Expectation values of operators are affected by the softened intra-system derivative discontinuity of populations.

- Similarly to the energy functional, also the populations as functional of the density show a softened intra-system derivative discontinuity.
- The exact Hohenberg-Kohn functional shows a softened intra-system derivative discontinuity in the low-density limit.

**Conclusion & Outlook**

We currently develop an approximate functional which incorporates the intra-system derivative discontinuity.

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**References**

We currently develop an approximate functional which incorporates the intra-system derivative discontinuity.

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**Soft-Coulomb molecules in 1D**

<table>
<thead>
<tr>
<th>Hamiltonian</th>
<th>Exact Kohn-Sham potential for two-electrons in spin singlet configuration (Belling et al. 2009) [2]</th>
</tr>
</thead>
<tbody>
<tr>
<td>( H(\alpha) = T + W + V(\alpha) )</td>
<td>( v_{\text{eff}}(t) = \frac{\sqrt{v(t)}}{\sqrt{t}} )</td>
</tr>
</tbody>
</table>

Exact solution of static inter-electron Schrödinger equation with one-frag (A. Cerri et al. 2015)

\( f(z) = \sum_{\chi} e^{2\pi i \chi z} \) for \( z = 3 \) Bohr

**High-density limit (small distance \( d = 3 \) Bohr)**

**Low-density limit (large distance \( d = 8 \) Bohr)**

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**Softened intra-system derivative discontinuity**

- We choose softened intra-system derivative discontinuity also for soft-Coulomb molecules in 1D.
- We currently develop an approximate functional which incorporates the intra-system derivative discontinuity.

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**Hohenberg-Kohn functional**

- The exact Hohenberg-Kohn functional shows a softened intra-system derivative discontinuity in the low-density limit.
- Expectation values of operators are affected by the softened intra-system derivative discontinuity of populations.