Supplemental Material

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CONTENTS

S1. ASSESSMENT OF LOCAL CONDITIONS ACROSS AVAILABLE APPROXIMATIONS

We utilize an exhaustive grid search to determine whether local conditions are satisfied for a given approximation. For LDAs, we consider 10000 evenly spaced values of $r_s \in [0.0001, 5]$ and 100 evenly spaced values of $\zeta \in [0, 1]$. For GGAs, we consider 10000 evenly spaced values of $r_s \in [0.0001, 5]$, 500 evenly spaced values of $s \in [0, 5]$, and 100 evenly spaced values of $\zeta \in [0, 1]$. For MGGAs, we consider 5000 evenly spaced values of $r_s \in [0.0001, 5]$, 100 evenly spaced values of $s \in [0, 5]$, 20 evenly spaced values of $\zeta \in [0, 1]$, and 100 evenly spaced values of $\alpha \in [0, 5]$ or $q \in [-10, 10]$. The number of values checked per variable is less in MGGAs to alleviate computational effort due to the combinatorial nature of the exhaustive search.

In determining whether local conditions are satisfied, a reasonable tolerance threshold of at most ± 0.001 is employed to approximately account for numerical errors arising from the numerical precision used and the finite difference method used to calculate numerical derivatives (further details can be found in our public code [1]). However, the numerical errors introduced are not guaranteed to be within the tolerances used.

In the following tables below, we report the fraction of local condition violations found in our exhaustive search. That is, we divide the number of violations found by the total number of configurations considered in the extensive grid search parameter space. If we find 0 such violations, then we conclude that the corresponding exact condition is satisfied for any reasonable density. We do not assess the LO bound condition on approximations that are for correlation only.

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TABLE S1. LDA functionals: numerical assessment of corresponding local conditions.

	$E_{\mathrm{C}}[n]$ non-positivity	$E_{\mathrm{C}}[n_\gamma]$ uniform scaling inequality	$T_{\mathrm{C}}[n]$ upper bound	concavity of $\lambda^2 E_{\mathrm{C}}[n_{1/\lambda}]$	LO extension to E_{XC}	LO	conjecture: $T_c \leq -E_c$
BR78 [2]	0	0	0	0	—	—	0
CHACHIYO-MOD [3, 4]	0	0	0	0	—	—	0
CHACHIYO [4]	0	0	0	0	—	—	0
GDSMFB [5]	1e-04	2e-05	0	0	0	0	6e-04
GK72 [6]	0	1e-04	0.999	1e-04	—	—	0
GL [7]	0	0	0	0	—	—	0
GOMBAS [8]	0	0	0	0	—	—	0
HL [9]	0	0	0	0	—	—	0
KARASIEV-MOD [3, 10]	0	0	0	0	—	—	0
KARASIEV [10]	0	0	0	0	—	—	0
KSDT [11]	0	0	0	0	0	0	0
LDA0 [12]	0	0	0	0	0	0	0
LP-A [13]	0	0	0	0	0	0	0
LP-B [13]	0	0	0.989	0.935	0	0	0
LP96 [14, 15]	0.515	0.726	0	0.845	—	—	0
MCWEENY [2, 16]	0	0	0	0	—	—	0
ML1 [17, 18]	0	9e-05	0	0.004	—	—	6e-05
ML2 [17, 18]	0	9e-05	0	0.004	—	—	8e-06
OB-PW [19–21]	0	0	0	0	—	—	0
OB-PZ [19, 20]	0	0	0	1e-04	—	—	0
OW-LYP [22]	0	0	0	0	—	—	0
OW [22]	0	0	0	0	—	—	0
PK09 [23, 24]	0	0	0	4e-04	—	—	0
PMGB06 [25]	0	0	0	0	—	—	0.970
PW-MOD [21]	0	0	0	0	—	—	0
PW-RPA [26]	0	0	0	0	—	—	0
PW [26]	0	0	0	0	—	—	0
PZ-MOD [27]	0	0	0	0	—	—	0
PZ [28]	0	0	0	1e-04	—	—	1e-04
RC04 [29]	0	0	0	0	—	—	0
RPA [30]	0	0.336	0.999	0.602	—	—	0
RPW92 [31]	0	0	0	0	—	—	0
TETER93 [32]	0	0	0	0	0	0	0
UPW92 [31]	0	0	0	0	—	—	0
VBH [33]	0	0	0	0	—	—	0
VWN-1 [34]	0	0	0	0	—	—	0
VWN-2 [34]	0	0	0	0	—	—	0
VWN-3 [34]	0	0	0	0	—	—	0
VWN-4 [34]	0	0	0	0	—	—	0
VWN-RPA [34]	0	0	0	0	—	—	0
VWN [34]	0	0	0	0	—	—	0
W20 [35]	0	0	0	0	—	—	0
WIGNER [22, 36]	0	0	0	0	—	—	0
XALPHA [37]	0	0	0	0	—	—	0
ZLP [38]	0	0	0.999	0.915	0	0	0

TABLE S2. GGA functionals: numerical assessment of corresponding local conditions.

	$E_{\mathrm{C}}[n]$ non-positivity	$E_{\mathrm{C}}[n_\gamma]$ uniform scaling inequality	$T_{\mathrm{C}}[n]$ upper bound	concavity of $\lambda^2 E_{\mathrm{C}}[n_{1/\lambda}]$	LO extension to E_{XC}	LO	conjecture: $T_c \leq -E_c$
ACGGAP [39, 40]	0	0	0	0	—	—	0.414
ACGGA [39, 40]	0	0	0	0	—	—	0
AM05 [41, 42]	0	0	0	0	0	0	0
APBE [43]	0	0	0	0	0	0	0.004
B97-D [44]	0.632	0.503	0.559	0.608	0.268	0.183	0.633
B97-GGA1 [45]	0.636	0.514	0.557	0.612	0.390	0.317	0.639
BEEFVDW [46]	0	0	0	0	0.003	0.013	0
BMK [47]	0.627	0.304	0.648	0.621	—	—	0.616
CCDF [48]	0	0	0	0	—	—	0
CHACHIYO [3]	0	0	0.044	0	0.217	0.217	0.010
CS1 [49, 50]	0.604	0.204	0.528	0.530	—	—	0.601
EDF1 [51]	0.605	0.245	0.002	0.231	0.162	0.203	0.527
FT97 [52, 53]	0	0	1e-05	0.003	—	—	0
GAM [54]	0.598	0.459	0.560	0.578	0.145	0.083	0.596
GAPC [55]	0.004	0.011	2e-04	0.005	—	—	0.015
GAPLOC [55]	4e-04	2e-04	2e-04	0.005	—	—	0.033
HCTH-120 [56]	0.495	0.310	0.327	0.450	0.065	0.061	0.507
HCTH-147 [56]	0.467	0.290	0.298	0.422	0.113	0.093	0.478
HCTH-407P [57]	0.536	0.445	0.428	0.508	0.105	0.075	0.543
HCTH-407 [58]	0.481	0.382	0.365	0.450	0.112	0.079	0.489
HCTH-93 [59]	0.435	0.196	0.258	0.386	0.266	0.237	0.446
HCTH-A [59]	0.493	0.289	0.355	0.454	0	0	0.501
HCTH-P14 [60]	0	0	0	0	0	0.029	0
HCTH-P76 [60]	0.986	0.929	0.999	0.991	0.011	0.005	0.978
HLE16 [61]	0.481	0.305	0.364	0.447	0.477	0.473	0.487
HYB-TAU-HCTH [62]	0.615	0.439	0.520	0.585	—	—	0.620
KT1 [63]	0.791	0.434	0.096	0.169	0.153	0.076	0.664
KT2 [63]	0.832	0.477	0.106	0.177	0.156	0.077	0.686
KT3 [64]	0.862	0.461	0.120	0.192	0.164	0.077	0.678
LM [65, 66]	0	0.119	0.464	0.384	—	—	0
LYPR [67]	0.320	0.113	0.801	0.590	—	—	0.438
LYP [68, 69]	0.576	0.218	0.003	0.203	—	—	0.511
MGGAC [70]	0	0	0	0	—	—	0.007
MOHLYP2 [71]	0.576	0.174	0.002	0.193	0.340	0.337	0.509
MOHLYP [72]	0.243	0.092	0	0.092	0.048	0.096	0.328
MPWLYP1W [73]	0.500	0.190	4e-07	0.168	0.003	0.004	0.474
N12 [74]	0	0	0	0	0.150	0.170	0
NCAP [75]	0.455	0.299	0.029	0.277	0.231	0.207	0.403
OBLYP-D [76]	0.595	0.246	0.002	0.243	0.019	0.020	0.505
OP-B88 [77]	0	2e-04	6e-04	0.002	—	—	7e-04
OP-G96 [77, 78]	0	2e-04	6e-04	0.002	—	—	7e-04
OP-PBE [77, 78]	0	2e-04	6e-04	0.002	—	—	7e-04
OP-PW91 [77, 78]	0	0.001	0.001	0.002	—	—	0.001
OP-XALPHA [77, 78]	0	2e-04	6e-04	0.002	—	—	7e-04
OPBE-D [76]	0	0	0	0	0.009	0.009	0.006
OPTC [79]	3e-06	0	0	0	—	—	0
OPWLYP-D [76]	0.596	0.247	7e-04	0.240	0.019	0.022	0.507
P86-FT [80]	0.454	0.298	0.027	0.276	—	—	0.402
P86VWN-FT [80]	0.447	0.297	0.026	0.275	—	—	0.389
P86VWN [80]	0.447	0.297	0.026	0.275	—	—	0.389
P86 [80]	0.454	0.298	0.027	0.276	—	—	0.403
PBE-JRGX [81]	0	0	0	0	—	—	0.006
PBE-MOL [82]	0	0	0	0	0	0	0.004
PBE-SOL [83]	0	0	0	0	0	0	0.006
PBE-VWN [84–86]	0	0	0	0	—	—	6e-04
PBE1W [73]	0	0	0	0	0	0	0
PBEFE [87]	0	0	0	0	0	0	0.006
PBEINT [88]	0	0	0	0	0	0	0.005
PBELOC [89]	0	0	0	0.003	—	—	0.271
PBELYP1W [73]	0.414	0.157	0	0.141	0	0	0.427
PBE [85, 86]	0	0	0	0	0	0	0.005

TABLE S3. GGA functionals: numerical assessment of corresponding local conditions.

	$E_{\mathrm{C}}[n]$ non-positivity	$E_{\mathrm{C}}[n_\gamma]$ uniform scaling inequality	$T_{\mathrm{C}}[n]$ upper bound	concavity of $\lambda^2 E_{\mathrm{C}}[n_{1/\lambda}]$	LO extension to E_{XC}	LO	conjecture: $T_c \leq -E_c$
PW91 [90–92]	3e-06	0	0	0	0	0	0
Q2D [93]	0	0.041	0.012	0.032	0	0	0.002
REGTPSS [94]	0	0	0	0	—	—	0.406
REVTCA [95]	0	0	0.003	0.051	—	—	0.024
RGE2 [96]	0	0	0	0	0	0	0.005
SCAN-E0 [97]	0	0	0	0	—	—	0
SG4 [98]	0	0.048	0.327	0.385	8e-04	0.007	0.050
SOGGA11 [99]	0	0.003	0.064	0.229	0	1e-04	0.002
SPBE [100]	0	0	0	0	—	—	0
TAU-HCTH [62]	0.595	0.491	0.492	0.567	—	—	0.603
TCA [101]	0	0	0	0	—	—	0
TH-FCFO [102]	0.223	0.772	0.233	0.237	0.787	0.228	0.226
TH-FCO [102]	0.200	0.795	0.211	0.214	0.781	0.205	0.203
TH-FC [102]	0.988	0.009	0.994	0.996	0.822	0.990	0.989
TH-FL [102]	0	1.000	0	0	0.498	0	0
TH1 [103]	0.215	0.780	0.224	0.225	0.295	0.220	0.218
TH2 [104]	0.061	0.935	0.070	0.070	0.323	0.065	0.063
TH3 [105]	0.217	0.781	0.217	0.219	0.284	0.218	0.218
TH4 [105]	0.103	0.894	0.106	0.106	0.238	0.105	0.105
TM-LYP [106]	0.575	0.209	0.122	0.173	—	—	0.565
TM-PBE [106]	0	0	0	0	—	—	0.509
W94 [107]	0	0	0	3e-05	—	—	0
WI0 [108]	0.614	0.004	0.002	0.014	—	—	0.603
WI [108]	0.900	0.008	0.008	0.023	—	—	0.896
WL [109]	0.590	0.166	0.595	0.581	—	—	0.377
XLYP [110]	0.576	0.218	0.003	0.203	0.013	0.019	0.511
XPBE [111]	0	0	0	0	0	0	0
ZPBEINT [112]	0	0.020	0.343	0.299	—	—	2e-04
ZPBESOL [112]	0	0.013	0.375	0.263	—	—	2e-04
ZVPBEINT [113]	0	0.093	0.273	0.226	—	—	0.001
ZVPBELOC [114]	0	3e-04	0.199	0.112	—	—	0.075
ZVPBESOL [113]	0	0.080	0.299	0.212	—	—	0.001

TABLE S4. MGGA functionals: numerical assessment of corresponding local conditions.

	$E_C[n]$ non-positivity	$E_C[n_\gamma]$ uniform scaling inequality	$T_C[n]$ upper bound	concavity of $\lambda^2 E_C[n_{1/\lambda}]$	LO extension to E_{XC}	LO	conjecture: $T_c \leq -E_c$
B88 [115]	0	0	0	0	—	—	0
B94 [116]	0	0	0	0	—	—	0
BC95 [117]	0	0	0	0	—	—	0
CC06 [118]	0	0	0	0	0	0	0
CS [68, 119]	0.352	0.166	0.252	0.275	—	—	0.481
HLE17 [120]	0	0	0	0	0.092	0.093	0
HLTAPW [121]	0	0	0	0	—	—	0
KCISK [122–126]	0	0	0	0.012	—	—	0.041
KCIS [122–126]	0	0	0	0	—	—	0
LP90 [13]	0	0.963	0.998	0.990	0	0	0
M06-L [127, 128]	0.700	0.661	0.705	0.696	0.228	0.181	0.698
M11-L [129]	0.385	0.194	0.004	0.153	0.425	0.456	0.478
MN12-L [130]	0.424	0.266	0.022	0.227	0.048	0.086	0.506
MN15-L [131]	0.462	0.184	3e-04	0.156	2e-04	0.006	0.594
OTPSS-D [76]	0	0	0	0	0	0	0.007
PKZB [132]	0	0	0	0	0	0	0.006
R2SCANL [133–135]	0	0	0	0	0	0	0
R2SCAN [134, 135]	0	0	0	0	0	0	0
REVM06-L [136]	0.777	0.702	0.835	0.783	5e-05	7e-05	0.767
REVSCAN [137]	0.212	0.063	0	0.084	0	0	0.288
REVTM [138]	0	0	0	0	0	0	0.329
REVTPSS [94, 139]	0	0	0	0	0	0	0.424
RSCAN [140]	0	0.008	0.101	0.160	0	0	0
SCANL [97, 141, 142]	0	0	0	0	0	0	0
SCAN [97]	0	0	0	0	0	0	0
TM [143]	0	0	0	0	0	0	7e-04
TPSSLOC [89]	0	0	0	0.003	—	—	0.280
TPSSLYP1W [73]	0.408	0.179	0	0.138	0	0	0.420
TPSS [144, 145]	0	0	0	0	0	0	0.008
VSXC [146]	0.298	0.084	0.190	0.260	—	—	0.294
ZLP [38]	0	0.943	0.998	0.981	0.343	0.285	0

TABLE S5. Hybrid GGA functionals: numerical assessment of corresponding local conditions.

	$E_{\mathrm{C}}[n]$ non-positivity	$E_{\mathrm{C}}[n_\gamma]$ uniform scaling inequality	$T_{\mathrm{C}}[n]$ upper bound	concavity of $\lambda^2 E_{\mathrm{C}}[n_{1/\lambda}]$	LO extension to E_{XC}	LO	conjecture: $T_c \leq -E_c$
APBE0 [114]	0	0	0	0	0	0	0.004
APF [147]	0	0	0	0	0	0	0
B1LYP [148]	0.576	0.218	0.003	0.203	0	0	0.511
B1PW91 [148]	0	0	0	0	0	0	0
B1WC [149]	0	0	0	0	0	0	0.005
B3LYP-MCM1 [150]	0.753	0.282	0.681	0.455	0	0	0.590
B3LYP-MCM2 [150]	0.558	0.210	4e-04	0.187	0	0	0.504
B3LYP3 [151]	0.457	0.174	0	0.154	0	0	0.451
B3LYP5 [151]	0.457	0.174	0	0.154	0	0	0.451
B3LYPS [152]	0.414	0.159	0	0.137	0	5e-05	0.442
B3LYP [151]	0.414	0.159	0	0.137	0	8e-05	0.442
B3P86 [153]	0.074	0.141	0	0.209	0	0	0.265
B3PW91 [154]	0	0	0	0	0	0	0
B5050LYP [155]	0.457	0.174	0	0.154	0	0	0.451
B97-1P [45]	0.666	0.463	0.634	0.649	0.056	0.042	0.663
B97-1 [59]	0.698	0.476	0.686	0.687	0.002	0.001	0.693
B97-2 [156]	0.665	0.479	0.605	0.643	0.065	0.048	0.666
B97-3 [157]	0.612	0.464	0.601	0.601	0.089	0.050	0.608
B97-K [47]	0.330	0.004	0.520	0.342	0	0	0.291
B97 [158]	0.645	0.359	0.612	0.626	0.003	0.003	0.641
BHANDHLYP [153, 159]	0.576	0.218	0.003	0.203	0	0	0.511
BHANDH [153, 159]	0.576	0.218	0.003	0.203	0	0	0.511
BLYP35 [160, 161]	0.576	0.218	0.003	0.203	0	0	0.511
CAP0 [162]	0	0	0	0	0.080	0.081	0.005
CASE21 [163]	0	0	0	0	0	0	0.259
EDF2 [164]	0.362	0.132	0	0.125	0	0	0.398
HAPBE [114]	0	0	0	0	0	0	0.012
HFLYP [68, 69]	0.576	0.218	0.003	0.203	0	0	0.511
HPBEINT [165]	0	0	0	0	0	0	0.005
KMLYP [166]	0.121	0.052	0	0.054	0	0	0.279
MB3LYP-RC04 [167]	0.359	0.143	0.001	0.126	0	1e-04	0.375
MPW1K [168]	0	0	0	0	0	0	0
MPW1LYP [169]	0.576	0.218	0.003	0.203	0	0	0.511
MPW1PBE [169]	0	0	0	0	0	0	0.005
MPW1PW [169]	0	0	0	0	0	0	0
MPW3LYP [170]	0.462	0.178	0	0.153	0	0	0.465
MPW3PW [169]	0	0	0	0	0	0	0
MPWLYP1M [72]	0.576	0.218	0.003	0.203	3e-04	3e-04	0.511
O3LYP [79, 171]	0.457	0.174	0	0.154	0.017	0.028	0.451
PBE-2X [172]	0	0	0	0	0	0	0.005
PBE-MOL0 [82]	0	0	0	0	0	0	0.004
PBE-MOLB0 [82]	0	0	0	0	0	0	0.005
PBE-SOL0 [82]	0	0	0	0	0	0	0.006
PBE0-13 [173]	0	0	0	0	0	0	0.005
PBE38 [174]	0	0	0	0	0	0	0.005
PBE50 [175]	0	0	0	0	0	0	0.005
PBEB0 [82]	0	0	0	0	0	0	0.005
PBEH [176, 177]	0	0	0	0	0	0	0.005
QTP17 [178]	0.407	0.156	0	0.135	0	0	0.439
REVB3LYP [179]	0.438	0.168	0	0.145	0	0	0.453
SB98-1A [180]	0.803	0.435	0.903	0.809	0	0	0.786
SB98-1B [180]	0.267	0.049	0.055	0.215	0.013	0.019	0.278
SB98-1C [180]	0.635	0.363	0.593	0.615	0.004	0.004	0.633
SB98-2A [180]	0	0	0	0	0.002	0.012	0
SB98-2B [180]	0.478	0.180	0.327	0.432	2e-05	4e-04	0.484
SB98-2C [180]	0.632	0.371	0.586	0.611	0.001	0.002	0.629
SOGGA11-X [181]	0	0.042	0.176	0.169	0	0.003	0
WC04 [182]	0	0	0	0	0.123	0.240	0
WP04 [182]	0	0	0	0	0.349	0.468	0
X3LYP [110]	0.462	0.178	0	0.153	0	0	0.465

TABLE S6. Hybrid MGGA functionals: numerical assessment of corresponding local conditions.

	$E_C[n]$ non-positivity	$E_C[n_\gamma]$ uniform scaling inequality	$T_C[n]$ upper bound	concavity of $\lambda^2 E_C[n_{1/\lambda}]$	LO extension to E_{XC}	LO	conjecture: $T_c \leq -E_c$
B0KCIS [126]	0	0	0	0	0	0	0
B86B95 [117]	0	0	0	0	0	9e-04	0
B88B95 [117]	0	0	0	0	0	9e-04	0
B98 [183]	0.202	0.004	0.145	0.119	0	0	0.172
BB1K [184]	0	0	0	0	0	1e-03	0
BR3P86 [185]	0.290	0.336	0.005	0.247	0	6e-04	0.305
DLDF [186]	0.543	0.455	0.523	0.532	0.298	0.241	0.540
EDMGGAH [187]	0.351	0.166	0.254	0.276	0.015	0.013	0.481
M05-2X [188]	0.745	0.696	0.760	0.743	0.070	0.042	0.741
M05 [189]	0.748	0.559	0.767	0.729	0.075	0.073	0.731
M06-2X [128]	0.681	0.613	0.720	0.682	0.058	0.036	0.674
M06-HF [190]	0.298	0.232	0.382	0.313	0.049	0.105	0.284
M06 [128]	0.419	0.229	0.257	0.375	0.329	0.330	0.423
M08-HX [191]	0.039	0.008	0	0.007	0.070	0.259	0.136
M08-SO [191]	0.079	0.019	0	0.015	0.149	0.260	0.196
MN15 [192]	0.785	0.612	0.396	0.631	0.288	0.276	0.860
MPW1B95 [170]	0	0	0	0	0	9e-04	0
MPW1KCIS [193]	0	0	0	0	0	0	0
MPWB1K [170]	0	0	0	0	0	1e-03	0
MPWKCIS1K [193]	0	0	0	0	0	0	0
PBE1KCIS [194]	0	0	0	0	0	0	0
PW6B95 [195]	0	0	0	0	0	9e-04	0
PW86B95 [117]	0	0	0	0	0	9e-04	0
PWB6K [195]	0	0	0	0	0	1e-03	0
REVM06 [196]	0.676	0.591	0.685	0.670	0.003	0.002	0.670
REVTPSSH [197]	0	0	0	0	0	0	0.424
TPSS0 [198]	0	0	0	0	0	0	0.008
TPSS1KCIS [199]	0	0	0	0	0	0	0
TPSSH [200]	0	0	0	0	0	0	0.008
X1B95 [170]	0	0	0	0	0	0	0
XB1K [170]	0	0	0	0	0	4e-05	0

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