

Orbital choice in constructing model Hamiltonians

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Model Hamiltonians (e.g., for the Hubbard model, Heisenberg model, or Spin Hamiltonians) were originally developed to provide a clear human-understandable interpretation of various physical phenomena, and to establish a connection between experimental measurements and the underlying physical interactions. However, they rely on a notion of effective orbitals, which---although many options are available to quantitatively construct or approximate them---cannot be unambiguously chosen from physical principles alone. While the associated choices are rarely questioned in the literature, we have found that variations in the construction and shape of the effective orbitals significantly impact the parameters of model Hamiltonians and the spectra obtained with them. I will discuss how the choice of the model space and different localization schemes impact the quality of model Hamiltonians.