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Computational studies of a 2D tight-binding model of randomly dispersed hydrogenic centers[1] JAYSON PAULOSE, Department of Physics, Princeton University, Princeton, NJ 08544; School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, RAVINDRA BHATT, Department of Electrical Engineering and Princeton Center for Theoretical Physics, Princeton University, Princeton, NJ 08544 — The impurity band arising from s-orbitals of randomly dispersed hydrogenic dopants in semiconductors in two dimensions is studied via exact diagonalization of a tight-binding model. Ensemble averaged density of states (DOS) and inverse participation ratio (IPR) of eigenstates are obtained as a function of energy at low to intermediate doping densities, where small clusters of sites are most significant. A similar calculation is done for p-orbitals for comparison. A strong peak in the DOS is seen about the impurity level. Increasing the density of sites weakens this peak and produces asymmetry in the DOS and the IPR. A nearest-neighbour pair approximation qualitatively explains several features in the DOS at low densities but does not reproduce the singularity. This motivates a comparison to a hierarchically constructed pair model, as well as random bipartite systems, which is pursued further via a renormalization group approach in a concurrent study.

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