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Variational Ground State Approach for A Tunnelling Exciton Coupled to Phonons

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Abstract: In this paper a variational study of a tunnelling exciton (Frenkel exciton) coupled to an arbitrary number of phonon modes is presented. The results of our model are presented both for weak non-adiabatic cases and for strong cases; and we come to the conclusion that the tunnelling reduction factor, the ground state energy of the tunnelling exciton-phonons system, and the mean number of ground state phonons, as the functions of the exciton-phonons coupling strength, are continuous, a condition that does not apply in cases of the tunnelling exciton-phonons models presented in the previous studies. In comparison with the previous studies, the presented model leads to a significant decrease of the ground state energy both of the small polaron and of the tunnelling exciton-phonons system, mainly for weak non-adiabatic cases.

Key Words: Hamiltonian, Ground state approximation, Vacuum state