

Bibliography

- [1] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B 864 (1964).
- [2] J. Perdew, in *Electronic Structure of Solids '91*, edited by P. Ziesche and H. Eschrig (Akademie Verlag, Berlin, 1991).
- [3] J. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).
- [4] G. Ortiz and P. Ballone, Phys. Rev. **B 56**, 9970 (1997).
- [5] W. Kohn and L. Sham, Phys. Rev. **140**, A 1133 (1965).
- [6] L.J. Sham and M. Schlüter, Phys. Rev. Lett. **51**, 1888 (1983).
- [7] L.J. Sham and M. Schlüter, Phys. Rev. **B 32**, 3883 (1985).
- [8] W. Kohn, Phys. Rev. **B 33**, 4331 (1986).
- [9] J.P. Perdew, R.G. Parr, M. Levy, and J.L. Balduz, Phys. Rev. Lett. **49**, 1691 (1982).
- [10] A. Seidl *et al.*, Phys. Rev. **B 53**, 3764 (1996).
- [11] S. Sharma, J.K. Dewhurst, and C. Ambrosch-Draxl, Phys. Rev. Lett. **95**, 136402 (2005).
- [12] D. Pines, *Elementary excitations in solids* (W.A. Benjamin, New York, 1963).
- [13] D. Pines and P. Nozieres, *Theory of Quantum Liquids: Normal Fermi Liquids, Vol. 1* (Perseus Books, Cambridge, Mass., 2000).
- [14] G. Giuliani and G. Vignale, *Quantum Theory of the Electron Liquid* (Cambridge University Press, Cambridge, UK, 2005).
- [15] M. Grüning, A. Marini, and A. Rubio, J. Chem. Phys. **124**, 154108 (2006).
- [16] S. Goedecker and C. Umrigar, Phys. Rev. Lett. **81**, 866 (1998).
- [17] G. Vignale and M. Rasolt, Phys. Rev. Lett. **59**, 2360 (1987).

- [18] G. Vignale and M. Rasolt, Phys. Rev. **B 37**, 10685 (1988).
- [19] P. Skudlarski and G. Vignale, Phys. Rev. **B 48**, 8547 (1993).
- [20] N. Helbig, Diploma thesis, Universität Würzburg (2001).
- [21] D.A. Maziotti, Phys. Rev. **A 57**, 4219 (1998).
- [22] D. Mazziotti and R. Erdahl, Phys. Rev. **A 63**, 042113 (2001).
- [23] T. Gilbert, Phys. Rev. **B 12**, 2111 (1975).
- [24] J. Cioslowski, K. Pernal, and P. Ziesche, J. Chem. Phys. **117**, 9560 (2002).
- [25] B.C. Carlson and J.M. Keller, Phys. Rev. **121**, 659 (1961).
- [26] E. Lieb, Pys. Rev. Lett. **46**, 457 (1981).
- [27] M. Levy, in *Density matrices and density functionals*, edited by R. Erdahl and V.H. Smith (D. Reidel Publishing Company, Dordrecht, Holland, 1987), pp. 479–498.
- [28] K. Yasuda, Pys. Rev. **A 63**, 032517 (2001).
- [29] H. Shull and P.-O. Löwdin, J. Chem. Phys. **30**, 617 (1959).
- [30] W. Kutzelnigg, Theoret. chim. Acta **1**, 327 (1963).
- [31] O. Gritsenko, K. Pernal, and E.J. Baerends, J. Chem. Phys. **122**, 204102 (2005).
- [32] C. Kollmar and B. Heß, J. Chem. Phys. **120**, 3158 (2004).
- [33] D.R. Hartree, Proc. Cambridge Phil. Soc. **24**, 89,111,426 (1928).
- [34] V. Fock, Z. Phys. **61**, 126 (1930).
- [35] A. Müller, Phys. Lett. **105A**, 446 (1984).
- [36] T.H. Dunning, Jr., J. Chem. Phys. **90**, 1007 (1989).
- [37] M. Buijse and E. Baerends, Mol. Phys. **100**, 401 (2002).
- [38] V. Staroverov and G. Scuseria, J. Chem. Phys. **117**, 2489 (2002).
- [39] N.N. Lathiotakis, N. Helbig, and E.K.U. Gross, cond-mat/0605531 .
- [40] G. Ortiz and P. Ballone, Phys. Rev. **B 50**, 1391 (1994).
- [41] J. Cioslowski and K. Pernal, J. Chem. Phys. **111**, 3396 (1999).
- [42] G. Csányi and T. Arias, Phys. Rev. **B 61**, 7348 (2000).

- [43] G. Csanyi, S. Goedecker, and T. Arias, Phys. Rev. **A 65**, 032510 (2002).
- [44] M. Städele *et al.*, Phys. Rev. **B 59**, 10031 (1999).
- [45] R.G. Parr and W. Yang, *Density-Functional Theory of Atoms and Molecules* (Oxford University Press, New York, 1989).
- [46] E.H. Lieb, in *Density Functional Methods in Physics*, edited by R.M. Dreizler and J. da Providencia (Plenum Press, New York, 1985), pp. 31–80.
- [47] A. Coleman, Rev. Mod. Phys. **35**, 668 (1963).
- [48] M. Krein and D. Milman, Studia Acta Mathematica **9**, 133 (1940).
- [49] J.A. Montgomery, Jr., J.W. Ochterski, and G.A. Petersson, J. Chem. Phys. **101**, 5900 (1994).
- [50] E.R. Davidson *et al.*, Phys. Rev. **A 44**, 7071 (1991).
- [51] M. W. Schmidt *et al.*, J. Comp. Chem. **14**, 1347 (1993).
- [52] R.E. Christoffersen, *Basic Principles and Techniques of Molecular Quantum Mechanics* (Springer, New York, 1989).
- [53] A. Shukla, M. Dolg, P. Fulde, and H. Stoll, Phys. Rev. **B 57**, 1471 (1998).
- [54] A. Shukla, M. Dolg, and H. Stoll, Phys. Rev. **B 58**, 4325 (1998).
- [55] A. Abdurahman, A. Shukla, and M. Dolg, J. Chem. Phys. **112**, 4801 (2000).
- [56] U. von Barth and L. Hedin, J. Phys. C **5**, 1629 (1972).
- [57] S.H. Vosko, L. Wilk, and M. Nusair, Can. J. Phys. **58**, 1200 (1980).
- [58] A.D. Becke, J. Chem. Phys. **98**, 5648 (1993).
- [59] R. Dovesi *et al.*, Phys. Rev. **B 29**, 3591 (1984).
- [60] R. Dovesi, B. Civalleri, R. Orlando, and V.R. Saunders, in *Reviews in Computational Chemistry, Vol. 21*, edited by K.B. Lipkowitz, R. Larter, and T.R. Cunardi (John Wiley & Sons, Inc., New York, 2005), p. chapter 1.
- [61] A.A. Radzig and B.M. Smirnov, *Reference Data on Atoms and Molecules* (Springer Verlag, Berlin, 1985).
- [62] J.J. De Groote and M. Masili, J. Chem. Phys. **120**, 2767 (2004).
- [63] H.R. Ihle and C.H. Wu, J. Chem. Phys. **63**, 1605 (1975).
- [64] S.B. Sharp and G.I. Gellene, J. Chem. Phys. **113**, 6122 (2000).

- [65] D. Pudewill *et al.*, J. Chem. Phys. **65**, 5226 (1976).
- [66] J. Krieger, Y. Li, and G. Iafrate, Phys. Rev. **A 46**, 5453 (1992).
- [67] K. Capelle and G. Vignale, Phys. Rev. Lett. **86**, 5546 (2001).
- [68] K. Capelle and G. Vignale, Phys. Rev. **B 65**, 113106 (2002).
- [69] K. Capelle and E.K.U. Gross, Phys. Rev. Lett. **78**, 1872 (1997).
- [70] J.D. Talman and W.F Shadwick, Phys. Rev. **A 14**, 36 (1976).
- [71] T. Grabo, T. Kreibich, S. Kurth, and E. Gross, in *Strong Coulomb Correlations in Electronic Struchture: Beyond the Local Density Approxiamtion*, edited by V. Anisimov (Gordon & Breach, Tokyo, 2000), pp. 203–311.
- [72] S. Kümmel and J. Perdew, Phys. Rev. Lett. **90**, 043004 (2003).
- [73] S. Kümmel and J. Perdew, Phys. Rev. **B 68**, 035103 (2003).
- [74] S. Sharma *et al.*, cond-mat/0510800 (2005).
- [75] R.T. Sharp and G.K. Horton, Phys. Rev. **90**, 317 (1953).
- [76] M. A. Reed *et al.*, J. Vac. Sci. Technol. **B 4**, 358 (1986).
- [77] A. Wensauer and U. Rössler, Phys. Rev. **B 69**, 155301 (2004).
- [78] A. Wensauer and U. Rössler, Phys. Rev. **B 69**, 155302 (2004).
- [79] H. Saarikoski *et al.*, Eur. Phys. J. **B 26**, 241 (2002).
- [80] H. Saarikoski *et al.*, Phys. Rev. **B 67**, 205327 (2003).
- [81] M. Ferconi and G. Vignale, Phys. Rev. **B 50**, 14722 (1994).
- [82] K. Pernal, Phys. Rev. Lett. **94**, 233002 (2005).
- [83] P.-O. Löwdin, Phys. Rev. **97**, 1474 (1955).

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Phys. Rev. **A** **72**, 030501 (2005)