Interesting title

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MONTH YEAR

Part a), setting up the basis.

Since we use hydrogen-like single particle states, we consider the quantum numbers nlm_lsm_s. We constrain ourselves to only look at $n = 1, 2, 3$, with $l = 0$ implying $m_l = 0$ In addition, since electrons are fermions, all single particle states (SPS) must have $s = 1/2$, giving two possible spin projections $m_s = 1/2, -1/2$, which we will write as $\uparrow, \downarrow$ respectively. Due to these restrictions, the only relevant quantum numbers are nm_s.

We begin by setting up an ansatz (educated guess) for the helium ground state $|\Phi_0\rangle$. The one body energy $\langle i|\hat{h}_0|i\rangle$ is increasing with n, thus it makes sense that the lowest energy multi particle state (MPS) should prioritize the $n = 1$ SPS. No two fermions can be in the same state, thus setting both electrons in $n = 1$ requires antiparallel spin. Thus, using the creation and annihilation operators $(a^\dagger_{nm_s}, a_{nm_s})$ from the second quantization formalism, we conclude:

$$|\Phi_0\rangle = a^\dagger_{1\uparrow} a^\dagger_{1\downarrow} |0\rangle$$

With $|0\rangle$ representing the vacuum state. Working with $|0\rangle$ becomes cumbersome when we wish to look at excitations of $|\Phi_0\rangle$, especially if $|\Phi_0\rangle$ contains many electrons. Therefor we "redefine the vacuum", that is set $|\Phi_0\rangle$ as the Fermi level. This means that we will add and remove particles from $|\Phi_0\rangle$ to represent excited states, instead of constructing these from $|0\rangle$. This introduces the language of *particles* and *holes*. A particle state is a filled state above the Fermi level, that is adding a $n = 2$ or 3 state to $|\Phi_0\rangle$. On the contrary a hole state is a non-filled state below the Fermi level, that is removing one of the $n = 1$ electrons from $|\Phi_0\rangle$. We will refer to hole states using letters $i, j, k, ...$ and particle states using letters $a, b, c, ...$.

Part b), Second quantized Hamiltonian.

Part c), Limiting ourselves to one-particle-one-hole excitations.

Part d), Moving to the Beryllium atom.

Part e), Hartree-Fock.

Part f), The Hartree-Fock matrices.

Part g), Writing a Hartree-Fock code.

A Appendix entry

some appendix things [1]

References

[1] John P. Perdew et al. "Understanding band gaps of solids in generalized Kohn–Sham theory". In: *Proceedings of the National Academy of Sciences* 114.11 (2017), 2801–2806. ISSN: 1091-6490. DOI: 10.1073/pnas.1621352114. URL: http://dx.doi.org/10.1073/pnas.1621352114.