Frozen Planet

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Article 1-Potential energy surfaces in atomic structure: The role of Coulomb correlation in the ground state of helium.

Abstract

"For the S states of two-electron atoms, we introduce an exact and unique factorization of the internal eigenfunction in terms of a marginal amplitude, which depends functionally on the electron-nucleus distances r1 and r2, and a conditional amplitude, which depends functionally on the interelectronic distance r12 and parametrically on r1 and r2." - Donde podemos mirar los conceptos básicos?, como lo de amplitud marginal... (Densidad de probabilidad) - La amplitud condicional la define uno? en que se basan para definir tales condicionales?

"Applying the variational principle, we derive pseudoeigenvalue equations for these two amplitudes, which cast the internal Schrodinger equation in a form akin to the Born-Oppenheimer separation of nuclear and electronic degrees of freedom in molecules." - Principio variacional? Método para no usar aproximaciones? Principio variacional, no se puede demostrar es un principio.

"The marginal equation involves an effective radial Hamiltonian, which contains a nonadiabatic potential energy surface that takes into account all interparticle correlations in an averaged way, and whose unique eigenvalue is the internal energy." - Trabajar en superficie de energía no abiabática significa trabajar sin aproximaciones? como es una superficie no adiabática? - Que el valor propio solo sea la energía interna es consecuencia de trabajar con superficies no adiabáticas o por como definen la la ecuación marginal?

"At each point (r1,r2), such surface is, in turn, the unique eigenvalue in the conditional equation. Employing the ground state of He as prototype, we show that the nonadiabatic potential energy surface affords a molecularlike interpretation of the structure of the atom, and aids in the analysis of energetic and spatial aspects of the Coulomb correlation, in particular correlation-induced symmetry breaking and quantum phase transition" - Con las superficias adiabáticas no se puede obtener la interpretación tipo molecular de la estructura del átomo?

"In the quantum-mechanical framework, this notion is put in on the basis of the topography of a Born-Oppenheimer (BO) potential energy surface (PES)" - La noción de que las moléculas y otros agregados atómicos poseen formas bien

definidas se puede basar en otro tipo de superficies de energía portencial o solo está la de BO?

- Cómo es un sistema doblemente excitado?

Concepts

- Conditional
- Marginal function