Homework 2 (due on May 10th)

Problem 1 - doing quasi-degenerate perturbation theory carefully

Obtain the formulas for the 2nd order effective Hamiltonian by carefully retracing the steps from the lecture. We start with the Hamiltonian $H = H_0 + H_1 + H_2$ which acts on Hilbert space spanned by states from group A and group B, with $H_0 |n\rangle = E_n |n\rangle$, where n belongs to either A or B, and E_n are zeroth-order energies (the whole method is most useful when the zeroth-order energies of states from group A are well separated from zeroth-order energies of states from group B). The operator H_1 is block-diagonal (BD), i.e. it has nonzero matrix elements only within A or B. The operator H_2 is block off-diagonal (BOD) - it has only matrix elements between states from A and B. Both of them are treated as perturbation to H_0, and in order to make the book-keeping of orders of perturbation easier it is convenient to write the Hamiltonian as

$$H = H_0 + \lambda H_1 + \lambda H_2$$

and keep track of powers of λ in the derivations below.

We perform a unitary transformation $\tilde{H} = UHU^\dagger$ where $U = e^{-S}$. S has to be an anti-hermitian operator ($S^\dagger = -S$) for U to be unitary. We expand S in powers of λ:

$$S = \lambda S^{(1)} + \lambda^2 S^{(2)} + \dots$$

and we want construct such an approximation to S that the BOD terms in the effective $\tilde{H}$ vanish to given order in λ.

1. Prove (or at least check that it works as advertised in low orders of expansion) the Baker-Hausdorff lemma:
$$e^{-S} H e^{S} = \sum_{n=0}^{\infty} \frac{1}{n!} [H, S]^{(n)} \,,$$
where $[H, S]^{(n)} = [[\dots[H, S], S], \dots, S]$, and $[H, S]^{(0)} = H$.
Hint: Write S as $\alpha S'$ with α a dimensionless c-number, and differentiate the lemma with respect to α.

2. Check what happens when we multiply two BD operators, two BOD operators, or a BD with a BOD operator.

3. Using the B-H lemma write down the expressions for BD and BOD parts of the transformed Hamiltonian. Organize them by order in λ. See that requiring S to be BOD is a good decision.

4. Obtain the operator equation for $S^{(1)}$:
$$[H_0, S^{(1)}] = -H_2 \,.$$
Derive the operator equations for $S^{(n)}$ with $n = 2$ and 3.

5. Derive the operator formula for $\tilde{H}^{(2)}$, the lowest-order nontrivial term in $\tilde{H}$ (BTW, what is $\tilde{H}^{(1)}$?)

6. Write our the matrix elements of $\tilde{H}^{(2)}$.

7. Now assume that $E_n - E_l = \Omega + \delta_{nl}$ with for $n \in A$ and $l \in B$. Write the simplest approximation for $S^{(1)}$ and $\tilde{H}^{(2)}$ when $\delta_{nl} \ll \Omega$.

8. *Optional:* Derive the formula for $\tilde{H}^{(3)}$.

Problem 2

Apply the above method to problem 3 from the previous HW. Derive the effective Hamiltonian (to 2nd order in t) acting within the set A of singly-occupied orbitals (states in set B are the two doubly-occupied ones). As you know, it should have a form of Heisenberg Hamiltonian. Note that the eigenstate of the effective $\tilde{H}$ corresponding to $\approx -4t^2/U$ energy is **not the same** as the exact eigenstate that you derived previously. This difference comes from the fact that we have transformed the Hamiltonian, but we have neglected the transformation of states while doing the unitary transformation. Convince yourself that the inaccuracy caused in this way is small, and that it is physically more transparent to forget about it.

Problem 3

Consider the so-called *central spin Hamiltonian*

$$H = \Omega S^z + \sum_k \omega_k J_k^z + \sum_k A_k \mathbf{S} \cdot \mathbf{J}_k \ ,$$

where S is the central spin operator, J_k are the "environmental spins" (both S and J_k are spin 1/2), the energy splittings fulfill $\Omega \gg \omega_k$, and the couplings A_k are also $\ll \Omega$.
Derive the effective Hamiltonian for J_k spins to the second order in A_k. *Hint:* consider the two spaces corresponding to $S^z = 1/2$ and $S^z = -1/2$.
Completely optional additional question: is $A_k \ll \Omega$ enough for convergence of perturbation theory when we have N environmental spins in the problem?