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Effective Hamiltonian approach to bright and dark excitons in single-walled carbon nanotubes SANGKOOK CHOI, JACK DESLIPPE, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — Recently, excitons in single-walled carbon nanotubes (SWCNTs) have generated great research interest due to the large binding energies and unique screening properties associated with one-dimensional (1D) materials. Considerable progress in their theoretical understanding has been achieved by studies employing the ab initio GW-Bethe-Salpeter equation methodology. For example, the presence of bright and dark excitons with binding energies of a large fraction of an eV has been predicted and subsequently verified by experiment. Some of these results have also been quantitatively reproduced by recent model calculations using a spatially dependent screened Coulomb interaction between the excited electron and hole, an approach that would be useful for studying large diameter and chiral nanotubes with many atoms per unit cell. However, this previous model neglects the degeneracy of the band states and hence the dark excitons. We present an extension of this exciton model for the SWCNT, incorporating the screened Coulomb interaction as well as state degeneracy, to understand and compute the characteristics of the bright and dark excitons, such as the bright and dark level splittings. Supported by NSF #DMR07-05941, DOE #De-AC02-05CH11231 and computational resources from Teragrid and NERSC.

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