Behavior of von Neumann entropy in atomic systems

Abstract
We show the behavior of the entanglement in atomic systems near the ionization threshold for both ground and first excited states. Bound and resonant states of two-electron quantum dot are studied using a variational expansion with a real basis-set functions. The von Neumann entropy is proposed as a method for the determination of the energy of a resonance.

Von Neumann Entropy
The von Neumann entropy $S$ is a measure of entanglement when consider pure quantum states. If we consider the ground state of the atomic system, the density matrix for a single electron, then $S$ is defined for:

$$S = -\sum_i \lambda_i \ln \lambda_i$$

where the $\lambda_i$'s are the eigenvalues of one-particle density matrix, which is

$$\rho = \text{Tr}_1 |\psi\rangle\langle\psi|$$

Where the $\psi$ is the two-particle wave function.

Different models of atomic systems

1) Spherical Helium: 
   $$H = \hbar^2 \frac{\nabla^2}{2m} - \frac{1}{r_1}$$

2) Helium: 
   $$V = \frac{1}{|r_1 - r_2|}$$

3) Quantum dot with a spherical well: 
   $$H = -\frac{\hbar^2}{2m} \nabla^2 + V(r_1) + V(r_2) + \frac{\alpha^2}{|r_2 - r_1|}$$ 
   $$V(r) = \begin{cases} V_0, & r < R \\ 0, & r \geq R \end{cases}$$

4) Quantum dot with an exponential well: 
   $$H = -\frac{\hbar^2}{2m} \nabla^2 - \frac{1}{r_1^2} - \frac{1}{r_2^2} - V_0 e^{-r_1} - V_0 e^{-r_2} + \frac{\alpha}{|r_2 - r_1|}$$
   $$V(r) = -(V_0/r_0) \exp(-r/r_0)$$

Von Neumann entropy for ground state
We analyze the scaling properties of the von Neumann entropy near the ionization threshold. Using the finite size scaling methods we calculate the critical charge and critical exponent associated to the von Neumann entropy.

Variational solution
The Hamiltonian is solved using the Ritz variational method with a complete basis. The number of elements of the basis is $M(N)$ and $N$ is the number of different radial functions used. In this way approximations to the eigenvalues of the Hamiltonian are obtained and the von Neumann entropy $E^{(N)}_\lambda(S^{(R)})$.

Possible basis are:

$$|\Phi_i\rangle \equiv \{|n_1, n_2; l\} = |\phi_n(r_1)\phi_n(r_2), \lambda^{n_1}_{n_2} (\Omega_1, \Omega_2) \rangle \chi$$

$$\lambda^{n_1}_{n_2} (\Omega_1, \Omega_2) = \frac{(-1)^{l_1}}{\sqrt{2l_1 + 1}} \sum_{m=\chi} (-1)^m Y_{m}^{l_1}(\Omega_1) Y_{m}^{l_2}(\Omega_2)$$

$$\phi_n^{(r)}(r) = \left[ \frac{\alpha^{2n+3}}{(2n+2)!} \right]^{1/2} r^n e^{-\alpha r^2}$$

$$\phi_n^{(r)}(r) = \sqrt{\frac{\beta^3}{4\pi(m+1)(m+2)}} e^{-\beta r} Y_{m}^{l_1}(\Omega_2)$$

The von Neumann entropy for excited states
In the figures we sketched qualitatively the envelope following the minima of the curves $S_1, S_2...$ This envelope is quite stable against $N$ and provides a method to obtain the real part of the energy of the resonant state.

Perspectives
The models presented here have spherical symmetry. We started to work with systems which have a constant magnetic field. In this case the symmetry is cylindrical and we need to study the behavior of the spins. For this reason, we need to change the variational basis considering angular moment different of zero.

References: