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The pseudo Hamiltonian approach for effective atoms in Difussion Monte Carlo revisited[1] FERNANDO REBOREDO, JARON KROGEL, Oak Ridge National Laboratory — Pseudo-Hamiltonians were initially proposed[1] as a method for removing computationally costly core electrons from diffusion Monte Carlo (DMC) calculations with purely differential operators. The approach, however, was largely abandoned. Pseudo-Hamiltonians were claimed to be very difficult to obtain specifically for transition elements. Instead, non-local pseudopotentials with the standard form used in single particle electronic structure have been used with relative success using the locality and later the T-moves approximations. However, these approximations give rise to systematic errors, in addition to the fixed-node, that largely depend on the quality of the trial wave function used to guide the DMC run. Since pseudo-Hamiltonians do not present those localization errors, we have revisited the idea for the case of transition metal ions. In this presentation we will discuss the cost and benefits of a pseudo-Hamiltonian treatment of the 3d Sc-Zn atomic series. [1] G. B. Bachelet, D. M. Ceperley, and M. G. B. Chiocchetti Phys. Rev. Lett. 62, 2088 (1989).

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