius, while $a = 5$ and $\omega = 1$

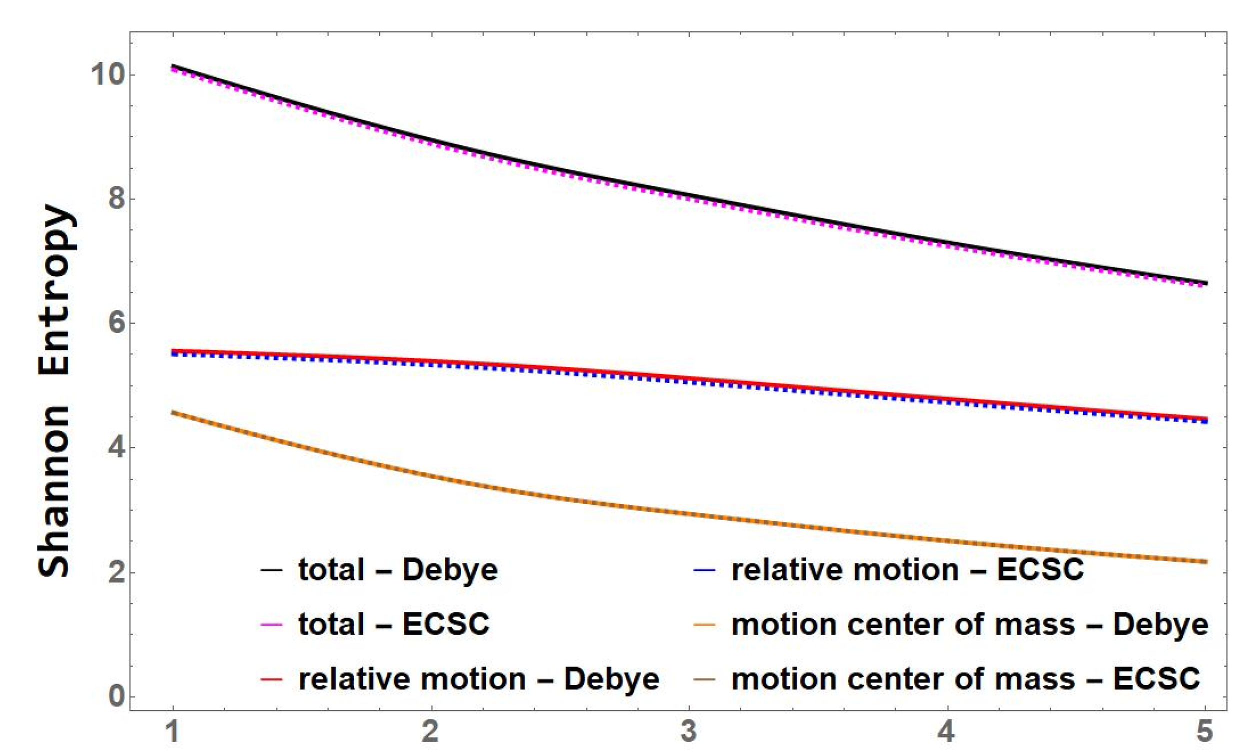

Figure 3: Variation of Shannon entropy with the force constant, while $a = 5$ and $1/\lambda_d = 1$

From the graphs shown in the figures above it can be seen that the values for Shannon entropy are slightly larger for Debye potential, but they follow the same trend for both potentials. This fact implies that the electron localization is slightly greater with ECSC potential compared to Debye potential. It can be noted that as the confinement radius increases, Shannon entropy increases until reaching a certain value (Fig. 1). As the inverse of λ increases, Shannon entropy stays almost the same (Fig. 2) and it decreases as force constant increases (Fig. 3).

References

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