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Variational Wavefunctions for a Quantum Wire of Cylindrical
J.E. HASBUN, State University of West Georgia — In previous work, the quantum level structure in a quantum wire was investigated.[1] As in that work, an electron is considered to be free to move along the z coordinate of a cylindrical wire but confined along the ρ direction and include the Hartree term and exchange-correlation a la DFT, as done previously.[2] However, whereas in ref.1 a numerically obtained ground state was compared to a ground state variational model based on the wave function $f(\rho) = 2\sqrt{2b_0}exp(-2b_0\rho^2)$, the present treatment makes use of a variational model ground state of the form $f(\rho) = J_0[a(1 + b_0R^2)\rho/R_p]exp(-b_0\rho^2)$, where J_0 is the zeroth order Bessel function, b_0 is the variational parameter, R is the radius of the wire, a is a zero of the Bessel function, and R_p is an adjustable effective radius. As will be shown, the motivation for this wavefunction is that it can be extended to at least two excited states and still be able to go beyond the Hartree approximation to include exchange-correlation using the LDA, and get reasonable convergence as well as reasonable agreement with the full numerical results.
[1] J. Hasbun, APS Bull. 49, 1135 (2004).
[2] J. Hasbun, APS Bull. 48, 888 (2003).

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