Exam in Quantum Embedding Theory (M2 RCTGE course)

January 2022 – Duration: 30 minutes

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a) [**6 pts**] Briefly motivate and explain the concept of quantum embedding in electronic structure theory. **Hint:** *You are expected to explain, in your answer, why solving the electronic structure problem for strongly correlated molecular systems or materials is a challenging task, even when substantial simplifications are made, like in Kohn–Sham density-functional theory. You should then explain with simple words what a quantum embedding is, what it is made for, and what are the different ways it can be implemented. In case you decide to complement your answer with equations, you should always explain (with words) how to read them and how they are (or could be) used in practical calculations.*

b) [**1 pt**] Let $\tilde{\boldsymbol{\gamma}} \equiv \{\tilde{\gamma}_{JI}\}$ denote the ground-state one-electron reduced density matrix (1RDM) of a **non-interacting** electronic system. Explain why $\tilde{\boldsymbol{\gamma}}$ is an idempotent matrix, *i.e.*, $\tilde{\boldsymbol{\gamma}}^2 = \tilde{\boldsymbol{\gamma}}$. **Hint:** *Give the structure of the 1RDM in the basis of the molecular spin-orbitals (i.e., the basis that diagonalizes the one-electron Hamiltonian) and conclude.*

c) [**3 pts**] We recall that the matrix elements of $\tilde{\boldsymbol{\gamma}}^2$ read as $\left[\tilde{\boldsymbol{\gamma}}^2\right]_{JI} = \sum\limits_{K\geq 0} \tilde{\gamma}_{JK}\tilde{\gamma}_{KI}$. The $I = 0$ (so-called **impurity**) spin-orbital is embedded into the single $I = 1$ (so-called **bath**) spin-orbital when

$$\tilde{\gamma}_{K0} \underset{K\geq 2}{=} 0. \tag{1}$$

Show that, in the latter case, the idempotency of $\tilde{\boldsymbol{\gamma}}$ implies that

$$\left[\tilde{\boldsymbol{\gamma}}^2\right]_{J0} = \tilde{\gamma}_{J0}\tilde{\gamma}_{00} + \tilde{\gamma}_{J1}\tilde{\gamma}_{10} = \tilde{\gamma}_{J0}. \tag{2}$$

Conclude from Eqs. (1) and (2) that, when the impurity is not disconnected from the rest of the system (*i.e.*, $\tilde{\gamma}_{10} \neq 0$), we have $\tilde{\gamma}_{J1} = 0$ for $J \geq 2$. What is the physical implication of this key mathematical result?

d) [**2 pts**] The "impurity+bath" cluster contains $N^{\mathscr{C}} = 2\left(\tilde{\gamma}_{00} + \tilde{\gamma}_{11}\right)$ electrons. Show, by considering the particular case $J = 1$ in Eq. (2), that $N^{\mathscr{C}} = 2$. Why is this result particularly interesting from a quantum embedding point of view?