Herman Skillman Potential Notes

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Contents

1 HS potential

The HS potential was obtained using the Cowan-code. The resulting points were fitted using these function:

$$U(r) = -\left(a\mathrm{e}^{-rb+c} + d\mathrm{e}^{-re+f} + g\mathrm{e}^{-rh+i} - j\right) \tag{1a}$$

$$E(r) = -\boldsymbol{\nabla} U(r) = -\left(ab\mathrm{e}^{-rb+c} + de\mathrm{e}^{-re+f} + gh\mathrm{e}^{-rh+i}\right) \tag{1b}$$

The parameters are given in tables 1 and 2.

Figure 1 shows the HS potential and field. Notice the discontinuity where it becomes coulombic. This discontinuity is due to the fact that the even though the potential reaches the Coulomb values, at this distance r_{max} the derivative, and thus the field, is discontinuous.

2 Preventing the discontinuity

Since the important aspect in a Molecular Dynamics code is the force, the field cannot have a discontinuity without introducing errors. To correct this:

a) The HS field is multiplied by a constant to shift it upward and match Coulomb at r_{max}

$$E'(r) = \frac{\text{Coulomb}(r_{max})}{E(r_{max})} E(r) \tag{2}$$

Charge state	r_{max} (Bohr)
Neutral	12.0
1+	3.20671
2+	3.4419260284993465
3+	2.5786383389900931
4+	2.3069998849855851
5+	2.1424931697942897
6+	1.9288708307182563

Table 1: Distance where HS potential reaches Coulombic values

	Neutral	1+	2+	3+	4+	5+	6+
a	3.14083382	6.68943368	1.08862692	1.26082951	8.33659368	8.13621709	7.52331956
b	2.23690529	5.46613511	1.12845509	1.24346292	15.53383795	15.39455048	15.56584267
c	2.45999159	3.50223818	2.40634711	2.48202614	4.69224278	4.6973397	4.77821787
d	1.04922253	9.84854609	7.5231977	7.60391482	5.66740119	1.33881001	2.17218048
e	0.758964055	16.33928308	11.80857511	14.20436211	4.93161199	1.40783802	1.51817071
f	0.916259659	4.55862051	4.40029841	4.63976132	3.58851214	2.72036815	2.38100923
g	6.43949225	2.05998631	3.5171341	5.75320941	1.33122023	5.60695758	5.09462365
h	5.57500308	1.79149357	4.02105327	4.57482337	1.36069086	4.96351559	5.11830058
i	3.46700894	2.67105113	3.70863489	3.45935956	2.65699251	3.59035494	3.70739486
j	-2.22471387e-3	-0.216514733	-0.33244088	-0.55091234	-0.90941801	-1.33283627	-1.84326541

Table 2: HS parameters

b) This multiplication factor must be applied to the potential too for the field to match the derivative of the potential:

$$U'(r) = \frac{\text{Coulomb}(r_{max})}{E(r_{max})} U(r) \tag{3}$$

c) But since the potential energy is now shifted by this multiplication, an additive constant is added so the potential match the Coulomb values at r_{max}:

$$U''(r) = U'(r) + \text{Coulomb}(r_{max}) - \frac{\text{Coulomb}(r_{max})}{E(r_{max})} U(r_{max}) \tag{4}$$

This addition constant does not change the field.

Figure 2 shows this scaling and how it prevent discontinuities at the boundary between Coulombic and HS.

This is performed in function Set_HermanSkillman_Lookup_Tables_Xe() in HermanSkillman.cpp.

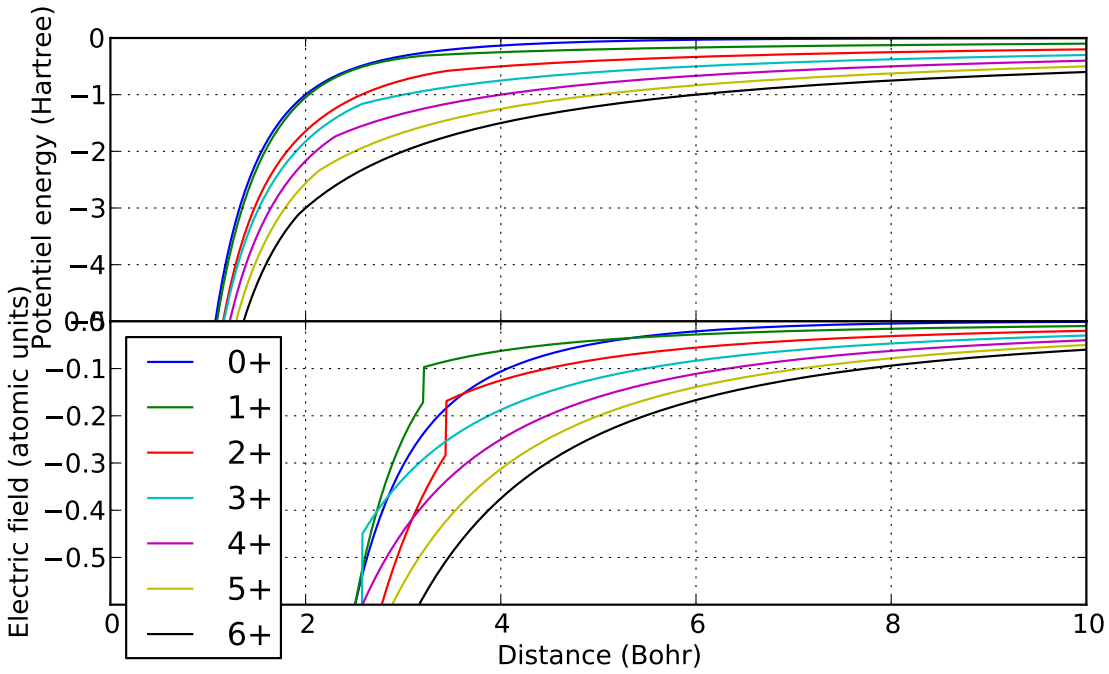

Figure 1: Raw HS Potential energy and electric field

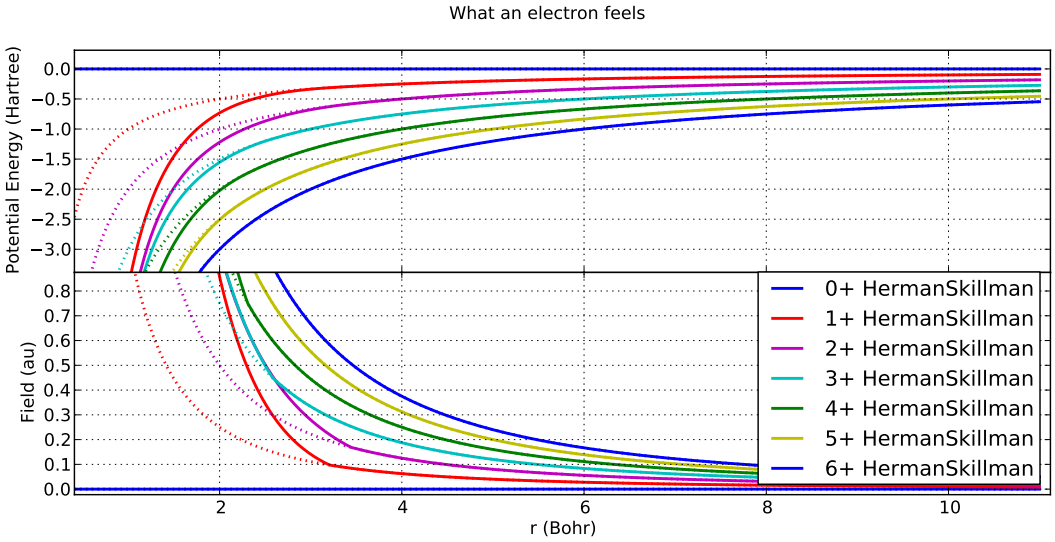

Figure 2: Coulomb-HS smooth boundary (doted line is Coulomb)

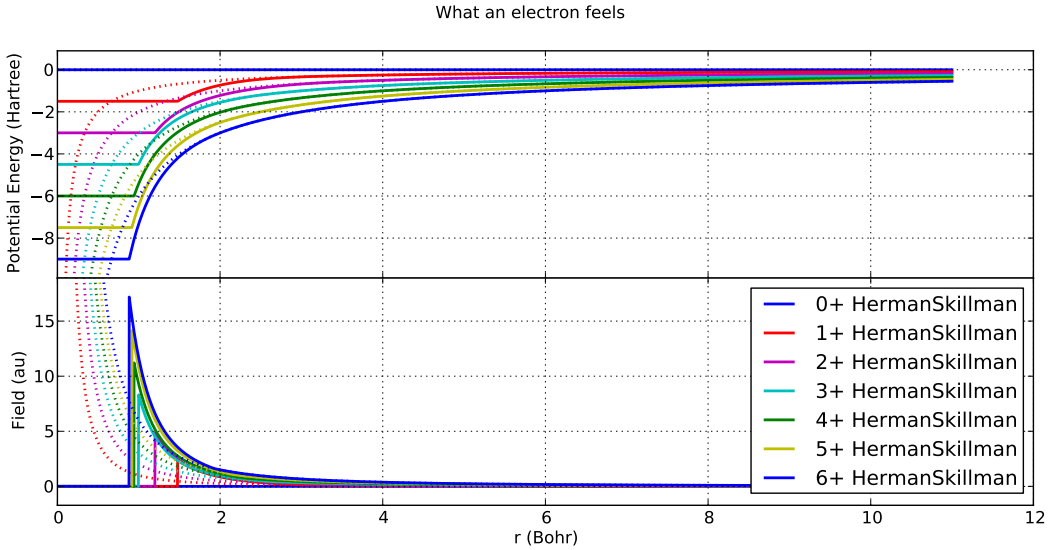

Figure 3: HS with hard cutoff (doted line is Coulomb)

3 Cutoff

3.1 Hard Cutoff

In the code, the depth of the potential is chosen. In the "Symmetric" potential case, it will affect the width of the charge distribution. In the HS case, fixing the max potential depth causes problems. Figure 3 shows what a hard cutoff creates. The potential is "capped" at a maximum value but since the derivative of this section is zero, the field becomes null. The distance at which the cutoff occurs will have a discrepancy in the field. A particle crossing that boundary will feel the drop in the field and will numerically heat. Because of that problem, a system consisting of many electrons and ions will create energy rendering any measurement of the energy futile, as is the case in an IBH study. To have a energy conserving system, the field has to go to zero smoothly.

3.2 Cubic Spline Cutoff

Even though the HS potential is fitted using the analytic function (1), making the field go from its maximum value to zero smoothly is hard. This is accomplished using a cubic spline of three points. See libpotentials.git/doc/cubic_spline/cubic_spline.pdf for how to do the spline.

The first of the three points is taken to be $r = 0$ and $E = 0$. The second and third points are taken really close to each other: the third point is the 10^{th} point after the second.

Taking these points arbitrarily will create problems though: the potential and field must match with $E = -\boldsymbol{\nabla} U$. To enforce this constraint, a bisection method is used to find the right

placement of the second (and thus also the third) point. The bisection will find the distance where the second point is to be taken by checking if the field's integration from 0 to this distance matches the HS potential at that distance.

Instead of finding the optimal distance, the code will search for an optimal fraction of the maximum field. The optimal distance is then obtained by finding where the field match the field.

First, the index of the maximum field is found and the bisection is performed between where the field is half and one tenth of that maximum. The bisection starts with the middle point (one sixth) as the fraction:

a) Find the index where the field is the maximum times the fraction;

b) Put the spline's second point there, and the spline's third point a bit further (an offset of 10);

c) Calculate the spline's parameters and the resulting potential at the third point's location;

- If the calculated potential is higher then the HS potential at the point's location, the spline's field gets too high. Increase the fraction (thus reducing the spline's maximum field) and start again.
- If the calculated potential is lower then the Hs potential at the point's location, the spline's field is too low. Decrease the fraction (thus increasing the spline's maximum field) and start again.

d) When the upper and lower bounds for the fraction converge, stop bisection.

This procedure is done for every charge state. Figure 4 shows the resulting potential. Note that the deepest potential has the right value (in this case 1.5 Hartree) and both the potential and field are smooth.

With such a potential, the energy of a system will stay constant over time and the physics can then be trusted. A nice addition too is that since the system does not (numerically) heat anymore, a bigger time step can be used.

The only issue is that, as can be seen on figure 5 where the Symmmetric potential is also plotted, the maximum field value is lower then the symmetric case. When an electron collide with an ion (thus coming from large distances) the HS field will increase faster than the Symmetric potential, but the Symmetric will have a slightly higher maximum field. It could affect the IBH.

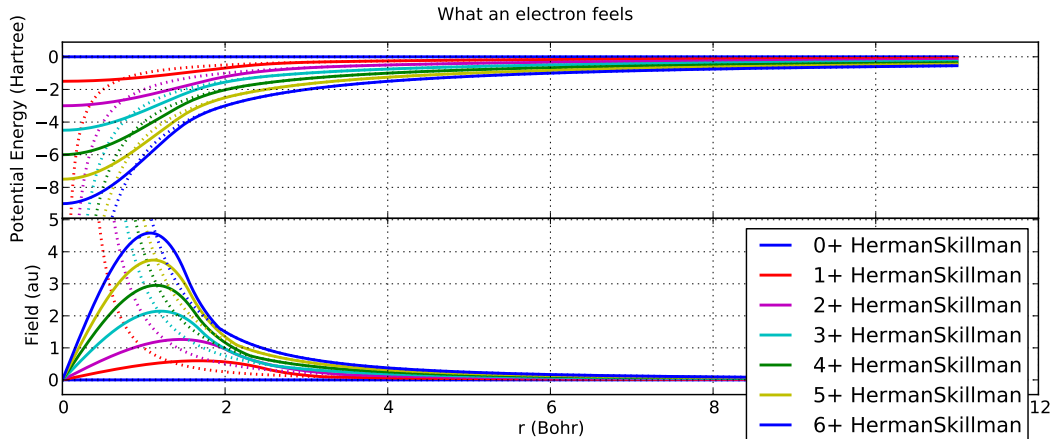

Figure 4: HS with spline cutoff (doted line is Coulomb)

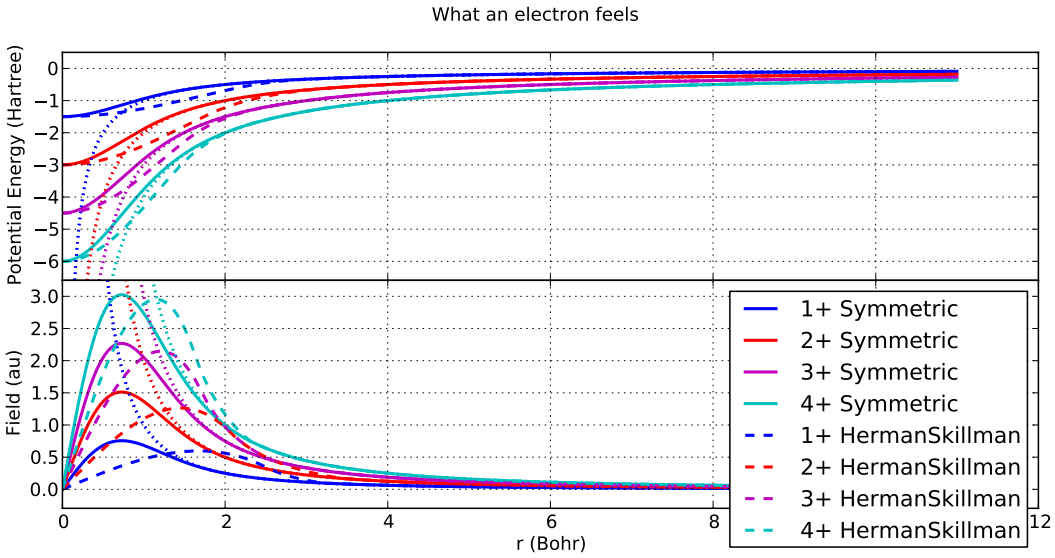

Figure 5: HS with spline cutoff compared to Symmetric potential (doted line is Coulomb)