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Impurity-based Quantum Circuits in Si

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Recent advances in manipulation of impurities in Silicon by STM techniques, both dangling bonds on Si surface [1] and dopant atoms in Si [2], enable the realization of atomic scale circuits in Si. In this work we focus on phosphorus (P) donors in Si [3]. The 6-fold degenerate conduction band of Si combined with valley-orbit coupling results in a manifold of 6 states of a single P donor. We describe a quantum circuit of P atoms in Silicon with electron population controlled by external gate in analogy to gated quantum dots in GaAs [4]. The electronic properties of these atomic scale quantum dot circuits (QDC), including intra- and inter donor exchange, are described by an extended Hubbard-Kanamori Hamiltonian (HK). The HK parameters show strong dependence on the position of substitutional donors in the Si lattice including on site Coulomb repulsion (U), interdot hopping (t), direct interaction (V) and exchange (J) terms. The interdot, t, V and J, terms strongly depend on dopant position (R_D) in Si lattice—small changes in R_D strongly impact these parameters. We study the influence of QDC design, chains and rings, and how disorder in R_D impacts QDC electronic properties, in particular the interplay of disorder and interactions. With no disorder in R_D the energy spectrum (ES) of quantum dot chain at half-filling as a function of U/t (V,J =0) shows a transition from spectrum dominated by kinetic energy ($U/t \ll 1$) to ES dominated by Coulomb interactions for $U/t \gg 1$. For weak (strong) interactions the excited states group by single particle energy spacing (Hubbard bands). In the noninteracting regime, disorder leads to electron localization. Using Lanczos and Density Matrix Renormalization Group approaches we explore the effect of interactions and disorder on atomic scale circuits in Si and potential many-body localized phases in the HK model [5].

References

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