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Modeling quantum materials with disorder and interactions in and out of equilibrium

Realistic modeling of quantum materials with both interactions and disorder, while challenging, has been a fruitful endeavour in explaining and informing experiments in condensed matter physics. Disorder is not only ubiquitous, but has been shown to give rise to novel phenomena like localization, suppressed critical temperature and metal-insulator transition. Experimental investigations, which almost always deal with non-equilibrium conditions, necessitates a method capable of handling time-dependent systems. Recently, we have developed the DMFT-CPA quantum embedding framework, applicable to both systems in and out of equilibrium, which integrates dynamical mean field theory (DMFT) with the coherent potential approximation (CPA), and systematically probed the physics of the Anderson-Hubbard model subjected to various interaction quench protocols. Particular emphasis is placed on the influence of different disorder distributions, including box, binary, and Gaussian types. In equilibrium, it is seen that the types of disorder considered have qualitatively different effects on the phases, in particular, the binary disorder giving rise to a band insulating phase. Out of equilibrium, we compute the time evolution of single-particle distribution functions and the dynamics of energy following the quench, elucidating the role of disorder in shaping the relaxation pathways and thermalization behavior in strongly correlated, disordered quantum systems. We see that the different disorder types do not show any qualitative differences in the energy and occupation dynamics even in the large binary disorder case, where the equilibrium phase is a band insulator.

Topical Area

Hard matter: quantum, electronic, semiconducting materials

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