

# What can the transition structure factor tell us about finite size effects in metals?



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Initiative

(Thanks for \$)

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This poster will address:

Coupled cluster theory  
Many-body theory  
Electronic structure of solids (e.g. VASP/PySCF)  
Wavefunctions

so stick around if you're interested!

1. Our analysis of the CCD correlation FSE convergence rate show an  $N^{-1/3}$  convergence to the TDL
2. Analysis of the transition structure factor shows this will eventually cross back over to  $N^{-1}$

## Can I use coupled cluster theory for solids?

### Strengths:

- Good balance of cost and accuracy ( $\sim 1\text{kcal/mol}$ )
- Common benchmark in material science
- Exact for high density limit for finite electron gases

### Weaknesses:

- Cost scales with system size/k-points
- HF is not metallic
- Slow scaling of finite size effects (FSE)

### Work-to-date:

#### Most work focused on insulators and semi-conductors

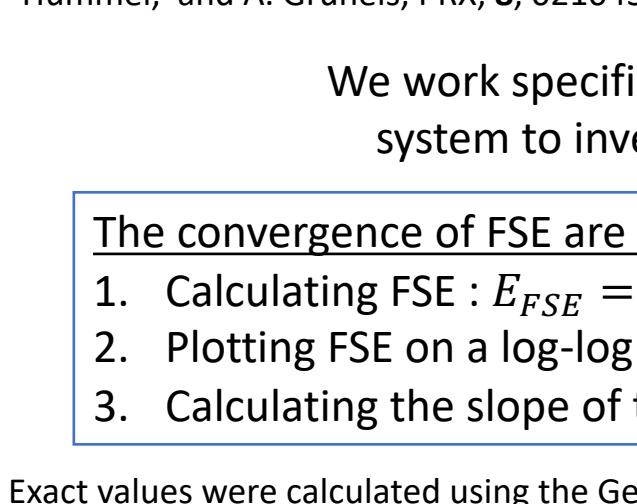
Studies include work by:

Grüneis

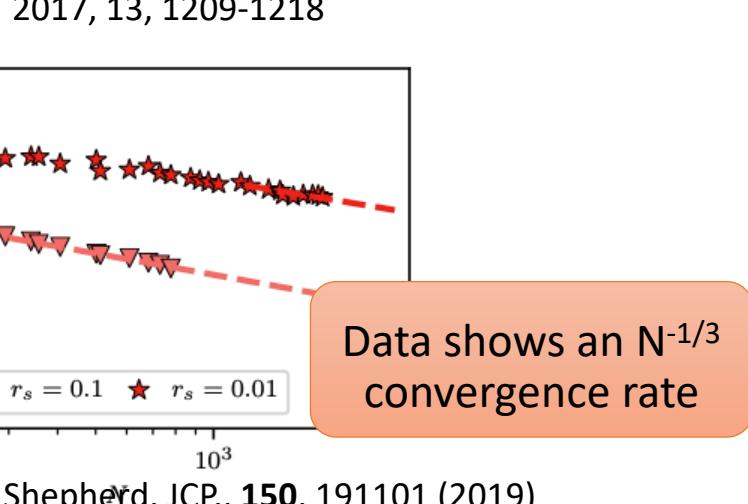
Berkelbach

Chan

Scuseria



Adapted from: T. Gruber, K. Liao, T. Tsatsoulis, F. Hummel, and A. Grüneis, PRX, **8**, 021043 (2018)



#### Still an open question for metals

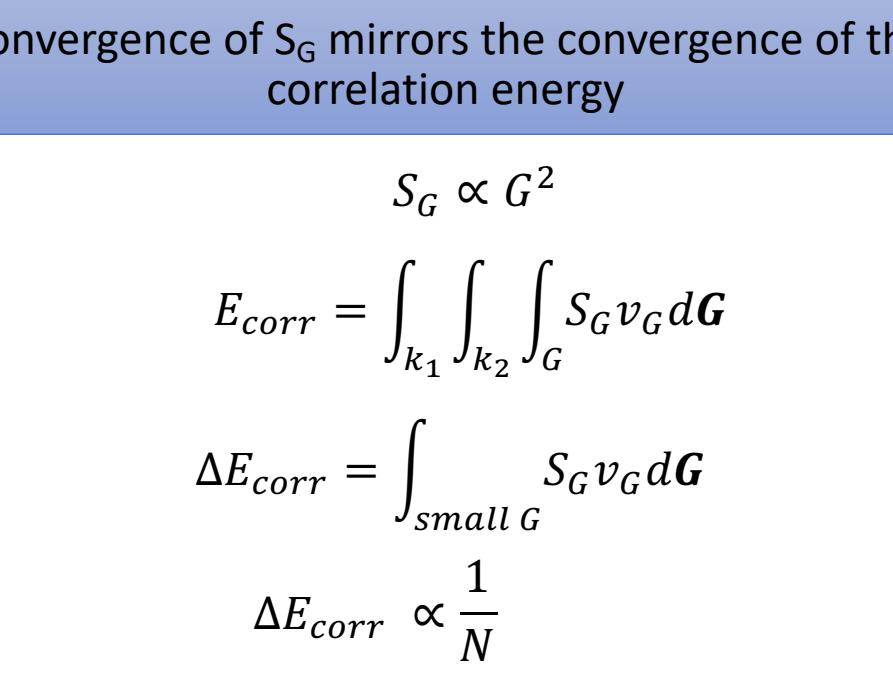
J. McClain, Q. Sun, G. Chan, T. Berkelbach JCTC 2017, **13**, 1209-1218

We work specifically with CCD on a metallic UEG model system to investigate FSE in the correlation energy

### The convergence of FSE are determined by:

1. Calculating FSE :  $E_{FSE} = E_{CCD} - E_{exact}$
2. Plotting FSE on a log-log plot
3. Calculating the slope of the plot to determine convergence

Exact values were calculated using the Gell-Mann and Brueckner method:  
M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957).



Data shows an  $N^{-1/3}$  convergence rate

## The Transition Structure Factor:

The transition structure factor is a new non-observable property in solids that contains all information on the correlation in the system

Derived from the coupled cluster correlation energy expression:

See A. Imler, a. Gallo, F. Hummel, A. Grüneis, PRL, **123**, 156401 (2019)

Convergence of  $S_G$  mirrors the convergence of the correlation energy

$$E_{corr} = \frac{1}{4} \sum_{ijab} v_{ijab} t_{ijab}$$

$$= \sum_G v_G S_G \quad , \text{ where } v_G = \frac{4\pi}{G^2}$$

$$S_G \propto \sum_{ijab} t_{ijab} \delta(k_i - k_a - G) \delta(k_j - k_b + G)$$

$S_G$  goes to 0 as correlation goes to 0

The transition structure factor can be used to evaluate the convergence rates of the FSE in solids

$$S_G \propto G^2$$

$$E_{corr} = \int_{k_1} \int_{k_2} \int_G S_G v_G dG$$

$$\Delta E_{corr} = \int_{small G} S_G v_G dG$$

$$\Delta E_{corr} \propto \frac{1}{N}$$



However, UEG data at high density shows an  $N^{-1/3}$  convergence rate

So what's happening?

## The structure factor shows a cross-over point between two convergence rates in the correlation energy:

We determined the analytical function of the transition structure factor and analyzed its convergence to the TDL

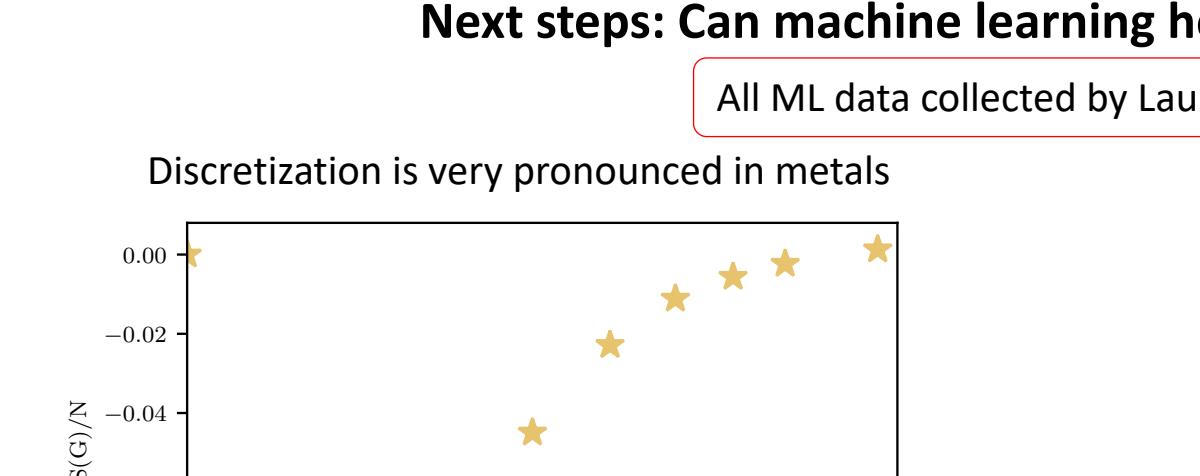
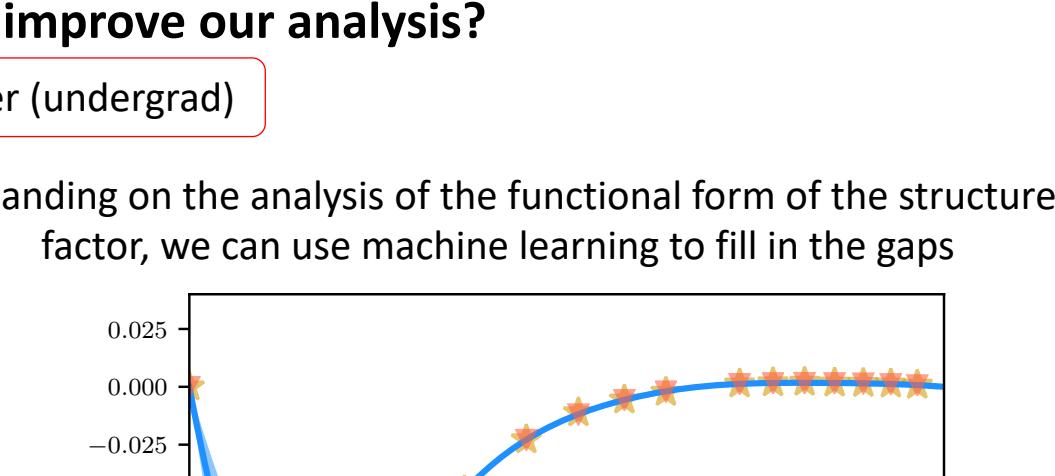


Figure shows the convergence of the remaining FSE after extrapolation to the TDL

$N^{-1/3}$  (equivalent to linear in G) will over-correct, good for sparse sampling in G

$N^{-1}$  (equivalent to cubic in G) will under-correct less



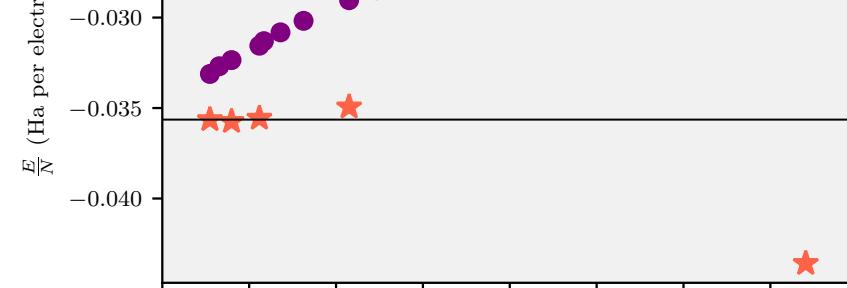
We see the cross-over in our UEG data at  $r_s = 1.0$

TM, B. Yang, and J. J. Shepherd – submitted to PRL

## Next steps: Can machine learning help us improve our analysis?

All ML data collected by Laura Weiler (undergrad)

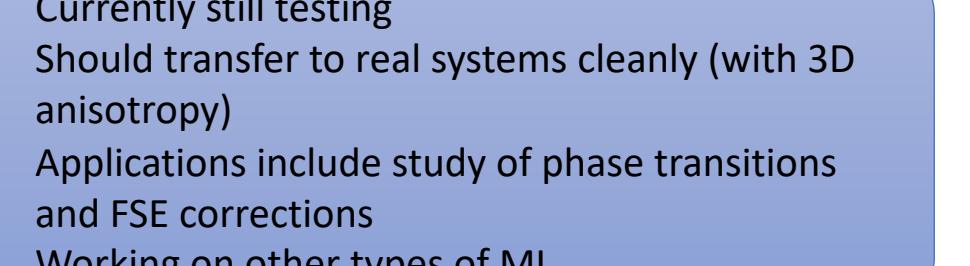
Discretization is very pronounced in metals



Preliminary results on TDL extrapolations shows promise for this approach

predicted CCD (red stars), TDL estimate (black line), original CCD (purple circles)

Expanding on the analysis of the functional form of the structure factor, we can use machine learning to fill in the gaps



(simple GPR from scikit-learn)

Currently still testing  
Should transfer to real systems cleanly (with 3D anisotropy)  
Applications include study of phase transitions and FSE corrections  
Working on other types of ML