TDL analysis of 2D HEG data from Gustav Baardsen's thesis (especially Fig 5.10)

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The problem with energies at a finite basis set size (M) and finite particle number (N) is that they suffer both from basis set incompleteness error, and from finite size effects. This means that convergence to known benchmarks can be difficult to quantitatively identify.

The aim of this analysis is to disentangle the two, and indeed this is successfully achieved. TDL estimates are therefore obtained for $r_s = 0.1, 0.5, 1.0$ and 2.0.

Gustav noted: "The CCD results for different finite systems seem to converge to approximately the same energy when the basis size approaches infinity" and my results say nothing substantially different to his. Indeed, qualitatively they are exactly the same. This is because Gustav's data set has obviously been diligently collected and is of high quality and very extensive!

Preliminaries:

- BSIE behaves *limitingly* as $1/M$ in 3D (Ref. 1), and perhaps $1/M^2$ in 2D (pers. comm.). (N.B. small system data $N = 10$ support a high-k turning point, or a $1/M$ limiting power-law).

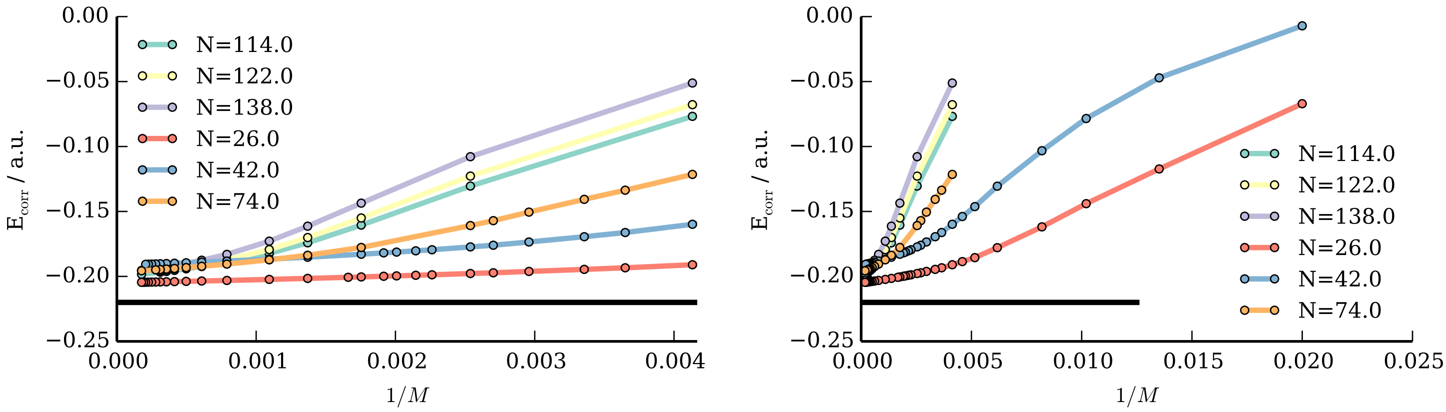
- Finite size error behaves as $1/N^{\frac{5}{4}}$ in 2D (Ref. 2), although this might be complicated by contributions from Hartree–Fock energy which we don't consider.

- Finite size error will be dominated by shell-filling effects rather than a clean representation of this power law, due to PBCs (c.f. TABCs) [2].

- Finite size error can be removed before basis set incompleteness error (Ref. 3). This requires $M \propto N$.

This is a little float-heavy, so there will be occasional unexpected page breaks.

We begin with a simple reproduction of the figure in question:

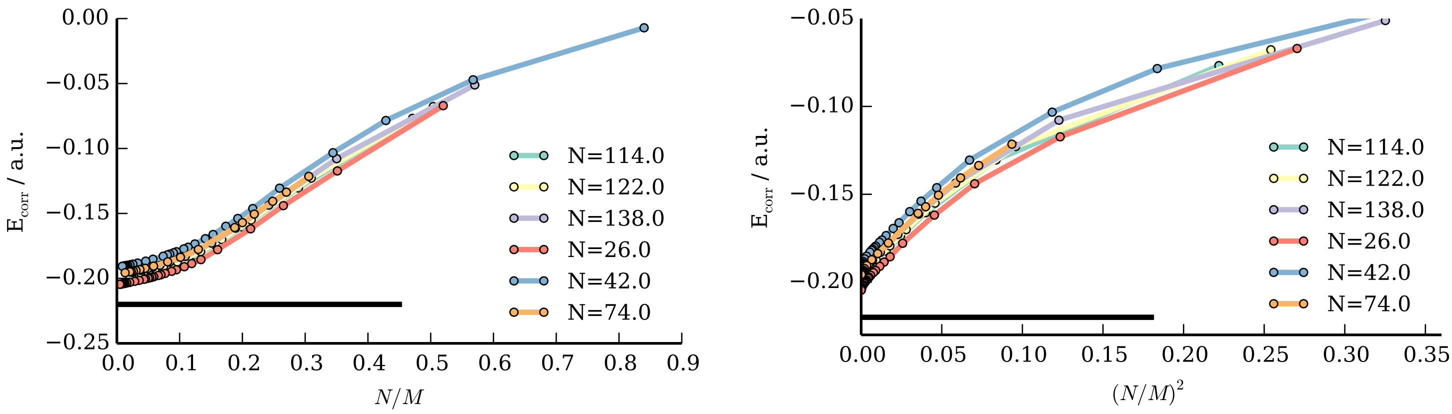


The small N data sets have been included for completeness and the black line is the GFMC result read from the thesis graph. The graph on the right is the whole data set available.

We now apply two transformations to the x-axis.

The first is due to Ref. 3, and just changes M to M/N to account for the dominant shifting of the shape of the lines. And the second is to look at the effect of using $1/M^2$ rather than $1/M$.

This yields:



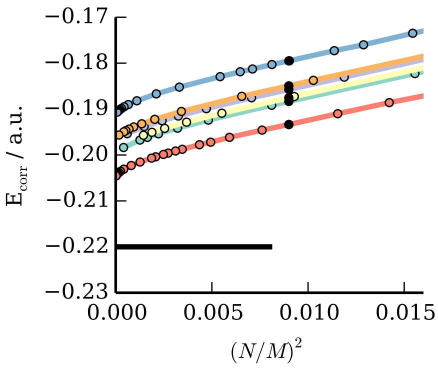
Overall, the transformation of M to N/M has achieved the effect of making the lines parallel as anticipated. This is just to say that the constant behind the basis set incompleteness error when measured as a function of N/M is particle-independent, which is also seen in Ref. 4.

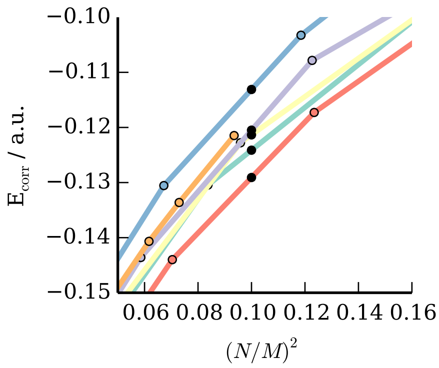
However, the lines are still offset from one another along the y-axis due to finite size effects. We can measure this N-dependent shift to the energy.

Since the lines no longer share x-dependent points, we need to measure this by linear interpolation. For a target value of $x = (N/M)^2$, x', we can find the points (x_1, y_1) and (x_2, y_2) on either side, then the shift can be computed:

$$E_\Delta(N) = y_2 + \frac{x' - x_2}{x_1 - x_2}(y_1 - y_2). \tag{1}$$

Since the lines are parallel, it should not matter unduly what shift we ultimately choose. In general, the larger the value then the worse the finite size effects, and the smaller the value the more *expensive* the calculations required.

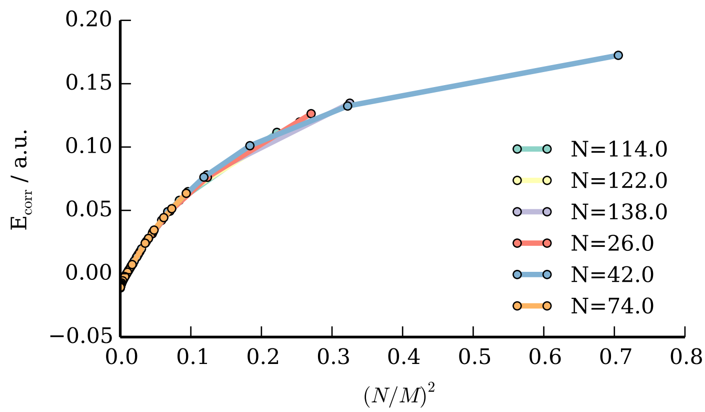




This shows two different possible regions for interpolation. These are very different to one another, but give the same qualitative results: the ordering of the lines is very similar.

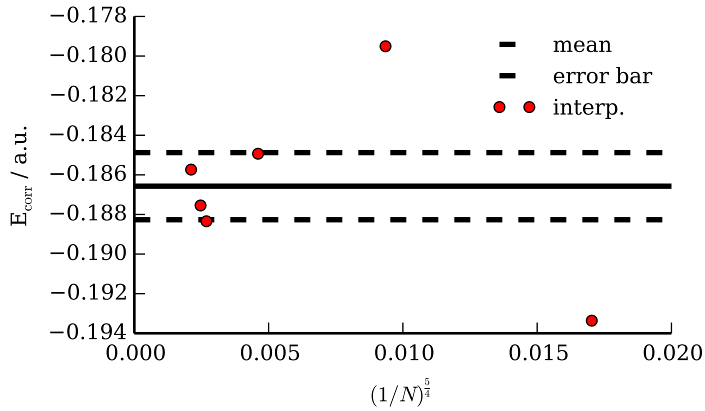
The graph on the left also shows strange behavior at high M, which I can't explain other than to say that there will be multiple $1/M^2$ contributions at high M and that this effect is unfortunate. I don't *think* that a $1/M$ power-law is expected, but it is possible.

Rescaling:



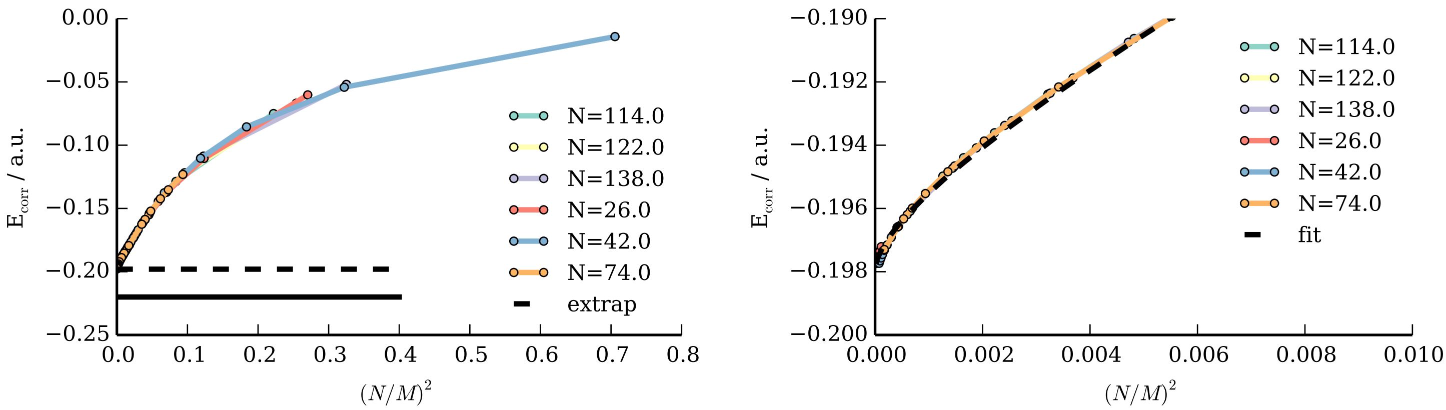
These lines now overlay one another to a very high accuracy.

The shift is far less clean, and has substantial finite size errors:



Although this might scale as $N^{-\frac{5}{4}}$, this is obviously unclear. The extrapolation would provide an estimate of the thermodynamic limit, but instead we just take the mean and associated error estimate: -0.1866 ± 0.0041.

We can now return to our graph with all the data and re-scale the energies again with this TDL correlation:



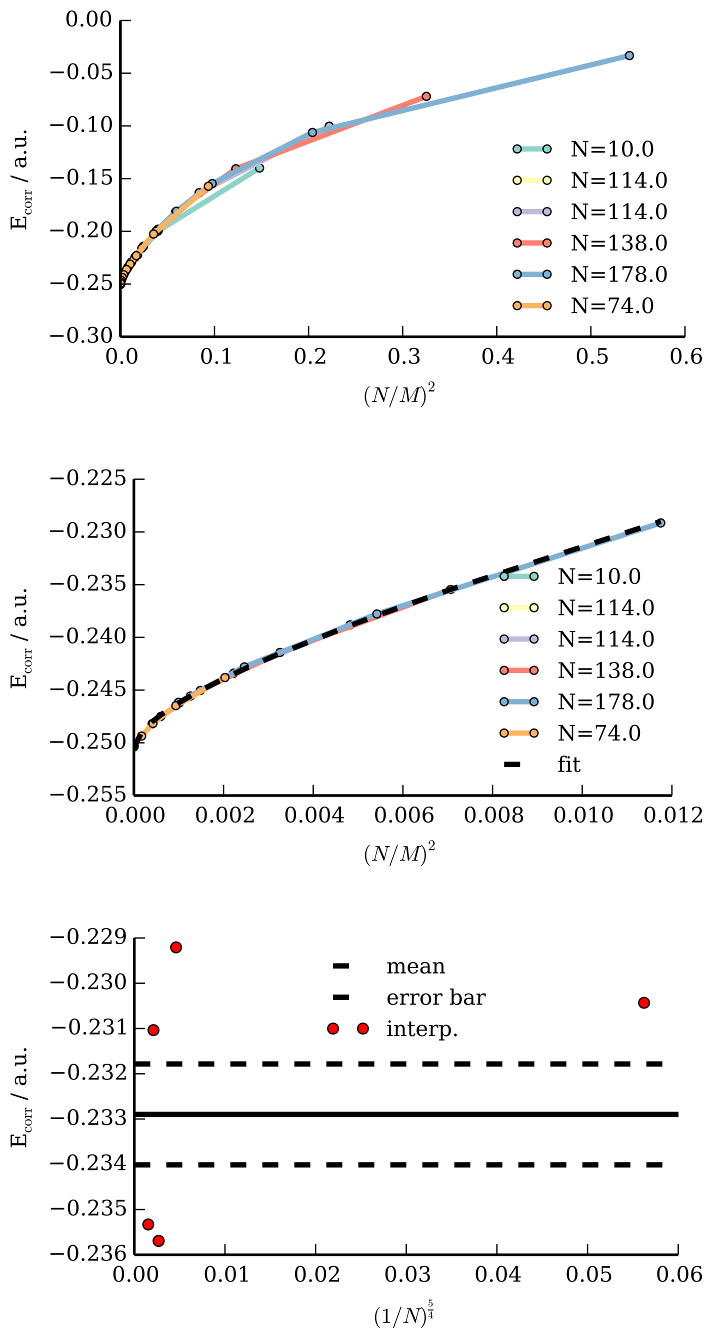
On the right, we have zoomed in and found an extrapolation that fit the last 10 data points of all lines:

$$E = -0.19801552 + 0.05726589\,(N/M) + 0.6905406\,(N/M)^2\,. \tag{2}$$

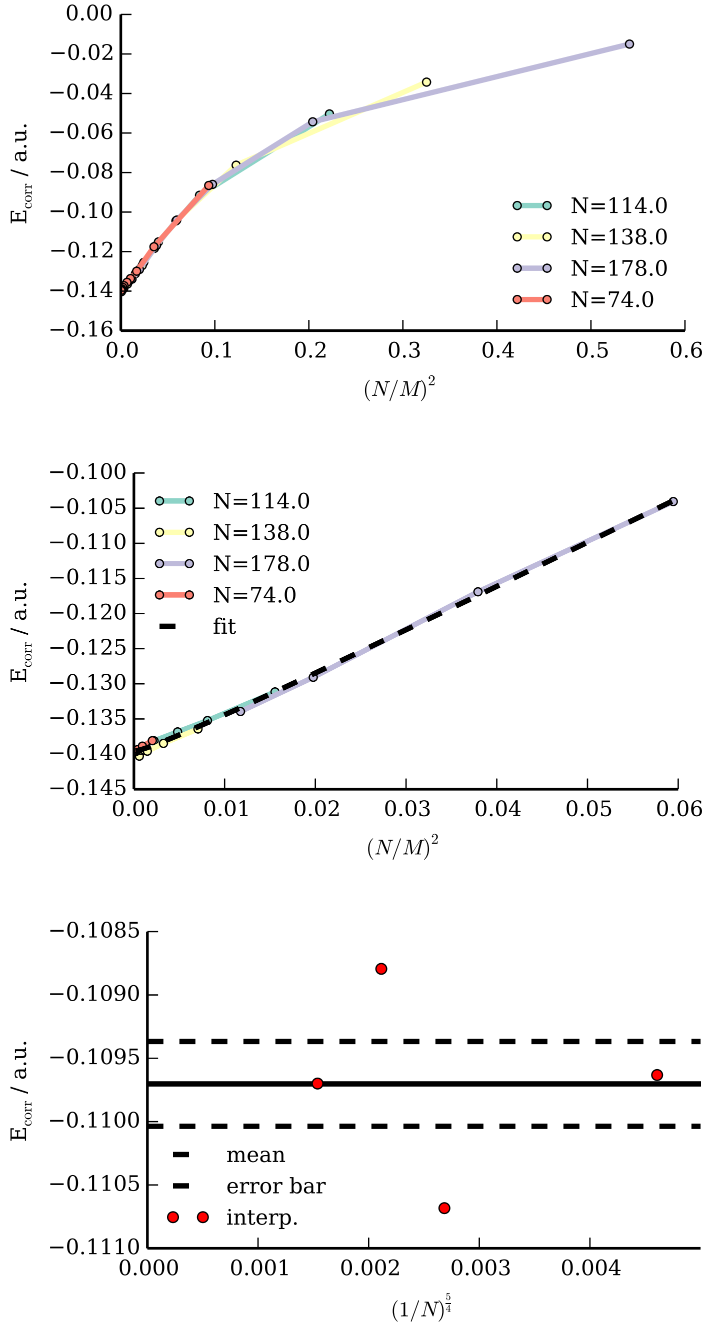
This is consistent with the power-law form that Gustav used, containing a linear term in $1/M$ which I cannot explain! This fit has substantially less error than our estimate for the TDL correction. Any problems with this extrapolation formula is also hard to quantify. The overall thermodynamic limit, complete basis set limit, value is therefore -0.1980 ± 0.0041, which is $(90 \pm 2)\%$ of the GFMC energy. This limit is then plotted back on the left graph.

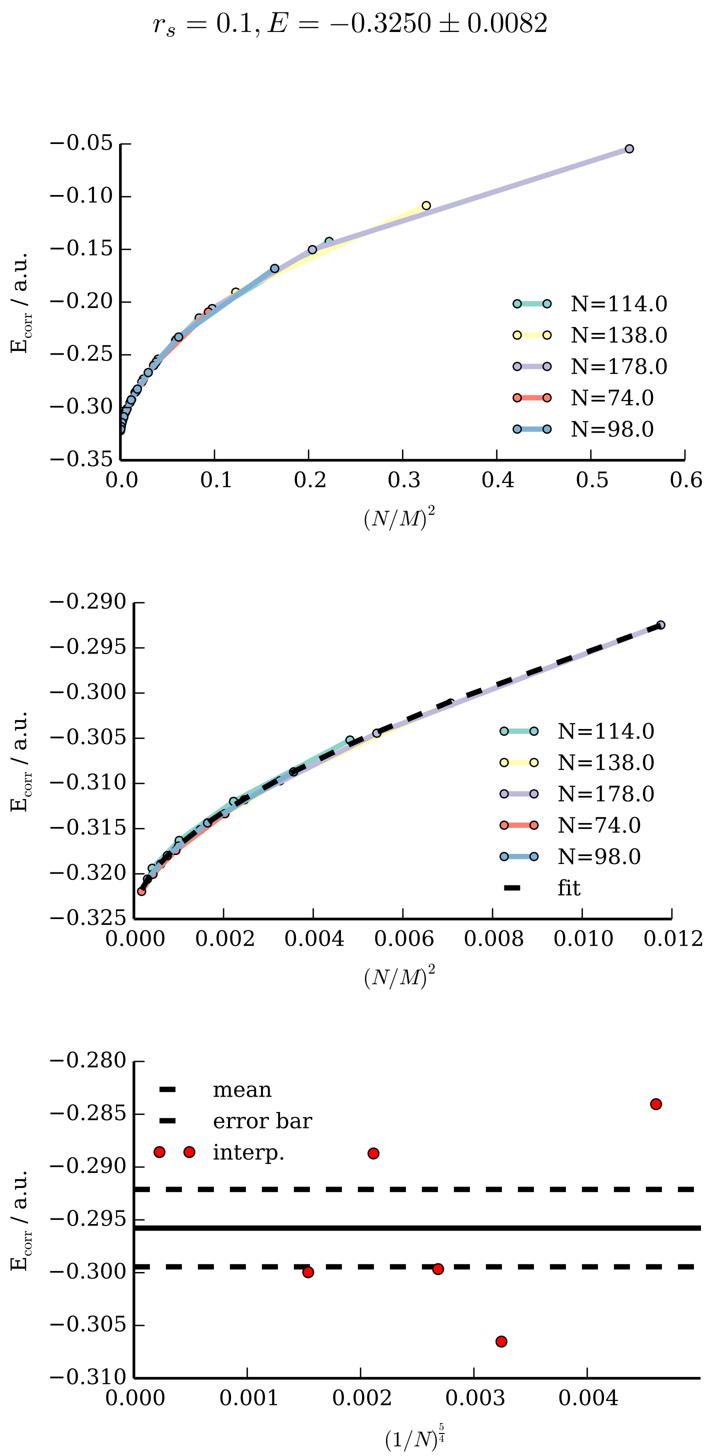
This separation in principle means that it is possible to converge the TDL and the CBS limits separately, although Gustav's data set is sufficiently complete that he has done lots of calculations both high N and high M. However, for more expensive methods this might not be possible. The analysis for other r_s values follows.

$r_s = 0.5, E = -0.2507 \pm 0.0027$



$r_s = 2.0, E = -0.13943 \pm 0.00067$





$r_s = 0.1, E = -0.3250 \pm 0.0082$
E$_{\mathrm{corr}}$ / a.u.
$(N/M)^2$
N=114.0
N=138.0
N=178.0
N=74.0
N=98.0
E$_{\mathrm{corr}}$ / a.u.
$(N/M)^2$
N=114.0
N=138.0
N=178.0
N=74.0
N=98.0
fit
E$_{\mathrm{corr}}$ / a.u.
$(1/N)^{\frac{5}{4}}$
mean
error bar
interp.

[1] J. J. Shepherd, A. Grüneis, G. H. Booth, G. Kresse, and A. Alavi, Phys. Rev. B **86**, 035111 (2012).
[2] N. D. Drummond, R. J. Needs, A. Sorouri, and W. M. C. Foulkes, Phys. Rev. B **78**, 125106 (2008).
[3] J. J. Shepherd and A. Grüneis, Phys. Rev. Lett. **110**, 226401 (2013).
[4] J. J. Shepherd and A. Grüneis, *Correlation Energy Divergences in Metallic Systems*, arXiv e-print 1208.6103 (2012).