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Anderson localization for chemically realistic systems¹ HANNA TERLETSKA, Louisiana State University. Ames lab.

Disorder which is ubiquitous for most materials can strongly effect their properties. It may change their electronic structures or even cause their localization, known as Anderson localization. Although, substantial progress has been achieved in the description of the Anderson localization, a proper mean-field theory of this phenomenon for more realistic systems remains elusive. Commonly used theoretical methods such as the coherent potential approximation and its cluster extensions [1] fail to describe the Anderson transition, as the average density of states (DOS) employed in such theories is not critical at the transition. However, near the transition, due to the spatial confinement of carriers, the local DOS becomes highly skewed with a log-normal distribution, for which the most probable and the typical values differ noticeably from the average value. Dobrosavljevic et.al., incorporated such ideas in their typical medium theory (TMT), and showed that the typical (not average) DOS is critical at the transition. While the TMT is able to capture the localized states, as a local single site theory it still has several drawbacks. For the disorder Anderson model in three dimension it underestimates the critical disorder strength, and fails to capture the re-entrance behavior of the mobility edge. We have recently developed a cluster extension of the TMT, which addresses these drawbacks by systematically incorporating non-local corrections. This approach converges quickly with cluster size and allows us to incorporate the effect of interactions and realistic electronic structure. As the first steps towards realistic material modeling, we extended our TMDCA formalisms to systems with the off diagonal disorder and multiple bands structures. We also applied our TMDCA scheme to systems with both disorder and interactions and found that correlations effects tend to stabilize the metallic behavior even in two dimensions. [1] M. Jarrell and H. R. Krishnamurthy, Phys. Rev. B 63, 125102 (2001). [2] V. Dobrosavljevic et. al, Eur. Phys. Lett. 62, 76 (2003). [3] C. E. Ekuma et.al., Phys. Rev. B89, 081107 (2014).

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