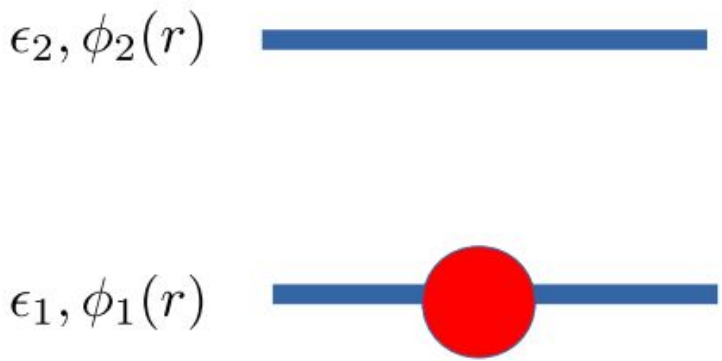
Exercises

RASESMA 2023

The Problem

Two levels system. Only level 1 occupied. No electron-electron interaction.



The Hamiltonian

1. Introduce the second quantization
2. Write the Hamiltonian

Densities and interaction

1. Calculate the bare electronic density $\mathrm{n}_0(r)$
2. Add to the Hamiltonian the interaction with an electric field oscillating at frequency ω
3. Calculate, within linear response, the change in the density induced by the interaction with the field $\Delta n(r,t)$

The electron-electron Interaction

1. Add to the Hamiltonian the electron-electron interaction assuming
   a. a constant integral of the Coulomb interaction, U
   b. zero self-interactions (no same indexes in the sum)
2. Under the above hypotheses demonstrate that the interaction term can be written as

$$H_{e-e} = \frac{U}{2} \sum_{ij} \hat{n}_i \hat{n}_j$$

With $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$

3. Calculate the Hartree-Fock potential and energies

The mean-field approximation

1. Assume now to replace the full electron-electron interaction (two bodies) with a mean-field approximation (one body)

$$\hat{H}_{e-e} \rightarrow \hat{V}_{e-e}$$

2. Within the mean-field approximation calculate the correction to the single-particle energies by using
   a. Static Rayleigh-Schrodinger Perturbation Theory
   b. Dyson equation