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A Unified Theory of Chemical Reactions and Application to Biochemistry

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We consider an (elementary) chemical reaction as a transition between two electronic states where the transient electronic state is a combination of the initial and final electronic states (tight-binding approximation). Then the dynamics of the chemical reaction is formally identical to those of a quantum pseudo-spin $\frac{1}{2}$ σ coupled to the nuclei coordinates. The coupling of the spin component σ^z generates the reorganization of the environment due to the electronic charge and favors ionic states while the transverse coupling favors covalent bonds. Using a standard mean field approximation (equivalent to consider the nuclei as classical particles) and representing the nuclei of the environment as a collection of harmonic normal modes, the nuclei degrees of freedom can be eliminate so that the dynamics of the electronic state is described by an extended Nonlinear Discrete Schroedinger Equation on a dimer with extra dissipative terms and random forces (describing the thermal fluctuations). Assuming the only existence of the σ^z coupling (charge or ionic) coupling, we recover identically the standard theory of electron transfer (redox) where there is systematically an energy barrier (except at the inversion point) and thus which obeys the Arrhenius law. The only existence of the transverse coupling yields covalent bonds (which are barrierless). The interesting situation is obtained when both couplings are present because for well-tuned parameters, we may obtain (nearly) flat energy profile for electronic transitions. We believe that biochemical reactions are systematically in that regime because they operate at relatively low temperature and release little heat (at the scale of the room temperature energy). Using this paradigm as a guide for constructing models for enzymes, we propose some primitive toys models for ultrafast electron transfer, funneling, long distance signal propagation, biomotors, bioluminescence etc... Because of the fine tuning of our model parameters, easy control of their enzymatic functions by relatively weak external perturbations is possible. Our theory can be readily extended to situations involving more than two electronic states for producing more complex chemical reactions. We speculate about new perspectives for understanding highly complex enzymes as complex logical networks made of many units ("q-bits") operating cascades of elementary electronic transition according to pre-encoded rules.