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A quantum Monte Carlo study of a spherical jellium with an embedded impurity MICHAL BAJDICH, FERNANDO A. REBOREDO, G. MALCOLM STOCKS, Materials Science and Technology Division, ORNL, Oak Ridge, TN, PAUL R.C. KENT, Center for Nanophase Materials Sciences, ORNL, Oak Ridge, TN, JEONGNIM KIM, National Center for Supercomputing Applications, UIUC, Urbana, IL — We study the effects of a model impurity in a spherical jellium with quantum Monte Carlo (QMC) methods. The closed-shell energies and densities of jellium spheres have been studied previously using density functional theory (DFT) as well as QMC methods [1,2]. In this study, we begin by reproducing the previous results. Second, we add an impurity to model the transition between delocalized jellium states and localized atomic-like states in correlated metallic systems. We obtain the phase space diagram of the system using Hartree–Fock, several DFT approximations and QMC methods. The differences between methods are further analyzed by comparing the ground state densities. Finally, using the inverse susceptibility scheme, we obtain the effective exchange-correlation potential and compare it with exciting approximations of DFT.

[1] L. M. Almeida et. al., Phys. Rev. B **66**, 075115 (2002).
[2] F. Sottile et. al., Phys. Rev. B **64**, 045105 (2001) and P. Ballone et. al,. Phys. Rev. B **45**, 6293 (1992).

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