DIRACX: Dirac exchange functional

$$
\begin{aligned}
K = {} & 0 \\
& + \sum_s \rho_s \varepsilon_{Xunif}\left(2\rho_s\right),
\end{aligned}
$$

where

$$\varepsilon_{Xunif}\left(n\right) = -3/4\,\frac{k_F\left(n\right)}{\pi}.$$

To avoid singularities in the limit $\rho_{\bar{s}} \to 0$

$$G = \rho_s \varepsilon_{Xunif}\left(2\rho_s\right).$$

PBEC: PBE correlation functional

$$
\begin{aligned}
K = {} & \rho\,\varepsilon_{Cpbe}\left(\rho, \frac{\rho_\alpha - \rho_\beta}{\rho}, \sqrt{\sigma}\right) \\
& + \sum_s 0,
\end{aligned}
$$

where

$$\varepsilon_{Cpbe}\left(n, \zeta, grad\right) = \varepsilon_{Cunif}\left(r_s\left(n\right), \zeta\right) + H\left(r_s\left(n\right), \zeta, T\left(n, \zeta, grad\right)\right),$$

$$H\left(rs, \zeta, t\right) = gama\left(\phi\left(\zeta\right)\right)^3 \ln\left(1 + \frac{\beta t^2\left(1 + A\left(rs, \zeta\right)t^2\right)}{gama\left(1 + A\left(rs, \zeta\right)t^2 + \left(A\left(rs, \zeta\right)\right)^2 t^4\right)}\right),$$

$$A\left(rs, \zeta\right) = \beta gama^{-1}\left(e^{-\frac{\varepsilon_{Cunif}\left(rs, \zeta\right)}{gama\left(\phi\left(\zeta\right)\right)^3}} - 1\right)^{-1},$$

$$gama = \frac{1 - \ln\left(2\right)}{\pi^2}$$

and

$$\beta = 0.066725.$$

To avoid singularities in the limit $\rho_{\bar{s}} \to 0$

$$G = \rho_s \varepsilon_{Cpbe}\left(\rho_s, 1, \sqrt{\sigma_{ss}}\right).$$

PBEX: PBE exchange functional

$$K = 0 + \sum_s \rho_s \varepsilon_{Xpbe}\left(2\rho_s, 2\sqrt{\sigma_{ss}}\right),$$

where

$$\varepsilon_{Xpbe}(n, grad) = \varepsilon_{Xunif}(n) F_{Xpbe}(S(n, grad)),$$

$$F_{Xpbe}(s) = 1 + \kappa - \kappa\left(1 + \frac{\mu s^2}{\kappa}\right)^{-1},$$

$$\mu = 1/3\,\beta\pi^2$$

and

$$\kappa = 0.804.$$

To avoid singularities in the limit $\rho_{\bar{s}} \to 0$

$$G = \rho_s \varepsilon_{Xpbe}\left(2\rho_s, 2\sqrt{\sigma_{ss}}\right).$$

PW92C: Perdew–Wang 1992 parametrization of LDA

$$K = \rho\,\varepsilon_{Cunif}\left(r_s(\rho), \frac{\rho_\alpha - \rho_\beta}{\rho}\right) + \sum_s 0,$$

where

$$\varepsilon_{Cunif}(rs, \zeta) = \varepsilon_{c0}(rs) + \frac{\alpha_c(rs) ff(\zeta)\left(1 - \zeta^4\right)}{ff0} + \left(\varepsilon_{c1}(rs) - \varepsilon_{c0}(rs)\right) ff(\zeta)\,\zeta^4,$$

$$ff(\zeta) = \frac{(1+\zeta)^{4/3} + (1-\zeta)^{4/3} - 2}{2\sqrt[3]{2} - 2},$$

$$ff0 = 1.709921,$$

$$\varepsilon_{c0}\left(rs\right) = \Gamma\left(rs, 0.0310907, 0.21370, 7.5957, 3.5876, 1.6382, 0.49294, 1\right),$$

$$\varepsilon_{c1}\left(rs\right) = \Gamma\left(rs, 0.01554535, 0.20548, 14.1189, 6.1977, 3.3662, 0.62517, 1\right),$$

$$\alpha_{c}\left(rs\right) = -\Gamma\left(rs, 0.0168869, 0.11125, 10.357, 3.6231, 0.88026, 0.49671, 1\right)$$

and

$$\Gamma\left(rs, A, a1, b1, b2, b3, b4, p\right) = -2A\left(1 + a1\,rs\right)\ln\left(1 + 1/2\,\frac{1}{A\left(b1\sqrt{rs} + b2\,rs + b3\,rs^{3/2} + b4\,rs^{p+1}\right)}\right).$$

SCANC: SCAN correlation functional

$$K = \rho\,\varepsilon_{Cscan}\left(\rho, \frac{\rho_\alpha - \rho_\beta}{\rho}, S\left(\rho, \sqrt{\sigma}\right), Alpha1\left(\rho, \frac{\rho_\alpha - \rho_\beta}{\rho}, \sqrt{\sigma}, 1/2\,\tau\right)\right) + \sum_s 0,$$

where

$$\varepsilon_{Cscan}\left(n, \zeta, s, a\right) = epsilonc1\left(n, \zeta, s\right) + Fc\left(a\right)\left(epsilonc0\left(n, \zeta, s\right) - epsilonc1\left(n, \zeta, s\right)\right),$$

$$Fc\left(a\right) = e^{-c1c\,a\,step\left(\frac{a}{1-a}\right)\left(1-a\right)^{-1}}step\left(1-a\right) - dc\,e^{c2c\,step\left(-\left(1-a\right)^{-1}\right)\left(1-a\right)^{-1}}step\left(a-1\right),$$

$$epsilonc1\left(n, \zeta, s\_\right) = \varepsilon_{Cunif}\left(r_s\left(n\right), \zeta\right) + H1\left(r_s\left(n\right), \zeta, T1\left(n, \zeta, s\_\right)\right),$$

$$H1\left(rs, \zeta, t\right) = gama\left(\phi\left(\zeta\right)\right)^3\ln\left(1 + w1\left(rs, \zeta\right)\left(1 - \frac{1}{\sqrt[4]{1 + 4A\left(rs, \zeta\right)t^2}}\right)\right),$$

$$A\left(rs, \zeta\right) = \frac{\beta\left(rs\right)}{gama\,w1\left(rs, \zeta\right)},$$

$$\beta\left(rs\right) = 0.066725\,\frac{1 + 0.1\,rs}{1 + 0.1778\,rs},$$

$$w1(rs,\zeta) = e^{-\frac{\varepsilon_{Cunif}(rs,\zeta)}{gama\,(\phi(\zeta))^3}} - 1,$$

$$gama = 0.031091,$$

$$epsilonc0(n,\zeta,s\_) = (epsilonclda0(r_s(n)) + H0(r_s(n),s\_))\,Gc(\zeta),$$

$$Gc(\zeta) = (3.3631 - 2.3631\,dx(\zeta))\left(1 - \zeta^{12}\right),$$

$$dx(\zeta) = 1/2\,(1+\zeta)^{4/3} + 1/2\,(1-\zeta)^{4/3},$$

$$ds(\zeta) = 1/2\,(1+\zeta)^{5/3} + 1/2\,(1-\zeta)^{5/3},$$

$$epsilonclda0(rs) = -\frac{b1c}{1 + b2c\sqrt{rs} + b3c\,rs},$$

$$H0(rs,s) = b1c\ln(1 + w0(rs)(1 - ginfzeta0(s))),$$

$$w0(rs) = e^{-\frac{epsilonclda0(rs)}{b1c}} - 1,$$

$$ginfzeta0(s) = \frac{1}{\sqrt[4]{1 + 4\,xiinf\,s^2}},$$

$$xiinf = 0.128026,$$

$$b1c = 0.0285764,$$

$$b2c = 0.0889,$$

$$b3c = 0.125541,$$

$$c1c = 0.64,$$

$$c2c = 1.5$$

and

$$dc = 0.7.$$

To avoid singularities in the limit $\rho_{\bar{s}} \to 0$

$$G = \rho_s \varepsilon_{Cscan}\left(\rho_s, 1, S\left(\rho_s, \sqrt{\sigma_{ss}}\right), Alpha1\left(\rho_s, 1, \sqrt{\sigma_{ss}}, 1/2\,\tau_s\right)\right).$$

SCANX: SCAN exchange functional

$$\begin{aligned} K = {} & 0 \\ & + \sum_s \rho_s \varepsilon_{Xscan}\left(2\,\rho_s, 2\,\sqrt{\sigma_{ss}}, \tau_s\right), \end{aligned}$$

where

$$\varepsilon_{Xscan}\left(n, grad, kin\right) = \varepsilon_{Xunif}\left(n\right) F_{Xscan}\left(S\left(n, grad\right), Alpha1\left(n, 0, grad, kin\right)\right),$$

$$F_{Xscan}\left(s, a\right) = \left(Hx1\left(s, a\right) + Fx\left(a\right)\left(hx0 - Hx1\left(s, a\right)\right)\right) Gx\left(s\right),$$

$$Fx\left(a\right) = \mathrm{e}^{-c1xastep\left(\frac{a}{1-a}\right)(1-a)^{-1}} step\left(1-a\right) - dx\,\mathrm{e}^{c2xstep\left(-(1-a)^{-1}\right)(1-a)^{-1}} step\left(a-1\right),$$

$$Hx1\left(s, a\right) = 1 + k1 - k1\left(1 + \frac{x\left(s, a\right)}{k1}\right)^{-1},$$

$$x\left(s, a\right) = muak\,s^2\left(1 + b4\,s^2 \mathrm{e}^{-\frac{|b4|s^2}{muak}} muak^{-1}\right) + \left(b1\,s^2 + b2\,\left(1-a\right)\mathrm{e}^{-b3\,(1-a)^2}\right)^2,$$

$$Gx\left(s\right) = 1 - \mathrm{e}^{-\frac{a1}{\sqrt{s}}},$$

$$a1 = 4.9479,$$

$$muak = \frac{10}{81},$$

$$b2 = \frac{1}{100}\sqrt{146},$$

$$b1 = \frac{511}{27000}b2^{-1},$$

$$b3 = 0.5,$$

$$hx0 = 1.174,$$

$$b4 = \frac{muak^2}{k1} - \frac{1606}{18225} - b1^2,$$

$$c1x = 0.667,$$

$$c2x = 0.8,$$

$$dx = 1.24$$

and

$$k1 = 0.065.$$

To avoid singularities in the limit $\rho_{\bar{s}} \to 0$

$$G = \rho_s \varepsilon_{Xscan}\left(2\rho_s, 2\sqrt{\sigma_{ss}}, \tau_s\right).$$

TPSSC: TPSS correlation functional

$$K = \rho\,\varepsilon_{Ctpps}\left(\varepsilon_{Crevpkzb}\left(\rho_\alpha, \rho_\beta, \sqrt{\sigma_{\alpha\alpha}}, \sqrt{\sigma_{\beta\beta}}, \sqrt{\sigma}, CC\left(\frac{\rho_\alpha - \rho_\beta}{\rho}, \Xi\left(\rho, Gradzeta\left(\rho, \frac{\rho_\alpha - \rho_\beta}{\rho}, \sigma_{\alpha\alpha}, \sigma_{\beta\beta}, \sigma_{\alpha\beta}\right)\right)\right)\right), Z\left(\rho, \sqrt{\sigma}, 1/2\,\tau\right)\right), Z\left(\rho\right.$$
$$+ \sum_s 0,$$

where

$$\varepsilon_{Ctpps}(epsiloncrvepkzb, z) = epsiloncrvepkzb\left(1 + depsiloncrvepkzb\, z^3\right),$$

$$d = 2.8,$$

$$\begin{aligned}&\varepsilon_{Crevpkzb}(\nu, nd, gradu, gradd, grad, Czetaxi, z)\\ &= \varepsilon_{Cpbe}\left(\nu + nd, \frac{\nu - nd}{\nu + nd}, grad\right)\left(1 + Czetaxi\, z^2\right) - (1\\ &\quad + Czetaxi)\, z^2\left(\nu\, mymax\left(\varepsilon_{Cpbe}\left(\nu + nd, \frac{\nu - nd}{\nu + nd}, grad\right), \varepsilon_{Cpbe}(\nu, 1, gradu)\right)(\nu + nd)^{-1}\right.\\ &\qquad\left. + nd\, mymax\left(\varepsilon_{Cpbe}\left(\nu + nd, \frac{\nu - nd}{\nu + nd}, grad\right), \varepsilon_{Cpbe}(nd, 1, gradd)\right)(\nu + nd)^{-1}\right),\end{aligned}$$

$$\begin{aligned}\varepsilon_{CrevpkzbU}(\nu, nd, gradd, grad, Czetaxi, z) = \varepsilon_{Cpbe}\left(\nu + nd, \frac{\nu - nd}{\nu + nd}, grad\right)&\left(1 + Czetaxi\, z^2\right.\\ &\left. - \frac{(1 + Czetaxi)\, z^2\nu}{\nu + nd}\right)\\ &- \frac{(1 + Czetaxi)\, z^2 nd\, \varepsilon_{Cpbe}(nd, 1, gradd)}{\nu + nd},\end{aligned}$$

$$CC(\zeta, \xi) = \frac{CC0(\zeta)}{\left(1 + 1/2\,\xi^2\left((1 + \zeta)^{-4/3} + (1 - \zeta)^{-4/3}\right)\right)^4}$$

and

$$CC0(\zeta) = 0.53 + 0.87\,\zeta^2 + 0.50\,\zeta^4 + 2.26\,\zeta^6.$$

To avoid singularities in the limit $\rho_{\bar{s}} \to 0$

$$G = \rho_s \varepsilon_{Ctpps}\left(\varepsilon_{CrevpkzbU}\left(0, \rho_s, \sqrt{\sigma_{ss}}, \sqrt{\sigma_{ss}}, CC0(1), Z(\rho_s, \sqrt{\sigma_{ss}}, 1/2\,\tau_s)\right), Z(\rho_s, \sqrt{\sigma_{ss}}, 1/2\,\tau_s)\right).$$

TPSSX: TPSS exchange functional

$$\begin{aligned}K = &\, 0\\ &+ \sum_s \rho_s \varepsilon_{Xtpss}\left(2\rho_s, 2\sqrt{\sigma_{ss}}, \tau_s\right),\end{aligned}$$

where

$$\varepsilon_{Xtpss}(n, grad, kin) = \varepsilon_{Xunif}(n)\, F_{Xtpss}(P(n, grad), Z(n, grad, kin)),$$

$$F_{Xtpss}(p,z) = 1 + \kappa - \kappa \left(1 + \frac{x_{tpss}(p,z)}{\kappa}\right)^{-1},$$

$$x_{tpss}(p,z) = \left(\left(\frac{10}{81} + \frac{cz^2}{(1+z^2)^2}\right)p + \frac{146}{2025}(q_b(p,z))^2 - \frac{73}{4050}q_b(p,z)\sqrt{18z^2+50p^2} + \frac{100}{6561}\frac{p^2}{\kappa} + \frac{4}{45}\sqrt{e}z^2 + e\mu p^3\right)\left(1+\sqrt{e}p\right)^{-2},$$

$$e = 1.537,$$

$$c = 1.59096,$$

$$q_b(p,z) = \frac{9}{20}\frac{Alpha(p,z) - 1}{\sqrt{1 + BAlpha(p,z)(Alpha(p,z) - 1)}} + 2/3\,p$$

and

$$B = 0.40.$$

To avoid singularities in the limit $\rho_{\bar{s}} \to 0$

$$G = \rho_s \varepsilon_{Xtpss}(2\rho_s, 2\sqrt{\sigma_{ss}}, \tau_s).$$