Behavior of von Neumann entropy in atomic systems

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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.

Different models of atomic systems

1) Spherical Helium: $H = h(1) + h(2) + \lambda V \qquad h(i) = \frac{1}{2}p_i^2 - \frac{1}{r_i}$

$\lambda = \frac{1}{Z} \qquad V = \frac{1}{r_>}$

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

3) Quantum dot with a spherical well:

$$H = -\frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}_1} - \frac{\hbar^2}{2m}\nabla^2_{\mathbf{r}_2} + V(r_1) + V(r_2) + \frac{e^2}{|\mathbf{r}_2 - \mathbf{r}_1|} \qquad V(r) = \begin{cases} -V_0, & r < R \\ 0, & r \geq R \end{cases}$$

4) Quantum dot with a exponential well:

$$H = -\frac{1}{2}\nabla^2_{\mathbf{r}_1} - \frac{1}{2}\nabla^2_{\mathbf{r}_2} - V_0 e^{-r_1} - V_0 e^{-r_2} + \frac{\lambda}{|\mathbf{r}_2 - \mathbf{r}_1|} \qquad V(r) = -(V_0/r_0^2)\exp(-r/r_0)$$

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, and ρ is the reduced density matrix for a single electron, then S is defined for:

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

when the λ's are the eigenvalues of one-particle density matrix, which is

$$\rho = \mathrm{Tr}_2 |\psi\rangle\langle\psi|$$

Where the ψ is the two-particle wave function.

Variational solution

The Hamiltonian is solved using the Ritz variational method with a complete basis {φ}. The number of elements of the base 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

$$E^{(N)}, \qquad S^{(N)}$$

Possible basis are:

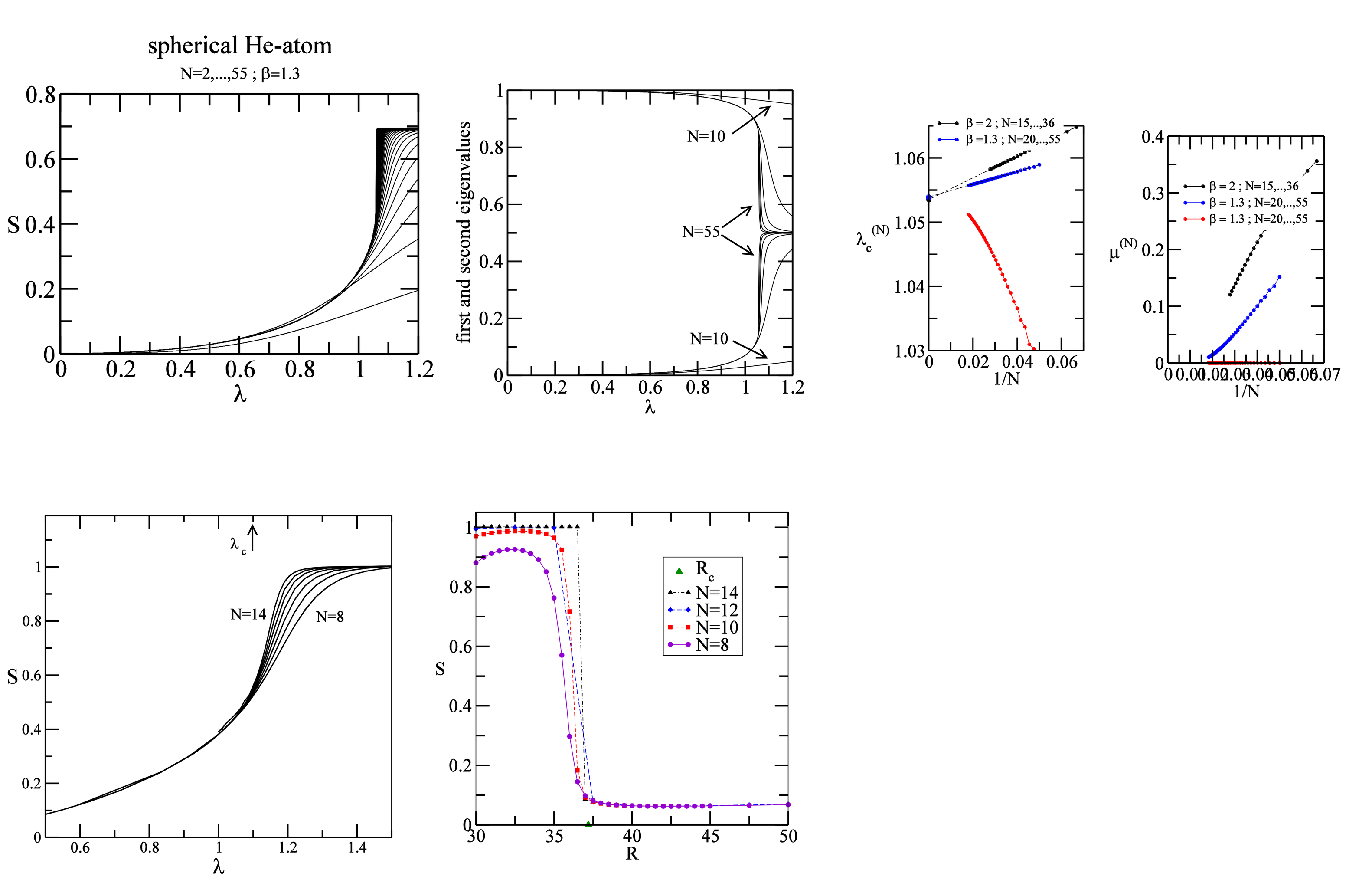
$$|\Phi_i\rangle \equiv |n_1, n_2; l\rangle = [\phi_{n_1}(r_1)\phi_{n_2}(r_2)]_s \mathcal{Y}^l_{0,0}(\Omega_1, \Omega_2)\chi_s$$

$$\mathcal{Y}^l_{0,0}(\Omega_1, \Omega_2) = \frac{(-1)^l}{\sqrt{2l+1}} \sum_{m=-l}^{l} (-1)^m Y_{lm}(\Omega_1) Y_{l-m}(\Omega_2)$$

$$\phi_n^{(\alpha)}(r) = \left[\frac{\alpha^{2n+3}}{(2n+2)!}\right]^{1/2} r^n e^{-\alpha r/2} \qquad \phi_m(r) = \sqrt{\frac{\beta^3}{4\pi(m+1)(m+2)}} e^{-\beta r/2} L_m^{(2)}(\beta r)$$

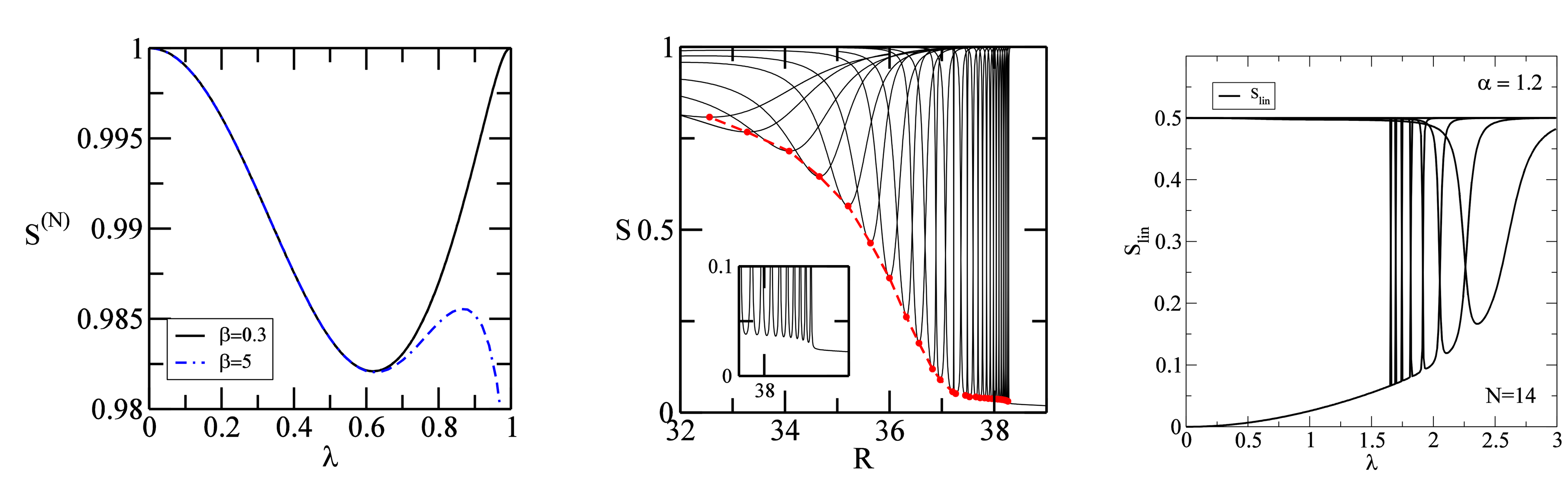
Von Neumann entropy for ground state

We analize 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.



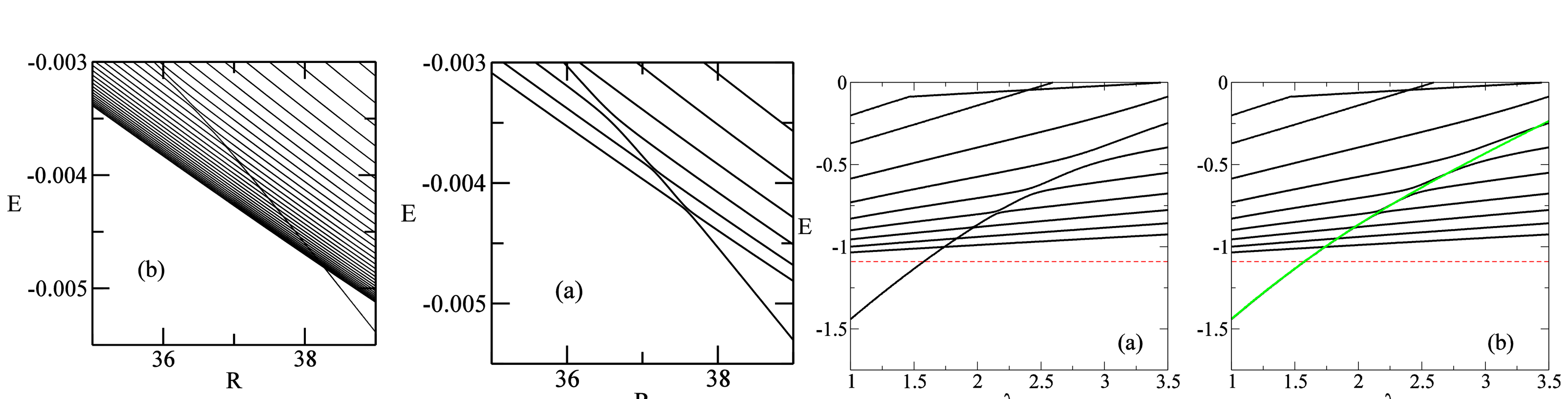
The von Neumann entropy for excited states

In the figures we sketched qualitatively the envelope following the minima of the curves S1, S2,… This envelope is quite stable against N and provides a method to obtain the real part of the energy of the resonant state.



Resonant states:

We have isolated complex eigenvalues, whose eigenfunctions are not square integrable. But this states can be analyzed using the spectrum obtained with a basis of square integrable functions.



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 staudy the behavior of the spins. For this reason, we need to change the variational basis considering angular moment different of cero.

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