Inter-dimensional degeneracies in van der Waals clusters

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Abstract

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\[ \text{\LaTeX with \texttt{proser.sty} does it all.} \]

(proser.sourceforge.net)
**Basic definitions**

- **$N$** atom cluster in $D$ dimensions; positions given by $D \times N$ matrix of Cartesian coordinates

\[
\mathbf{R} = (r_1 r_2 \ldots r_N),
\]

with

\[
\mathbf{r}_i = \begin{pmatrix}
x_{1i} \\
\vdots \\
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\end{pmatrix}.
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- Define difference vectors and their lengths

\[
\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i,
\]

\[
|r_{ij}| = |\mathbf{r}_{ij}|.
\]
Basic definitions

- Dimensionless Hamiltonian of $N$ bosonic van der Waals atoms with atomic mass $\mu$

$$H = -\frac{1}{2m} \sum_{i=1}^{N} \nabla_i^2 + \sum_{(i,j)} V(r_{ij}),$$
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• Inverse dimensionless mass is \( m^{-1} = \hbar^{2}/2^{\frac{1}{3}} \mu \sigma^{2} \epsilon \) proportional to the square of the de Boer parameter\(^{[1]} \); \( \epsilon \) and \( \sigma \) the standard Lennard-Jones parameters. [J. de Boer, Physica, 14, 139 (1948)]
Monte Carlo trial function optimization

- Generate a sample of configurations $\mathbf{R}_\sigma$ ($\sigma = 1, \ldots, s$) from a relative probability density function $\psi_g(\mathbf{R}_\sigma)^2$. 

In theory, for a complete set of elementary basis functions $i$ the Schrödinger equation becomes

$$
\hat{0}_i(\mathbf{R}) = \sum_{j=1}^{n} \hat{j}(\mathbf{R}) E_{ji}.
$$

In practice, solve for matrix $E$ in least-squares sense on Monte Carlo sample. Reproduces stationarity of energy w.r.t. linear parameters for infinite sample.
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- Generate a sample of configurations $\mathbf{R}_\sigma$ ($\sigma = 1, \ldots, s$) from a relative probability density function $\psi_g (\mathbf{R}_\sigma)^2$.
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• Re-weighted functions defined as $\hat{\beta}_i(R) = \psi_g(R)^{-1} \beta_i(R)$ and $\hat{\beta}'_i(R) = \psi_g(R)^{-1} H \beta_i(R)$ for least-squares.
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Monte Carlo trial function optimization

- Optimal linear combinations of the basis functions \( \beta_i \) computed by spectral decomposition of \( \mathcal{E} \):

\[
\mathcal{E}_{ij} = \sum_{k=1}^{n} d_{ik}^k \tilde{E}_k \hat{d}_{kj}^k
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with \( \hat{d}_{ij}^k \) and \( d_{i}^k \) left and right eigenvectors of \( \mathcal{E} \) with eigenvalues \( \tilde{E}_k \).
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- Yield: trial functions

$$\tilde{\psi}^k = \sum_{i=1}^{n} d_i^k \beta_i.$$
Monte Carlo trial function optimization

- Non-linear parameters of the $\beta_i$ are optimized by minimizing the variance of the local energy of the linearly optimized $\bar{\psi}^k$

$$
\chi^2 = \frac{\sum_{\sigma=1}^{s} [\hat{\psi}^{k'}(R_{\sigma}) - \tilde{E}_k \hat{\psi}^k(R_{\sigma})]^2}{\sum_{\sigma=1}^{s} \hat{\psi}^k(R_{\sigma})^2},
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where $\hat{\psi}^k = \psi_g^{-1} \bar{\psi}^k$ and $\hat{\psi}^{k'} = \psi_g^{-1} H \bar{\psi}^k$. 
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- For each choice of the non-linear parameters, new optimized linear parameters have to be computed.
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full optimization of all parameters consists of a linear optimization nested in a non-linear one.
Numerical results: three-body case

<table>
<thead>
<tr>
<th>$D$</th>
<th>$E_1$</th>
<th>$\Delta E_1$</th>
<th>$E_1$</th>
<th>$\Delta E_1$</th>
<th>$E_1$</th>
<th>$\Delta E_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-1.872 548 547 6</td>
<td>$-9 \times 10^{-1}$</td>
<td>-1.734 808 71</td>
<td>$-8 \times 10^{-1}$</td>
<td>-0.895 584</td>
<td>$-4 \times 10^{-1}$</td>
</tr>
<tr>
<td>2</td>
<td>-2.760 461 351 5</td>
<td>$2 \times 10^{-10}$</td>
<td>-2.552 953 22</td>
<td>$-1 \times 10^{-9}$</td>
<td>-1.302 484</td>
<td>$-7 \times 10^{-7}$</td>
</tr>
<tr>
<td>3</td>
<td>-2.760 555 278 7</td>
<td>$6 \times 10^{-10}$</td>
<td>-2.553 289 43</td>
<td>$1 \times 10^{-8}$</td>
<td>-1.308 442</td>
<td>$9 \times 10^{-6}$</td>
</tr>
<tr>
<td>4</td>
<td>-2.760 461 351 3</td>
<td>$-5 \times 10^{-11}$</td>
<td>-2.552 953 22</td>
<td>$-1 \times 10^{-9}$</td>
<td>-1.302 483</td>
<td>$-2 \times 10^{-6}$</td>
</tr>
<tr>
<td>5</td>
<td>-2.760 179 569 8</td>
<td>$-1 \times 10^{-9}$</td>
<td>-2.551 944 61</td>
<td>$-2 \times 10^{-8}$</td>
<td>-1.284 627</td>
<td>$-1 \times 10^{-5}$</td>
</tr>
<tr>
<td>6</td>
<td>-2.759 709 937 6</td>
<td>$5 \times 10^{-10}$</td>
<td>-2.550 263 64</td>
<td>$7 \times 10^{-9}$</td>
<td>-1.254 901</td>
<td>$5 \times 10^{-6}$</td>
</tr>
</tbody>
</table>

Ground state energies $E_1$ (with errors in the last significant digit) and deviations from quadratic fits $\Delta E_1$ for $\text{Kr}_3$, $\text{Ar}_3$ and $\frac{1}{2}\text{-Ne}_3$ in dimensions $D = 1$ through $D = 6$. 
**Numerical results: four-body case**

<table>
<thead>
<tr>
<th>$D$</th>
<th>$E_1$</th>
<th>$\Delta E_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-2.625 622 56</td>
<td>-2 $\times 10^{-0}$</td>
</tr>
<tr>
<td>2</td>
<td>-4.329 517 95</td>
<td>-8 $\times 10^{-1}$</td>
</tr>
<tr>
<td>3</td>
<td>-5.118 146 05</td>
<td>-2 $\times 10^{-9}$</td>
</tr>
<tr>
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<td>-5.118 653 84</td>
<td>3 $\times 10^{-9}$</td>
</tr>
<tr>
<td>5</td>
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</tr>
<tr>
<td>6</td>
<td>-5.116 622 70</td>
<td>1 $\times 10^{-9}$</td>
</tr>
</tbody>
</table>

Ground state energies (with errors in the last significant digit) and deviations from quadratic fits $\Delta E_1$ for $\text{Ar}_4$ in dimensions $D = 1$ through $D = 6$. 
Numerical results: excited states $\text{Ar}_3$

Comparison of the excited state energies $E_k$ (with errors in the last significant digit) of $\text{Ar}_3$ in $D = 2, 3$ and $4$ dimensions.

<table>
<thead>
<tr>
<th>$k$</th>
<th>$D = 2$</th>
<th>$D = 3$</th>
<th>$D = 4$</th>
</tr>
</thead>
<tbody>
<tr>
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<td>-2.250 185 5</td>
<td>-2.249 860</td>
</tr>
<tr>
<td>3</td>
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<td>-2.126 361</td>
<td>-2.126 039</td>
</tr>
<tr>
<td>4</td>
<td>-1.996 153</td>
<td>-1.996 43</td>
<td>-1.996 153</td>
</tr>
<tr>
<td>5</td>
<td>-1.946 3</td>
<td>-1.946 7</td>
<td>-1.946 3</td>
</tr>
</tbody>
</table>
**Numerical results: excited states $\text{Ar}_4$**

<table>
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<tr>
<th>$k$</th>
<th>$D = 3$</th>
<th>$D = 5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>-4.800 897 73</td>
<td>-4.800 897 75</td>
</tr>
<tr>
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<td>-4.725 156 7</td>
<td>-4.725 156 6</td>
</tr>
<tr>
<td>4</td>
<td>-4.630 025</td>
<td>-4.630 025</td>
</tr>
<tr>
<td>5</td>
<td>-4.586 389</td>
<td>-4.586 384</td>
</tr>
</tbody>
</table>

Comparison of the excited state energies $E_k$ (with errors in the last significant digit) of $\text{Ar}_4$ in $D = 3$ and 5 dimensions.
**Exact results**

- Schrödinger equation for an $N$ particle cluster in $D$ spatial dimensions has $ND$ variables.
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- Consider more general $D$-dimensional Schrödinger equation

$$\left( -\sum_{i=1}^{N} \frac{1}{2m_i} \nabla_i^2 + V \right) \psi = E\psi$$
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- Rotationally and translationally invariant potential, not necessarily a sum two-body contributions.
- Mass of each particle may be different.
Exact results

• Apply differential operator identity

\[ \frac{\partial}{\partial x_{\alpha i}} = \sum_{j \neq i} \frac{\partial r_{ij}}{\partial x_{\alpha i}} \frac{\partial}{\partial r_{ij}} \]
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- to obtain

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\nabla_i^2 = \sum_{j \neq i} a_{i;j} \frac{\partial}{\partial r_{ij}} + \sum_{j,k \neq i} g_{i;jk} \frac{\partial^2}{\partial r_{ij} \partial r_{ik}}
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where

\[
a_{i;j} = \sum_{\alpha=1}^{D} \frac{\partial^2 r_{ij}}{\partial x_\alpha^2} = \frac{D - 1}{r_{ij}}
\]

\[
g_{i;jk} = \sum_{\alpha=1}^{D} \frac{\partial r_{ij}}{\partial x_\alpha} \frac{\partial r_{ik}}{\partial x_\alpha} = \frac{r_{ij} \cdot r_{ik}}{r_{ij} r_{ik}} \text{ angle: no } D \text{ dependence}
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- Transform Schrödinger equation so that
  1. second-order operator is unchanged

$H = E \Gamma H_0 = E \Gamma$ with $\Gamma = \varepsilon$ and $H_0 = 1$ to be determined.
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- Use
  $$
  H\psi = E\psi \rightarrow H'\phi = E\phi
  $$

  with
  $$
  \psi = \chi\phi \quad \text{and} \quad H' = \frac{1}{\chi}H\chi
  $$
Exact results


$$H' = V - \sum_{i=1}^{n} \frac{1}{2m_i} (S_i + T_i + U_i)$$

with

$$S_i = \sum_{j, k \neq i} g_{i;jk} \frac{\partial^2}{\partial r_{ij} \partial r_{ik}},$$

$$T_i = \sum_{j \neq i} \left( a_{i;j} + 2 \sum_{k \neq i} g_{i;jk} \chi^{-1} \frac{\partial \chi}{\partial r_{ik}} \right) \frac{\partial}{\partial r_{ij}},$$

and a “centrifugal” contribution to the effective potential

$$U_i = \sum_{j \neq i} a_{i;j} \chi^{-1} \frac{\partial \chi}{\partial r_{ij}} + \sum_{j, k \neq i} g_{i;jk} \chi^{-1} \frac{\partial^2 \chi}{\partial r_{ik} \partial r_{ik}}.$$
Exact results

- Define $N$ matrices of order $N - 1$

$$\hat{G}_i = (r_{ij} g_{i;jk} r_{ik})_{j,k\neq i},$$

the Grammian associated with the $N - 1$ vectors $r_{ij}$ with $j = 1, \ldots, i - 1, i + 1, \ldots, N$. 
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- Volume squared of the parallelepiped formed by the vectors from particle $i$ to all other particles:

\[ \omega = \det (\hat{G}_i) \]
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• Volume squared of the parallelepiped formed by the vectors from particle $i$ to all other particles:

$$\omega = \det (\hat{G}_i)$$

• Linear differential operators $T_i$ vanish for the choice

$$\chi = \omega^{(1-D)/4}.$$
**Exact results**

- Contributions to effective potential

\[
U_i = \frac{1}{8} [(N - 1)^2 - (N - D)^2] \sum_{j \neq i} \frac{1}{r_{ij}} \frac{\partial \log \omega}{\partial r_{ij}} \\
= \frac{(N - 1)^2 - (N - D)^2}{16\omega^2} \sum_{j,k \neq i} \frac{\partial \omega}{\partial r_{ij}} g_{i;jk} \frac{\partial \omega}{\partial r_{ik}}.
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\]

- Amplitude is symmetric in \( D \) about \( D = N \).
- Schrödinger equation has the same energy eigenvalues in \( D = N - 1 \) and \( D = N + 1 \).
- Energy minimum at \( D = N \). (Last sum is sum of squares because \( g_{i;jk} \) is an inner product.)
Summary and discussion

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Resulting equation and its eigenvalue spectrum have an analytical continuation for $D < N$ and is symmetric about $D = N$. The same applies to the spectrum. Continuation unrelated to physical spectrum of $N$ particle clusters for $D = N$.

Fundamental problem with the work by Gonzalez and Leal [6]: $1 = D$ expansion estimates of energy levels of Lennard-Jones clusters in $D = 3$ with $N = 3; 4; \ldots; 7$ and $13$ obtained by analytic continuation from large $D$. 

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References