Introduction to Density Functional Theory (SS 2008)

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Problem set No. 1

Hand out : Thursday 17 April 2008
Hand in : Thursday 24 April 2008

1. The Rayleigh-Ritz principle for pure states

Given a Hamiltonian H with orthonormal eigenstates ψ_n (i. e. $< \psi_n \mid \psi_m >= \delta_{nm}$) and eigenvalues E_n obtained by:

$$H \; |\psi_n >= \; E_n \; |\psi_n > \tag{1}$$

with:

$$E_0 \leq E_1 \leq E_2 ... \tag{2}$$

(i.e. we allow for degeneracies).

(a) Prove that:

$$< \phi \; |H| \; \phi > \geq E_0 \tag{3}$$

for any normalized wavefunction ϕ. (2 points)

(b) In the case of q degenerate ground states, i.e. $E_0 = E_1 = \ldots = E_q$ and $E_{q+1} > E_q$, the orthonormal eigenstates $\psi_0, \ldots, \psi_q$ span a linear space $\mathbf{L}$. Prove that the " $=$ " sign in Eq. 3 holds if and only if $\phi \in \mathbf{L}$. (3 points)

2. The Hohenberg-Kohn (HK) theorem for degenerate systems

(a) Prove the HK theorem for degenerate systems, i.e. prove that the density of any one of the degenerate ground states uniquely determines the external potential. (3 points)

(b) Find an example where a given degenerate ground state density corresponds to two different ground state wavefunctions. (2 points)