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Propagation of strongly bound Frenkel excitons in LiF: An effective two-particle kinematic approach of super-atom in ab initio Wannier basis[1] CHEN-LIN YEH, HUNG-CHUNG HSUEH, Department of Physics, Tamkang University,Taiwan, WEI KU, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, NY, USA — A general new first-principles Wannier function based method is proposed to better understand the propagation of strongly bound Frenkel excitions. Specifically, long-standing debate of the Frenkel nature of the excitons in LiF is made apparent by the formation of a "super-atom" consisting of Wannier orbitals from both Li and F. On this basis, a new approach is proposed by formulating the kinematic contribution to the propagation of the exciton via an effective two-particle hopping kernel. The same kernel contains both the mass enhancement at strong binding and the decay into continuum at weak binding, and is thus exact in both limits. This kinematic effect is compared with found to overwhelm the conventional interaction-based propagations of exciton in LiF. This general theoretical framework can be directly applied to the study of propagation of local excitations of strongly correlated systems.

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