Supplementary Information for "Finding Density Functionals with Machine Learning"

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The purpose of this supplementary material is to provide the information necessary to reproduce our machine learning approximation (MLA) to the kinetic energy functional exactly, as well as extra details about the nature of the MLA. Table III gives the first 100 potential parameters a_i, b_i, and c_i to double precision. Along with the equations in the main paper and details of Numerov's method, one should be able to reproduce the corresponding weights a_j of the functional on line 4 of Table I in the main text.

SELF-CONSISTENT DENSITIES

Table I gives the percentage of variance lost, $(1 - \sum_{j=1}^{\ell}\lambda_j / \sum_{j=1}^{G}\lambda_j)\times 100\%$, in taking the first ℓ eigenvalues in the principle component analysis (PCA) projection. For each projection, there are $G = 500$ eigenvalues, but only a few are necessary to represent the local variation in the densities. For example, with $N = 1$, $m = 30$ and $\ell = 5$, we retain 99.98% of the variance when projecting onto the PCA subspace. In Table II, we coarsely optimize the parameters m and ℓ in the PCA projection.

$N\ell$	1	2	3	4	5	6	7	8
1	35	3	0.8	0.07	0.02	0.004	0.002	0.0003
2	45	15	3.7	0.36	0.10	0.019	0.006	0.0015
3	44	18	4.9	0.78	0.16	0.043	0.012	0.0037
4	48	24	9.5	1.9	0.40	0.087	0.023	0.0063

TABLE I. Percent of variance lost in taking the first ℓ PCA eigenvalues with $m = 30$. Averaged over 100 PCA projections $\boldsymbol{P}_{m,\ell}(\boldsymbol{n})$ with randomly chosen centers $\boldsymbol{n}$ in the test set.

$m\ell$	3	4	5	6
15	6.5	1.9	0.92	1.2
20	6.3	1.9	0.87	0.89
25	5.2	1.5	0.87	0.92
30	4.2	1.3	0.86	0.97
35	4.6	1.2	0.90	1.0
40	3.9	1.2	0.95	1.0
45	3.9	1.3	0.98	0.98

TABLE II. Mean absolute errors $\overline{|\Delta T|}$, in kcal/mol, on 100 randomly chosen self-consistent densities in the test set, averaged over $N = 1, 2, 3$ and 4. This coarse optimization gives $m = 30$, $\ell = 5$. Errors are less sensitive to m than ℓ. For $\ell \geq 7$, the gradient descent search fails to converge in some cases.

NUMEROV'S METHOD

We use Numerov's method [1] to solve Schrödinger's equation for N non-interacting spinless fermions confined to 1d box:

$$\left(-\frac{1}{2}\frac{\partial^2}{\partial x^2} + v(x)\right)\psi(x) = \epsilon\psi(x), \tag{1}$$

with boundary conditions $\psi(0) = \psi(1) = 0$. We discretize $\psi(x)$ and $v(x)$ on a uniform grid with spacing $\Delta x = 1/(G-1)$: $\psi_j = \psi(j/(G-1))$, $v_j = v(j/(G-1))$ for $j = 0, \ldots, G-1$. Starting from $\psi_0 = 0$ and $\psi_1 = 1$, we calculate the remaining ψ_j iteratively:

$$\psi_{j+1} = \frac{(2 - 5\Delta x^2 f_j/6)\psi_j - (1 + \Delta x^2 f_{j-1})/12)\psi_{j-1}}{1 + \Delta x^2 f_{j+1}/12}, \tag{2}$$

where $f_j = 2(\epsilon - v_j))$. To determine the eigenvalues $\epsilon^{(k)}$ and eigenfunctions $\psi^{(k)}$, we find the first N intervals that contain a root of $\psi_{G-1}(\epsilon)$, scanning from $\epsilon = -3\sum_{i=1}^{3} a_i$ in steps of $\Delta\epsilon = 1$. For each interval k, we perform a binary search for the root, reducing the length of the interval to less than 10^{-14}. The eigenvalue is taken as the midpoint of the interval (the error in ϵ_k is less than 5×10^{-15}). After normalizing the eigenfunctions $\psi^{(k)}$, the density and kinetic energy are given by:

$$n(x_j) = \sum_{k=1}^{N} \psi^{(k)}(x_j)^2, \quad T = \sum_{k=1}^{N} \epsilon_k - \sum_{j=1}^{G-1} n(x_j) v_j \Delta x. \tag{3}$$

[1] See e.g. E. Hairer, P. Nørsett, P. Syvert Paul and G. Wanner, *Solving ordinary differential equations I: Nonstiff problems* (Springer, New York, 1993).

j	α_j	a_1	b_1	c_1	a_2	b_2	c_2	a_3	b_3	c_3
1	14.342671597303580	1.180270056381577	0.071951010171267996	0.529934532594325 4	9.013205209842888	0.092675711955144	0.539643178767533 3	7.210302051717128	0.074083309285191 8	0.412034115072088 4
2	5.175360849250056	6.168939733519782	0.082993252991643	0.516722731523008 5	8.304951436191428	0.089014506021332	0.416912208159295	8.804876133493911	0.096594459684078	0.571105709443816
3	0.835534193378979	9.080904330470710	0.076853027746880 97	0.562268643606314 9	3.911674577648888	0.075518320091272 2	0.508664949777539	1.809709070880952	0.095976684502697	0.402422037149375
4	−5.373806223157635	8.697231487958999	0.063848716630704 96	0.585946429359627 7	8.673308770115531	0.087692878702095 7	0.485065025701083 9	4.189229162595343	0.045183680771276 09	0.581924487126040 9
5	−0.319073063815225	1.880199805158718	0.034255402984959 52	0.487404458713053 4	3.541514636747403	0.098366063995612 1	0.451515140419886	9.826680624097133	0.192	0.435264256453319
6	0.435131589094208 1	3.522977833467916	0.072180552006599 771	0.448917088761112 5	3.332712157375289	0.078525485307348 36	0.585294102801011 6	8.144612686919626	0.048489298817363 92	0.548478989434870 7
7	−5.783654943336363	5.286896436167961	0.049733245016520 48	0.465360994391444	7.135152688153955	0.095634924199585	0.440894944021174	2.243825016881491	0.058655883048217 63	0.568748117008862 6
8	5.857253335721763	1.896112874949486	0.032608978864389 52	0.450103328328055 7	5.885541925485173	0.062409322695931 34	0.561861175474473	6.486450948532671	0.072936337751454 38	0.569535908428756 2
9	0.362779597324067 8	7.516612508143043	0.099318409018399	0.569979329055005 55	5.262683987610352	0.097216963242874 8	0.472671160338163 8	8.89032075863951	0.056320911987425 37	0.405614805104374
10	29.95678925033907	8.493092481594 69	0.064750785330711 6	0.448137652738837 3	3.622632918136 46	0.040186592719782 59	0.525317396829749	1.155756643175955	0.091061502467220 8	0.587031705582734
11	−8.100865228495 75	7.105439309279282	0.084318444668049 3	0.422387132359130 2	4.606936643431428	0.063266930586471 06	0.538164319328688 5	2.832289239384128	0.079703846585840 57	0.417127569575901 1
12	−1.631527605278485	8.539550342890 36	0.072849047224670 74	0.583905823689045	1.340024891088 64	0.078159205157539	0.538335369598924 6	7.396341414064901	0.059451101645428 45	0.492404384218895 1
13	11.06175144743 51	7.853417776611835	0.070700773176797 58	0.508078736376261 7	4.408481706562826	0.062985283283884 89	0.461186076617371	7.905428673264 01	0.038879332787050 98	0.587222739753224 8
14	4.440893290111033	6.396984311399037	0.057306606685787 38	0.596441539875245	5.472334576900375	0.065701863688826 426	0.547378709183074	4.715521015256764	0.080362967406916 7	0.535417952099488
15	2.731504789238804	4.228544205571447	0.060718990099779 01	0.413523577681770 1	2.550224851908171	0.064247714683426 88	0.520339516711386 4	4.842862964307187	0.063339956033635 176	0.524412197522766 7
16	−12.355131455143 41	2.579686666551495	0.066431890544701 8	0.488852545063004 8	3.764107410086705	0.065767201995594 33	0.548168602005323 4	1.399253719979948	0.075404903025131 19	0.465545698896573 1
17	11.550952489211 01	1.107700596345898	0.059553891321719 3	0.535920752160894	2.706093393731662	0.065618410066717 81	0.426911496692299 4	1.501048590877154	0.063520349684316 2	0.433182104359277 1
18	0.170348485406411 9	8.264356247010 31	0.046241962647768 03	0.423623760829707 2	7.025290029097274	0.079807501972669 55	0.468392718402503 6	2.822503099972245	0.052225224116667 061	0.481099852143109 6
19	−0.130178554743 33	8.741245478785 86	0.062879314476838 1	0.473619642319636 4	8.591662514082 43	0.084738261964 188	0.456466250809403	8.228777497676 242	0.037277743249205 75	0.469735079819382 6
20	−1.646528531854399	4.545173787725101	0.034331896934214 91	0.491902159523417 7	1.726935494533148	0.031357965955056 73	0.580800322296872	2.502191185545461	0.085678880976874 75	0.590962133161188 8
21	−2.371179702223466	1.015154584908506	0.077265957085117 65	0.400898853773291 1	6.688534202733123	0.086954406374234 6	0.403293222827825	6.297133313147086	0.033453693281974 18	0.543307047009755 2
22	13.693832422144 02	3.283098134816701	0.068416178039579 27	0.430419549693744 25	5.887062834756559	0.051523994349496 422	0.432199560699743	3.207122477750064	0.073718083894043 21	0.496728453543185
23	−2.216419772035322	2.056773486230531	0.082569991594569 4	0.479224783903814	6.945590707033352	0.074086364568922 97	0.495775045654710 8	5.846222671659907	0.083645245447208 1	0.409472002085241 6
24	−6.000764355636 04	2.037033522054 63	0.076055175427939 95	0.450129151568358 5	1.452563564788	0.074336923739896 13	0.423396907604344	8.950593020194 88	0.057036156208371 87	0.467902365984293 5
25	8.164091086678 99	6.400475835681034	0.034255899491393 43	0.554409581884655	6.086484474478635	0.072828449561280 38	0.427259689718639 6	5.362076464433345	0.057806341606610 02	0.550317319865832 4
26	−22.389731490641 3	3.751807395744921	0.085262410735628	0.445345084866874 9	7.559337237117221	0.058409098679704 21	0.499022346701435	4.729884445483556	0.092921871230672 24	0.559050337471094 5
27	5.595799173773367	4.522456026868127	0.036202019468413 09	0.505021006076815	1.885091277540955	0.065217803858488 91	0.496160103595582	9.474219454963 29	0.055674013339615 9	0.483404574974009 1
28	1.946455825665 49	2.751346713386582	0.094819552851681 5	0.490120421250647 3	7.863592227266858	0.095179798395182 5	0.519662004980269 1	9.516086800352 75	0.077853773154636 09	0.580601559226294 5
29	−1.105559825330 69	5.725277193011525	0.030973031162614 06	0.551117778556780 3	7.988513342309234	0.092832317986858	0.514641511636756 9	1.101098863639624	0.088293902851979 1	0.526510863143027 2
30	−3.886381532777 54	4.958711729661 77	0.068232544387776 03	0.564595131300880 6	9.081352253176 34	0.044728569058404 44	0.429911712404620 1	8.249736378498 09	0.088544313618 56	0.541619364861009 3
31	−1.341930693678 109	6.451869235304859	0.054828048889270 922	0.569417017643024 2	4.416924335199 95	0.042122086127206 39	0.589712500067734 2	8.865211079845 57	0.086658179484255 7	0.531174423022763 5
32	−10.164671215713 73	6.705508349541454	0.093474969807761 9	0.442069317172849 5	2.858371131410651	0.037225575506068 529	0.421658050029743	6.670274811535954	0.097733247094632 1	0.538756085129185
33	−1.107633246744663	7.390220519784453	0.079706616741810 83	0.508194060224835	3.815123656821275	0.049655298633978 79	0.497023655525965	9.699452453117 18	0.070393411310230 45	0.499074429174679
34	10.394518718668 51	1.478170300165134	0.036021095092150 16	0.579911338104815 4	2.105782960173057	0.086192838023678	0.481252829377607	7.010226383015251	0.035353277899893 27	0.496998966457719
35	−0.139925361351959	4.045190240200832	0.035799555552582782	0.567836234859899 5	9.323868377350 74	0.085864897655904 4	0.569875299685558 2	9.818959037995 08	0.047040209565330 79	0.570869233757954 2
36	3.656124569605117	4.944179742822627	0.093191652533049	0.483464027797733 5	9.384797941949 1	0.084081006349773 5	0.409025472070404 5	3.673880603434117	0.071589340234893 80	0.559819680364353
37	8.067346791126 84	2.988178201634472	0.074821869475154 47	0.495014456966061 4	1.910770315838324	0.038771529030451 22	0.578665956849929 2	4.285706479098184	0.059404875507701 45	0.484451336881370 2
38	0.301156662183572 2	8.789962073643 55	0.048334523937733 47	0.459203937360375	9.934677577778 73	0.097396430307 1365	0.428034968453508	4.931948094146 225	0.096941028775526	0.456066035392976
39	−0.246917895832428 3	6.242957525364009	0.098956831423411 2	0.420566257052738 1	4.739832300049 83	0.045011022516167 8	0.559400017887981	9.119789479431 94	0.061898260311627 79	0.493100819449519
40	−5.704905642148452	4.447521595114223	0.067705232054577 97	0.504796589729867 5	3.987888630073714	0.035951366152543 31	0.592901104492553 6	5.221218237153 44	0.040294319054676 98	0.514129411681418
41	0.142579577968751 9	6.919606258393273	0.082175636897531 2	0.597679941866142 6	8.040990370181 68	0.031292621108814 38	0.468653088192583 1	3.421695873368174	0.051662157795870 51	0.420856080381851 3
42	0.684370289450278 9	8.272005873231 67	0.054701338843166 1	0.445325478642323 7	7.433883810628654	0.046122023438269 98	0.526973037029639	8.364161921824	0.079968793908048 05	0.503675571839614 4
43	−14.065717573691 53	6.220712308892191	0.047659565453437 692	0.489895929037135 3	8.722494312415 67	0.050599670523558 8	0.442127405287572 7	2.416276423317 33	0.073736609308282 08	0.540385065253599
44	8.323461094437 68	9.297160676629 43	0.065681060341482 7	0.496006685901146 6	6.796263459296078	0.040371161070977 55	0.438988573786915 8	2.206183147865627	0.080491098908105 6	0.580622132313237 3
45	−5.252317079780442	3.424683176707511	0.086752998557643	0.432254856047479 6	8.859255296971943	0.095596725294955 1	0.517620399931 194	5.826144924819697	0.091040844281354	0.416701440818250 1
46	6.186413888987 92	3.789578783769164	0.076173263043824 99	0.541849004576107 3	1.363177133649232	0.031972492452403 19	0.528499999290674 3	4.987900195533 8	0.041261253229208 61	0.489516720675473 5
47	0.482190632617353 2	1.195769022526768	0.049287490829701 99	0.528685947237834 7	8.767140633033632	0.087085241229527 8	0.598963815290328 5	2.489565114307663	0.055686854410478 115	0.578705695794220 9
48	5.707663438868804	4.058614230578957	0.047438753923945 99	0.498114989035443 6	1.015171237874 32	0.085826684646538	0.547034932077456 6	6.343764732288268	0.087876934185823	0.544945236749704 4
49	−0.185795867902261 2	5.159763617905121	0.085057042258765 9	0.531149128446558 8	7.238990148015965	0.058670487113936 52	0.566241078122187	8.706006093342 84	0.040888387548046 445	0.530514339249028 4
50	2.321594443893878	3.319181325761367	0.053910808697809	0.591443543460077 3	9.117760453774 91	0.035833540019189 01	0.466941368494417	6.117669336479262	0.045530141564225 49	0.413132426352717 5
51	2.451069994722774	4.005247740100538	0.076208610674944 49	0.575922543333295 5	6.743529978394792	0.096734728036000 8	0.498063985926895	5.505849306951131	0.097144036358688 3	0.451734677211 02
52	−0.961350897030818	7.710615861039985	0.071316171253071 38	0.400736252272210 2	3.372061685311945	0.045793354369674 17	0.484550326849621 7	8.602199592923 5	0.063468185108336 3	0.420724281082454 3
53	−10.679714906713 66	4.728468083127391	0.065092008062538 13	0.495940080135112 7	9.812664816064 75	0.095134676053071 9	0.504721201527784 2	3.180268423645401	0.068191338503702 3	0.575858078972047
54	1.375998039323297	2.740626958875014	0.064383238365668 41	0.507715816856486 6	1.813952930718781	0.084552323086903 1	0.407247659218711	1.054506345314588	0.099827478914431 6	0.595634442044153 9
55	−4.330863793299111	3.209443235555092	0.051508067670949 47	0.593243219531049	4.682408324655706	0.036413762266121 34	0.449194004317304 3	9.578004704242 46	0.089704223465467	0.470288773534834
56	6.961655278126058	3.013659237176324	0.080268421188334 9	0.573346079140423 5	7.441047648005995	0.092446253937035 9	0.521667146638173 9	8.154031319345 62	0.056119343505686 269	0.491048371900593 2
57	−5.305400832811 53	2.088882156026381	0.074640912274694 28	0.474007275624833 9	4.228694369663863	0.039931783489746 01	0.440294623814849 2	9.412298433960689	0.065283594922645 17	0.492358090684315 6
58	3.395100400983763	7.973368098629 92	0.091184358395522 36	0.531400787140655 6	6.375772536276909	0.093302636410837 9	0.447244215655568	7.387561983870292	0.097764338445491 2	0.479824590293356
59	1.330224789015745	5.105339790874075	0.063317182843429 62	0.550380470650627 5	9.574082164184 2	0.074635006441328 46	0.581448195254658 2	5.810342341443878	0.033276351278031 91	0.555021635636082 9
60	−0.292606495526307 9	6.773414983805557	0.075958199052591 91	0.521083462611455 3	4.229974804881476	0.035321775456335 47	0.572561513021506 3	8.884528325496 66	0.093298571068546	0.504638812485702 8
61	−26.418409905255 62	6.417011618542 83	0.062469446461726 64	0.425892344142607 1	1.379491105318868	0.063036379278181 08	0.453144303050720 2	2.189456974183496	0.098078005933584	0.517438456407929 9
62	6.630393088825135	6.476325542442256	0.075994356471882 18	0.434552870579566	6.969363897694016	0.066693020371761 08	0.517427894398595	3.961825639220393	0.092911532224498	0.462104357033659 5
63	3.065748817227897	1.300093759156537	0.067418850755991 73	0.486634511696751 3	6.942052331590217	0.071079639207560 23	0.493067278131158 8	7.834870626014938	0.064461156038706 24	0.536721921821626 6
64	−1.743105697039855	3.145607697855832	0.041529299276100 4	0.585941434322660 1	5.945295724435049	0.074143794063865 93	0.454862947673868 1	1.062923665624632	0.076362140803380 54	0.433029125433189 5
65	−1.631255302904965	3.121291975208031	0.031335617417523 11	0.524510056949801	8.031188798375 2	0.098737609241280 9	0.512855959951593	7.572783963151993	0.093619248113851 8	0.452324098733509 3
66	−9.509826926425 15	7.367027947839741	0.073981085154265 52	0.475325760046692 5	1.589160147317211	0.073985889423494 99	0.464410581491098 7	1.719981611302808	0.049869760634796 17	0.539470969839443 3
67	−4.496736421068983	8.564986505860 69	0.087095015579911 9	0.480700471087150 1	8.858154110695 66	0.093669052114511 4	0.412076459478655	2.422694718173737	0.056519232648803 63	0.483235154774881 5
68	−1.002977917543076	9.431218143626 08	0.036898943831728 01	0.480185091501836 5	6.762463110315146	0.097799013487549 5	0.588037729906973	8.482887773574 23	0.059837359550212 98	0.483756003501434
69	−9.231065451706 94	8.479296961594 59	0.054721412255576 1	0.494998970235259 8	4.776138672418544	0.083516226465965 4	0.578516621149568 9	4.459069855546714	0.068927721673633 42	0.590852931184479 1
70	14.999263048312 82	4.708917711658332	0.090736428406538 2	0.455003333495992 9	5.373320800648651	0.037399245362693 47	0.446813240661560 5	1.831662246071428	0.058255589142067 48	0.566434199642786
71	4.189181104505013	7.583635162152007	0.093682970842179 2	0.411067909912185 6	6.090022152191 53	0.058950447891399 01	0.545125369204061 4	6.851478307492325	0.047638403342314 68	0.501063316085022 4
72	8.328371883138842	3.414315967033806	0.050540846424766 5	0.504330741052470 6	3.070996567281799	0.069682763289745 09	0.570266970236848	5.360783854112533	0.038888833806669 67	0.578415546756623 7
73	−21.842008884915 82	1.625552430388586	0.045462368316544 88	0.542607857632417 9	4.091176923293506	0.038368850396528 42	0.504879512949007	4.527748284314512	0.059758941029279 81	0.467059850649671
74	6.604738977945651	3.421878979312 62	0.089444995069718 7	0.494148562897417 2	4.967497413312 63	0.060311512137835 82	0.411902863745698	4.581927607849956	0.087194896369227 9	0.417680575452423
75	15.279884232466 28	6.229538426957454	0.082152109121586 3	0.411878484925231 5	2.377028497509498	0.096311093310645 8	0.474673655680810 9	5.398545541594487	0.082257465678064 3	0.525894723319048 7
76	1.377130763885458	9.151763463337 75	0.048186824886185 07	0.574408949666749	2.366656226877287	0.050591997697459 39	0.473107499729489	4.342903653707 39	0.074929040494938 38	0.403865637589233 7
77	−0.775695935148424 4	8.152511280158 1	0.081297534421981	0.511285375196410 7	4.530310672134297	0.066529124861348 06	0.594624523185316 2	1.568860626254933	0.042568820256052 58	0.549102780104355 6
78	−9.504327928043 36	4.670517118870347	0.043982677995534 92	0.451947267371889 3	2.155276187476066	0.048941143618085 4	0.569475627865203 3	1.947130206816878	0.063213090412016 74	0.412231214773356 8
79	3.754137123031758	6.801389212739803	0.070033093426234 26	0.512921484248138 9	9.924339101493 23	0.093139282089872	0.410401649514640 4	5.230366081025 18	0.091952918204162	0.446529497438288
80	−4.499804654067136	4.406584351091798	0.097021115901162 6	0.477297593852152 7	2.270764431848441	0.085356275712211 6	0.466959692098883 9	4.425574133334857	0.051780050947379 9	0.564519180912112 8
81	−13.999906168852	8.304086221392 41	0.090394873809322	0.505320958374436 4	2.454354187669313	0.085768169040050 4	0.576877467653029	7.167289037979305	0.083120632017551 5	0.422133968079279 9
82	−4.878405649764898	7.975675712689654	0.080964951597413 9	0.583199015888957 1	1.696376490191135	0.067830461192706 37	0.578856072348660 3	5.118512758012828	0.065546170065123 21	0.557158655852978
83	−8.706116626901 58	3.078380132262833	0.063276262752935 22	0.401798898167941 8	2.138629261588504	0.053747333027151 09	0.543244322891937	7.596013793576791	0.099992446704472 9	0.511524562576321
84	3.578654662131496	4.294915349281119	0.066470664181728 1	0.556628916585203 6	3.387516420897519	0.066542282934132 48	0.430493549849486 2	8.432328281561 06	0.061217696939205 87	0.552707684390498
85	0.042325954115396 7	9.569366653534 94	0.068259638236415 94	0.553235306476861 8	7.233942984150266	0.077360329991033 62	0.427431654154194 1	8.960226930 99	0.039963477330609 68	0.509107313078646 2
86	−6.387446031119123	5.052123646744015	0.053069734537515 37	0.465729741846814 1	1.261670338009784	0.053922352609947 65	0.435557134047666	9.818841284758 22	0.043416419361416 2	0.546118275633825
87	3.029693711282459	1.767169254935782	0.038627305488900 3	0.417420242288104 8	9.991898828365 94	0.034710753522480 7	0.531658797486970 9	4.794411329362948	0.048663927171989 35	0.520281555759426 17
88	−0.791031105864576	8.380824270655 73	0.055212790770486 2	0.582180019492365 9	3.864226559651998	0.054621670805278 7	0.505154323978516 5	4.445064096761643	0.033869071793617 38	0.465908117746965
89	2.970836817385 8	9.227063637420 46	0.069121403865493 836	0.563002337818579 5	2.929880196570098	0.079666599068684 009	0.499226363393581	6.920427033384 97	0.031234074920227 2	0.407715660159876
90	−7.110772604917624	3.106633667560681	0.048739900253877 01	0.569704953589338 1	8.307007774637 54	0.052495016309893 04	0.566978376291061 2	1.134573939330 62	0.072007601353994 357	0.444672072474744
91	−7.162305080703513	5.387619660361665	0.045815003857453 13	0.519783506282974	8.225519917733 7	0.083122669390787	0.427498766760087	6.828948529150043	0.059433495931412	0.511586149713706
92	1.720368406482304	6.780548897314363	0.087001211193309 2	0.598490848442784	6.587571277412653	0.056941052371280 53	0.522669782534278 8	5.990056411944593	0.078379213223164 56	0.466823604075257 7
93	0.149488404564976 2	8.098185241717 48	0.097659525529836	0.484853559604263 7	2.153483785757176	0.047342111106742 12	0.407722222205073 15	7.143110762448606	0.046822103323860 52	0.509084643832387
94	−0.962821097034532	7.260437643310942	0.050833965752790 76	0.547453037159866	8.381629903060 18	0.057910509436882 69	0.579439562549738 2	2.722302743095399	0.083744615781603	0.539542847125162 4
95	0.935122045036145	2.317883014549977	0.059762949487823031	0.580920437623820 6	8.191724073542 63	0.068067781957685 99	0.547937441785378	9.939903362253 75	0.042669772301815 23	0.595990170586379 1
96	0.432827723650467 7	4.113414252906836	0.079884045133400 22	0.526207991092555 7	7.436994191924832	0.076416991961448 98	0.431628208551548 6	9.596718070162 01	0.071989665157052 08	0.456302497028836 9
97	0.853043516035702	3.229317247568396	0.046642883808967 379	0.491664178074803	9.195336151425 81	0.094421601252687 1	0.579263841357722	6.980966479991427	0.076473121261060935	0.540776396743738 5
98	−3.516191871248866	9.207695342396 92	0.072145990769657 883	0.411131207094635 6	7.568725646438693	0.080690203332229 7	0.495204295074376	8.949197474614 64	0.042634437772906 76	0.573526196085083
99	19.672437605496 39	2.270663590855083	0.097117017796776 5	0.461301796787272 8	8.224805604729 66	0.053602477256128 2	0.474530301185656 44	3.970009703387312	0.098203234925795 3	0.502918207513967
100	1.544060514744405	4.017102041449901	0.044370906450895 48	0.507365561530174 1	3.724036679477685	0.076227726459893 46	0.436888283799122 2	5.350823421126575 7	0.076591193976297 86	0.405624376399138 2

TABLE III. All the necessary information to construct our MLA, trained from 100 densities with $N = 1$ on a grid of 500 points, with $\lambda = 12 \times 10^{14}$ and $\sigma = 43$. For purposes of saving space, we do not list these densities. They may be reconstructed from these potentials via Numerov's method.