Abstract Submitted for the MAR05 Meeting of The American Physical Society

Quantum Corral Wave-function Engineering ALFREDO CORREA, Department of Physics, University of California at Berkeley and Lawrence Livermore National Laboratory, FERNANDO REBOREDO, Lawrence Livermore National Laboratory, CARLOS BALSEIRO, Centro Atómico Bariloche and Instituto Balseiro — We present a theoretical method for the design and optimization of quantum corrals^[1] with specific electronic properties. Taking advantage that spins are subject to a RKKY interaction that is directly controlled by the scattering of the quantum corral, we design corral structures that reproduce spin Hamiltonians with coupling constants determined a priori[2]. We solve exactly the bi-dimensional scattering problem for each corral configuration within the s-wave approximation [3] and subsequently the geometry of the quantum corral is optimized by means of simulated annealing[4] and genetic algorithms[5]. We demonstrate the possibility of automatic design of structures with complicated target electronic properties [6]. This work was performed under the auspices of the US Department of Energy by the University of California at the LLNL under contract no W-7405-Eng-48. [1] M. F. Crommie, C. P. Lutz and D. M. Eigler, Nature 403, 512 (2000) [2] D. P. DiVincenzo et al., Nature 408, 339 (2000) [3] G. A. Fiete and E. J. Heller, Rev. Mod. Phys. 75, 933 (2003) [4] M. R. A. T. N. Metropolis et al., J. Chem. Phys. 1087 (1953) [5] E. Aarts and J. K. Lenstra, eds. Local search in combinatorial problems (Princeton University Press, 1997) [6] A. A. Correa, F. Reboredo and C. Balseiro, Phys. Rev. B (in press).

> Alfredo Correa Department of Physics, University of California at Berkeley and Lawrence Livermore National Laboratory

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