Product state and mean field theory

The mean field approach is a very powerful method to get insights into the physics of many-body quantum systems which relies on a strong approximation. Within the mean field approximation, one assumes that quantum correlations shall be neglected, that is, the many-body wave function is constrained to be the product state:

$$\left|\psi\right\rangle = \sum_{\{m\}} \psi^{m_1 \ldots m_n} \left|m_1\right\rangle \otimes \ldots \otimes \left|m_N\right\rangle$$

$$= \sum_{m_1=1}^{d} \psi^{(1)}_{m_1} \left|m_1\right\rangle \otimes \sum_{m_2=1}^{d} \psi^{(2)}_{m_2} \left|m_2\right\rangle \otimes \ldots \otimes \sum_{m_N=1}^{d} \psi^{(\mathrm{N})}_{m_N} \left|m_N\right\rangle$$

$$= \left|\psi^{(1)}\right\rangle \otimes \left|\psi^{(2)}\right\rangle \otimes \ldots \otimes \left|\psi^{(\mathrm{N})}\right\rangle$$

Thus, the object of study has been simplified from an exponential to a linear problem in the number of lattice sites N. An additional assumption results in a further simplification: imposing translational invariance-all $|\psi^{(\mathrm{j})}\rangle$ are equal-recast the original problem into a problem independent of the system of the system size N. Indeed, the number of d.o.f. is d^N in the original problem, Nd in the mean field scenario and only d in the translationally invariant one.

It is then not surprising that within the mean field approximation, efficient algorithms or even analytical solutions exists to very complex problems. However, the drawback of this powerful of this approach is the fact that the introduction of product state is, in general, unjustified and uncontrolled. Indeed, independent checks of the mean field approximation are always needed, either via comparison with experimental results or by other means. Nevertheless, whenever quantum correlations do not play a major role, the mean field approximation can be very powerful and, it can give a powerful insight in the physics of the system and can serve as a guide and starting point for further, more refined, analysis.

Matrix product state and CI?

Two Lectures on DMRG in Quantum Chemistry

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