

# Finite-Size Corrections

## Structure Factor or MPC or both?

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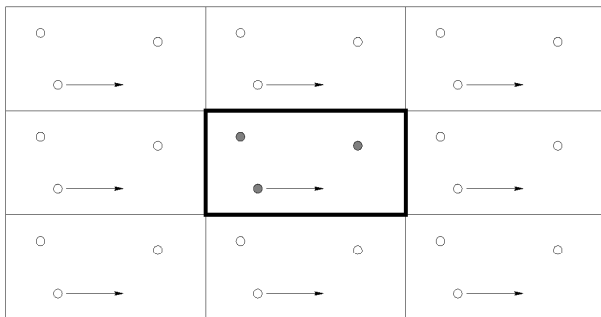
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# Outline

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  - Which Coulomb energy?
  - The Ewald interaction
- 3 Exchange and correlation
  - The exchange-correlation hole
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- 4 Finite-size errors
  - Real-space approach
  - Reciprocal-space approach
  - Link between the two approaches
  - Strengths and weaknesses

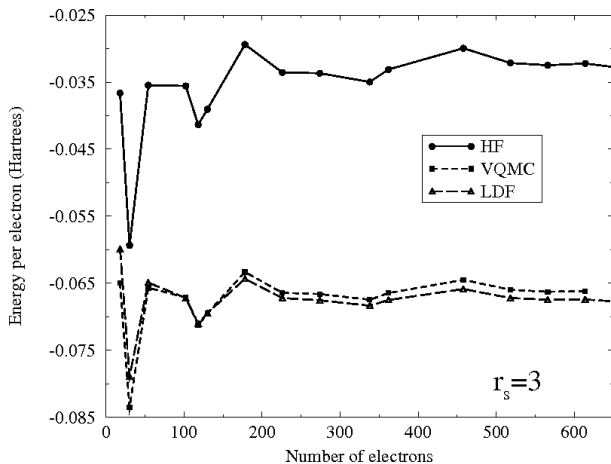
# Introduction

QMC simulations of solids study finite systems subject to periodic boundary conditions.

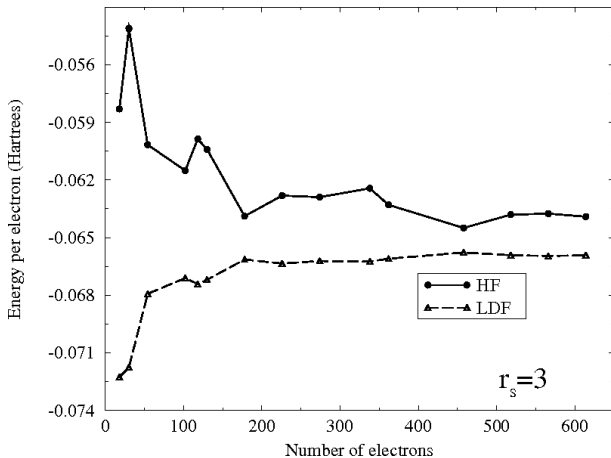


We *really* want to model infinite systems.

The small system size leads to finite-size errors.

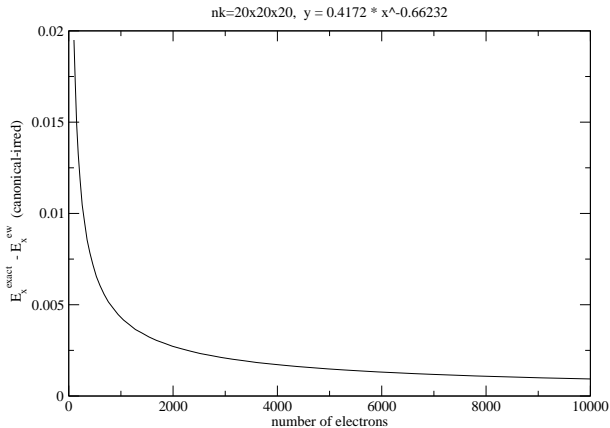


Since the QMC finite-size errors behave like the LDF (or HF) errors, we apply LDF (or HF) finite-size corrections.

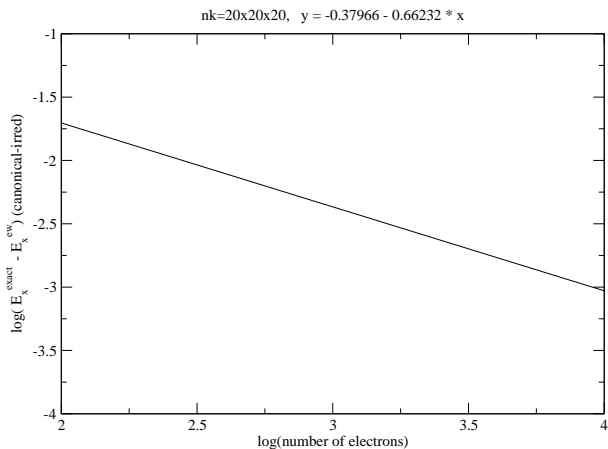


- The residual finite-size errors decay very slowly — roughly like  $1/N$ .
- They arise from the exchange-correlation part of the Coulomb energy.
- They can be problematic.

Similar errors are seen in HF calculations, but in this case we can study *very large systems* . . .



... and extract the scaling convincingly:





## Questions

- Does the XC energy really converge like  $1/N$ ?
- If so, why does the exchange energy converge like  $1/N^{2/3}$ ?
- Very recently, Chiesa, Ceperley, Martin and Holzmann, and, independently, Gaudoin and Pitarke, proposed a new way of dealing with Coulomb finite-size errors. How does this relate to the MPC method? Is it actually different? Is it better?

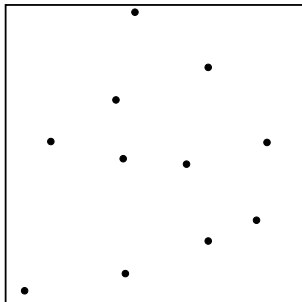
To answer these questions, we need to think hard about the treatment of Coulomb interactions in infinite periodic systems.

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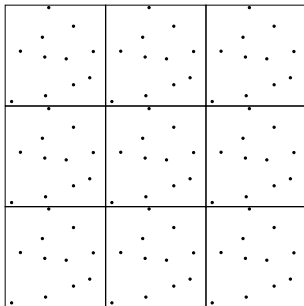
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# Which Coulomb energy?

- Consider a simulation cell containing  $N$  unit point charges plus a cancelling uniform background.

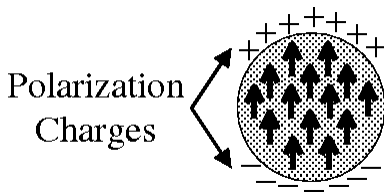


- To model a solid, embed the cell in a lattice of identical copies of itself.



- Calculate the Coulomb energy per cell as a function of lattice size and let the lattice size tend to infinity to get a result for the solid.

But which answer do you want?



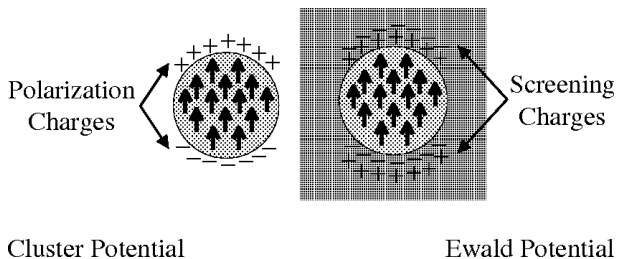
Because of the long range of the Coulomb interaction, result depends on cluster shape even in the limit as the cluster size  $\rightarrow \infty$ !

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# The Ewald interaction

It seems most natural to adopt “tin-foil” boundary conditions,



yielding the *periodic* Ewald interaction/potential.

## Reciprocal-space representation

To within an (irrelevant) arbitrary constant, the Ewald potential due to a point charge  $\delta(\mathbf{r})$ , its cancelling uniform background, and all its images, may be obtained by solving Poisson's equation

$$\nabla^2 v_{\text{Ew}}(\mathbf{r}) = -4\pi \left( \delta(\mathbf{r}) - \frac{1}{\Omega} \right),$$

within one unit cell subject to periodic boundary conditions.

Evaluating the reciprocal lattice vector Fourier components gives:

$$\begin{aligned} \int_{\Omega} e^{-i\mathbf{G}\cdot\mathbf{r}} \nabla^2 v_{\text{Ew}}(\mathbf{r}) d\mathbf{r} &= -4\pi \int_{\Omega} e^{-i\mathbf{G}\cdot\mathbf{r}} \left( \delta(\mathbf{r}) - \frac{1}{\Omega} \right) d\mathbf{r} \\ -G^2 \tilde{v}_{\text{Ew}}(\mathbf{G}) &= \begin{cases} -4\pi & \mathbf{G} \neq 0 \\ 0 & \mathbf{G} = 0 \end{cases}. \end{aligned}$$



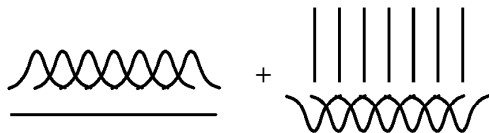
Although the Fourier components  $\tilde{v}_{\text{Ew}}(\mathbf{G})$  are well defined, the corresponding Fourier series

$$v_{\text{Ew}}(\mathbf{r}) = \frac{1}{\Omega} \sum_{\mathbf{G} \neq \mathbf{0}} \frac{4\pi}{G^2} e^{i\mathbf{G} \cdot \mathbf{r}}$$

does not converge and is just as useless as the real space sum of  $1/r$  potentials considered earlier.

# The Ewald formula

A practical method for evaluating the Ewald interaction is obtained by splitting up the charges as follows:



- The periodic potential corresponding to the first, smooth, distribution may be expressed as a rapidly convergent Fourier series.
- The short-range potential from a delta function plus its neutralising Gaussian may be evaluated in real space.

## Reciprocal space revisited

The Ewald formula is

$$v_{\text{Ew}}(\mathbf{r}) = \frac{4\pi}{\Omega} \sum_{\mathbf{G}(\neq \mathbf{0})} \frac{\exp\left(-\frac{\kappa^2 G^2}{2} + i\mathbf{G} \cdot \mathbf{r}\right)}{G^2} - \frac{2\kappa^2}{\pi} + \sum_{\mathbf{R}} \frac{\text{erfc}\left(\frac{|\mathbf{r}-\mathbf{R}|}{\sqrt{2}\kappa}\right)}{|\mathbf{r}-\mathbf{R}|}$$

where  $\kappa$  is the width of the auxiliary Gaussian charges.

Although numerically efficient, this formula is analytically awkward.

If we choose  $\epsilon = \kappa/\sqrt{2}$  very small and assume that  $|\mathbf{r}-\mathbf{R}| \gg \epsilon$ , then

$$v_{\text{Ew}}(\mathbf{r}) \approx \frac{1}{\Omega} \sum_{\mathbf{G}(\neq \mathbf{0})} \frac{4\pi e^{-\epsilon^2 G^2} e^{i\mathbf{G} \cdot \mathbf{r}}}{G^2}.$$

This convenient Fourier representation is far wrong in tiny regions of radius  $\epsilon$  about each lattice point, but very accurate elsewhere.

# The Madelung potential

The constant

$$v_M = \lim_{|\mathbf{r}| \rightarrow 0} \left( v_{\text{Ew}}(\mathbf{r}) - \frac{1}{r} \right)$$

is called the Madelung potential. It is the potential at a unit point charge due to the cancelling background and all the images of that charge.

Its approximate Fourier representation is

$$v_M \approx \frac{1}{\Omega} \sum_{\mathbf{G}(\neq \mathbf{0})} \frac{4\pi e^{-\epsilon^2 G^2}}{G^2} - \int_{\text{all space}} \frac{4\pi e^{-\epsilon^2 G^2}}{G^2} \frac{d\mathbf{G}}{(2\pi)^3}.$$

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# The exchange-correlation hole

## Definition

The pair density  $n(\mathbf{r}, \mathbf{r}')d\mathbf{r}d\mathbf{r}'$  is the probability of finding one particle in box  $d\mathbf{r}$  and a second particle in box  $d\mathbf{r}'$ .

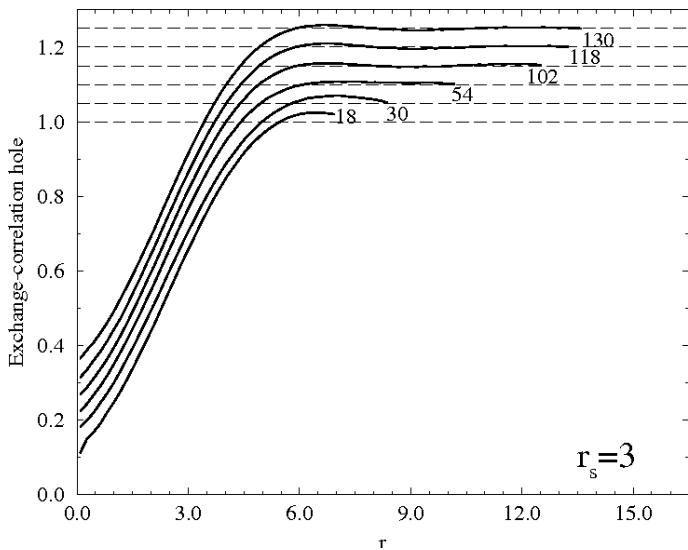
Writing

$$\begin{aligned}n(\mathbf{r}, \mathbf{r}') &= n(\mathbf{r})n(\mathbf{r}'|\mathbf{r}) \\n(\mathbf{r}'|\mathbf{r}) &= n(\mathbf{r}') + n_{\text{xc}}(\mathbf{r}', \mathbf{r})\end{aligned}$$

then defines the XC hole.

The sum rule

$$\int n(\mathbf{r}'|\mathbf{r})d\mathbf{r}' = N - 1 \quad \Rightarrow \quad \int n_{\text{xc}}(\mathbf{r}', \mathbf{r})d\mathbf{r}' = -1 .$$



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# The exchange-correlation energy

The energy expectation value in a QMC simulation contains several terms:

- Kinetic energy.
- Potential energy of interaction between electrons and ions.
- Hartree energy.
- Exchange-correlation energy.

Of these, it is the exchange-correlation energy — the term describing the effect of the pair correlations on the total energy — with which we are concerned here.

The XC energy arises from the interaction between the electrons and their XC holes

$$\begin{aligned}
 E_{\text{xc}} &= \frac{1}{2} \int n_{\text{xc}}^{\text{Av}}(\mathbf{r})(v_{\text{Ew}}(\mathbf{r}) - v_M) d\mathbf{r} \\
 &= \frac{1}{2} \int n_{\text{xc}}^{\text{Av}}(\mathbf{r})v_{\text{Ew}}(\mathbf{r}) d\mathbf{r} + \frac{v_M}{2}
 \end{aligned}$$

where  $v_M$  is the Madelung potential and  $n_{\text{xc}}^{\text{Av}}(\mathbf{r})$  is the system-averaged XC hole:

$$n_{\text{xc}}^{\text{Av}}(\mathbf{r}) = \frac{\int_{\Omega} n(\mathbf{r}')n_{\text{xc}}(\mathbf{r}', \mathbf{r}' + \mathbf{r}) d\mathbf{r}'}{\int_{\Omega} n(\mathbf{r}') d\mathbf{r}'}$$

## Why $v_{\text{Ew}}(\mathbf{r}) - v_M$ ?

- The Ewald potential  $v_{\text{Ew}}(\mathbf{r})$  includes contributions from
  - ▶ the electron at the origin,
  - ▶ its background,
  - ▶ all its images.
- Only the first of these ought to contribute to the XC energy.

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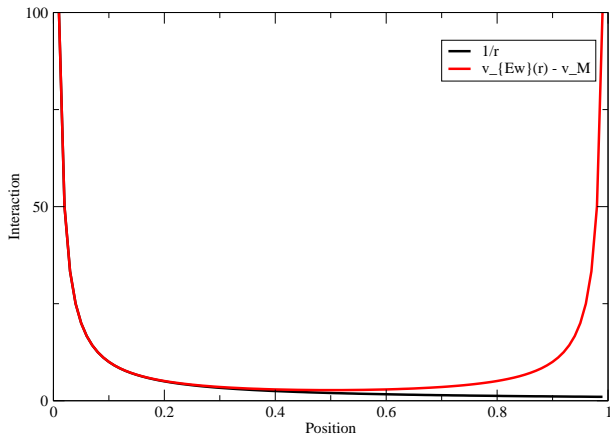
# Real-space approach to finite-size errors

$$E_{\text{xc}} = \frac{1}{2} \int n_{\text{xc}}^{\text{Av}}(\mathbf{r})(v_{\text{Ew}}(\mathbf{r}) - v_M) d\mathbf{r}$$

- Since  $n_{\text{xc}}^{\text{Av}}(\mathbf{r})$  converges quite rapidly to the infinite system-size limit, the error must be in the interaction.
- Expanding  $v_{\text{Ew}}(\mathbf{r}) - v_M$  about  $\mathbf{r} = 0$  gives

$$v_{\text{Ew}}(\mathbf{r}) - v_M = \frac{1}{r} + \frac{2\pi r^2}{3\Omega} + \mathcal{O}(r^4).$$

- In an infinite system, this reduces to  $1/r$  as expected; in a finite system, the quadratic term gives a  $1/\Omega \sim 1/N$  error.

Comparison of Ewald and  $1/r$  Interactions

# The modified periodic Coulomb interaction

Replace

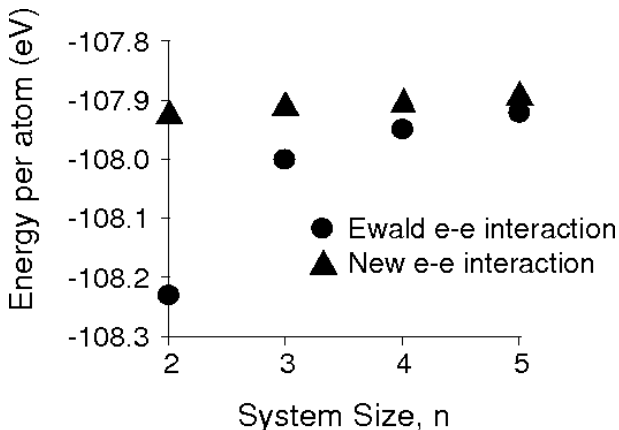
$$E_{\text{xc}} = \frac{1}{2} \int n_{\text{xc}}^{\text{Av}}(\mathbf{r})(v_{\text{Ew}}(\mathbf{r}) - v_M) d\mathbf{r}$$

by

$$E_{\text{xc}} = \frac{1}{2} \int \frac{n_{\text{xc}}^{\text{Av}}(\mathbf{r})}{r} d\mathbf{r}$$

- Use minimum image convention to extend  $1/r$  periodically.
- Keep Ewald interaction for Hartree energy terms.

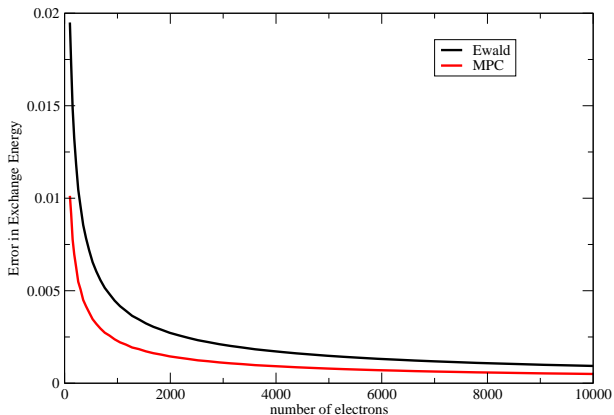
Fixes  $1/N$  error. Works well for exchange-correlation energy.





Doesn't fix  $1/N^{2/3}$  error seen in Hartree-Fock calculations.

Comparison of Ewald and MPC Interactions for Exchange



## Origin of HF error

- Since the MPC interaction is exactly correct within the cell, the HF error must arise from the form of  $n_x^{\text{Av}}(\mathbf{r})$ .
- For large  $r$  in a uniform electron gas

$$n_x^{\text{Av}}(\mathbf{r}) \sim r^{-4} .$$

- Hence

$$\int_L^\infty \frac{n_x^{\text{Av}}(\mathbf{r})}{r} 4\pi r^2 dr \sim \int_L^\infty r^{-3} dr \sim L^{-2} \sim \Omega^{-2/3} .$$

The exchange hole does not “fit in” to the simulation cell.

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# Reciprocal-space approach to finite-size errors

Re-expressing  $E_{xc}$  in  $k$ -space:

$$\begin{aligned}
 E_{xc} &= \frac{1}{2} \int_{\Omega} n_{xc}^{Av}(\mathbf{r}) v_{Ew}(\mathbf{r}) d\mathbf{r} + \frac{v_M}{2} \\
 &= \frac{1}{2\Omega} \sum_{\mathbf{G}(\neq\mathbf{0})} \frac{4\pi \tilde{n}_{xc}^{Av}(\mathbf{G}) e^{-\epsilon^2 G^2}}{G^2} \\
 &\quad + \left( \frac{1}{2\Omega} \sum_{\mathbf{G}(\neq\mathbf{0})} \frac{4\pi e^{-\epsilon^2 G^2}}{G^2} - \frac{1}{2} \int \frac{4\pi e^{-\epsilon^2 G^2}}{G^2} \frac{d\mathbf{G}}{(2\pi)^3} \right)
 \end{aligned}$$

and rearranging ...

... gives

$$E_{\text{xc}} = \frac{1}{2\Omega} \sum_{\mathbf{G}(\neq 0)} \frac{4\pi(\tilde{n}_{\text{xc}}^{\text{Av}}(\mathbf{G}) + 1)e^{-\epsilon^2 G^2}}{G^2} - \frac{1}{2} \int \frac{4\pi e^{-\epsilon^2 G^2}}{G^2} \frac{d\mathbf{G}}{(2\pi)^3}$$

- $\tilde{S}(\mathbf{G}) = \tilde{n}_{\text{xc}}^{\text{Av}}(\mathbf{G}) + 1$  is called the *static structure factor*.
- Since  $\tilde{S}(\mathbf{G})$  is (normally) proportional to  $G^2$  at small  $G$ , the summand does not diverge as  $G \rightarrow 0$ .
- The convergence factors are *required*.

In the  $\Omega \rightarrow \infty$  limit, the sum becomes an integral and we obtain the standard result

$$E_{\text{xc}} \rightarrow \frac{1}{2} \int \frac{4\pi(\tilde{S}(\mathbf{G}) - 1)e^{-\epsilon^2 G^2}}{G^2} \frac{d\mathbf{G}}{(2\pi)^3}.$$

$$E_{xc} = \frac{1}{2\Omega} \sum_{\mathbf{G}(\neq 0)} \frac{4\pi \tilde{S}(\mathbf{G}) e^{-\epsilon^2 G^2}}{G^2} - \frac{1}{2} \int \frac{4\pi e^{-\epsilon^2 G^2}}{G^2} \frac{d\mathbf{G}}{(2\pi)^3}$$

- Chiesa asserts that the leading contribution to the error arises from the omission of the  $\mathbf{G} = 0$  term.
- Expanding  $\tilde{n}_{xc}^{Av}(\mathbf{G})$  and  $\tilde{S}(\mathbf{G})$  about  $\mathbf{G} = 0$ ,

$$\tilde{n}_{xc}^{Av}(\mathbf{G}) = -1 + \alpha G^2 + \dots \quad \tilde{S}(\mathbf{G}) = \alpha G^2 + \dots ,$$

gives the finite-size correction

$$\Delta_{\text{Chiesa}} = \frac{2\pi\alpha}{\Omega} .$$

- The constant  $\alpha$  can be obtained from RPA theory or by extrapolating the calculated  $\tilde{S}(\mathbf{G})$  towards  $\mathbf{G} = 0$ .

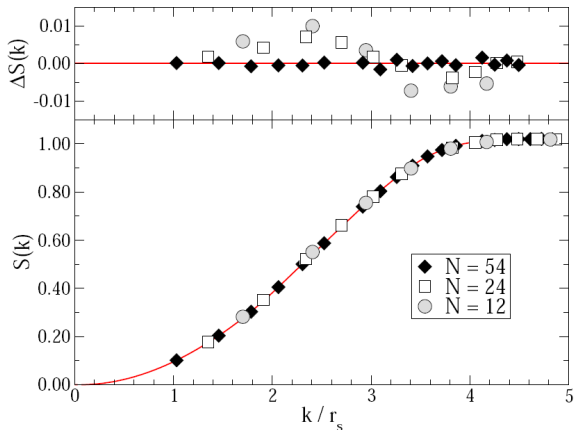


FIG. 1: Lower panel: Static structure factor for the electron gas at  $r_s = 10$ . Upper panel:  $\Delta S = S_N(k) - S_{66}(k)$ . The difference is computed using a spline function interpolation of  $S_{66}$ .



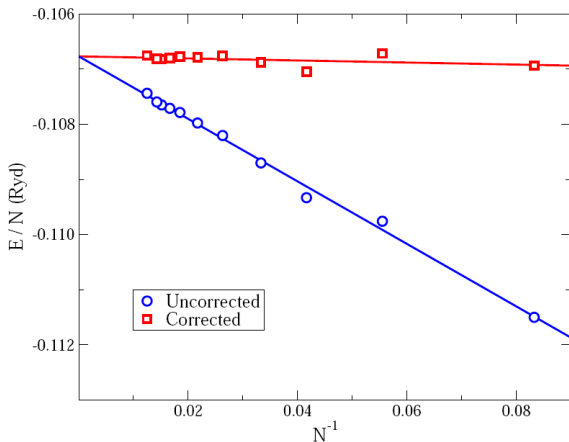
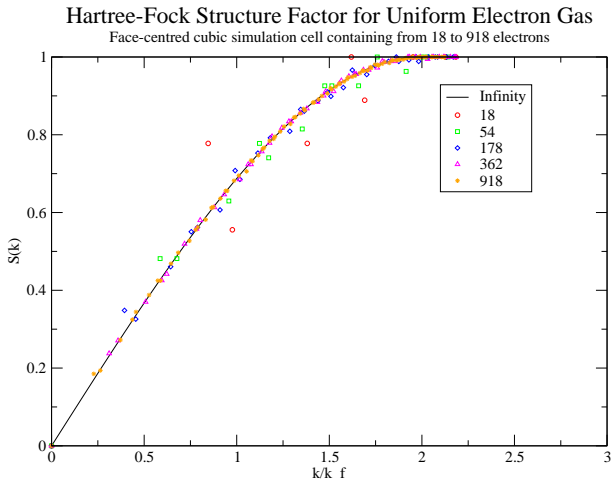


FIG. 2: Energies per particle of the electron gas at  $r_s = 10$  in Rydberg as a function of the inverse particle number. Circles are the Monte Carlo energies averaged over twist angles. Squares are the energies after the additional  $\hbar\omega_p/2N$  correction (see text).

# Scaling of the Hartree-Fock error

$S_{\text{HF}}(\mathbf{k})$  is *not* quadratic near  $\mathbf{k} = 0$ :



The missing  $\mathbf{G} = 0$  term in

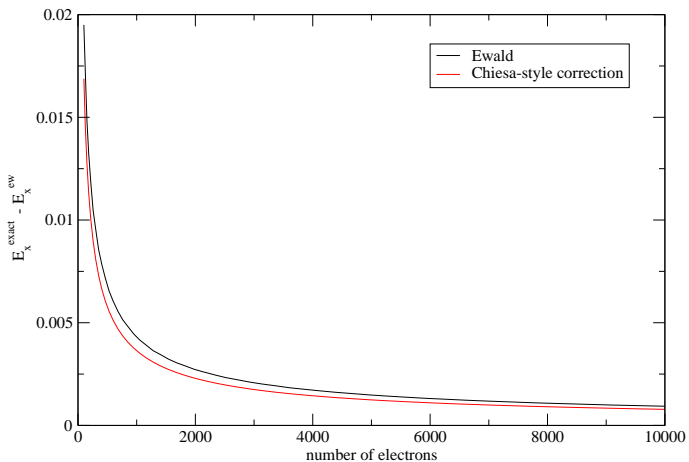
$$E_x = \frac{1}{2\Omega} \sum_{\mathbf{G}(\neq 0)} \frac{4\pi S_{\text{HF}}(\mathbf{G})e^{-\epsilon^2 G^2}}{G^2} - \frac{1}{2} \int \frac{4\pi e^{-\epsilon^2 G^2}}{G^2} \frac{d\mathbf{G}}{(2\pi)^3}$$

is therefore infinite!

Instead, add analytic integral of  $4\pi S_{\text{HF}}(\mathbf{k})/k^2$  over small sphere of volume equal to the volume of  $k$ -space per reciprocal lattice vector.

This correction scales like  $N^{-2/3}$ .

## Exchange Energy of Electron Gas



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# Link between the two approaches

According to Chiesa,

$$E_{\text{xc}} = E_{\text{xc}}^{\text{Ew}} + \frac{2\pi\alpha}{\Omega}, \quad \text{where} \quad \tilde{n}_{\text{xc}}^{\text{Av}}(\mathbf{G}) = -1 + \alpha\mathbf{G}^2 + \dots$$

$$\begin{aligned} \text{Since } \tilde{n}_{\text{xc}}^{\text{Av}}(\mathbf{G}) &= \int_{\Omega} n_{\text{xc}}^{\text{Av}}(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} d\mathbf{r} \\ &= -1 - \frac{1}{6}\mathbf{G}^2 \int_{\Omega} n_{\text{xc}}^{\text{Av}}(\mathbf{r}) r^2 d\mathbf{r} + \dots, \end{aligned}$$

it follows that

$$\alpha = -\frac{1}{6} \int_{\Omega} n_{\text{xc}}^{\text{Av}}(\mathbf{r}) r^2 d\mathbf{r}.$$

Hence, the reciprocal-space correction is equivalent to

$$E_{\text{xc}} = E_{\text{xc}}^{\text{Ew}} - \frac{\pi}{3\Omega} \int_{\Omega} n_{\text{xc}}^{\text{Av}}(\mathbf{r}) r^2 d\mathbf{r}.$$

According to the real-space MPC approach,

$$\begin{aligned} E_{\text{xc}} &= \frac{1}{2} \int_{\Omega} \frac{n_{\text{xc}}^{\text{Av}}(\mathbf{r})}{r} d\mathbf{r} \\ &= \frac{1}{2} \int_{\Omega} n_{\text{xc}}^{\text{Av}}(\mathbf{r}) \left( v_{\text{Ew}}(\mathbf{r}) - v_M - \frac{2\pi r^2}{3\Omega} + \dots \right) d\mathbf{r} \\ &= E_{\text{xc}}^{\text{Ew}} - \frac{\pi}{3\Omega} \int_{\Omega} n_{\text{xc}}^{\text{Av}}(\mathbf{r}) r^2 d\mathbf{r} + \dots \end{aligned}$$

## Conclusion

Reciprocal-space correction is a quadratic approximation to the MPC

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# Strengths and weaknesses (provisional)

- If the XC hole “fits in” to the simulation cell, the reciprocal-space approach is inferior to the real-space approach.
- If not, the two differ:
  - ▶ The real-space approach uses the right interaction but the approximate “squashed” hole; it therefore overestimates the magnitude of the XC energy.
  - ▶ The reciprocal-space approach can employ an analytic approximation to  $\tilde{S}(\mathbf{G})$  for small  $\mathbf{G}$ . This can be substantially better than “squashing” the hole.
- Would you rather modify the Hamiltonian or apply a correction after the simulation?

# When is the real-space approach exact?

The real-space approach is exact if

- The shape of the XC hole is right.
- The XC hole “fits in” to the simulation cell.

# When is the reciprocal-space approach exact?

The reciprocal-space approach is exact if

- The shape of the XC hole is right (so that calculated  $\tilde{S}(\mathbf{G})$  is correct).
- The exact  $\tilde{S}(\mathbf{k})$  is obtained by interpolation from  $\tilde{S}(\mathbf{G})$  and the  $k$ -space integral is evaluated exactly.

In practice, the second of these seems unlikely . . . .

# Quadrature and the sampling theorem

Suppose that

$$\phi(\mathbf{r}) = \int \tilde{\phi}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} \frac{d\mathbf{k}}{(2\pi)^3}$$

is a smooth and rapidly decaying function of  $\mathbf{r}$ .

Consider a lattice of replicas

$$\phi^{\text{per}}(\mathbf{r}) = \sum_{\mathbf{R}} \phi(\mathbf{r} - \mathbf{R}) .$$

Since  $\phi^{\text{per}}(\mathbf{r})$  is periodic, it has a Fourier series

$$\phi^{\text{per}}(\mathbf{r}) = \frac{1}{\Omega} \sum_{\mathbf{G}} \tilde{\phi}^{\text{per}}(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}} .$$

The Fourier components are

$$\begin{aligned}\tilde{\phi}^{\text{per}}(\mathbf{G}) &= \int_{\Omega} \sum_{\mathbf{R}} \phi(\mathbf{r} - \mathbf{R}) e^{-i\mathbf{G}\cdot\mathbf{r}} d\mathbf{r} = \sum_{\mathbf{R}} \int_{\Omega} \phi(\mathbf{r} - \mathbf{R}) e^{i\mathbf{G}\cdot(\mathbf{r}-\mathbf{R})} d\mathbf{r} \\ &= \int \phi(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} d\mathbf{r} = \tilde{\phi}(\mathbf{G}).\end{aligned}$$

Thus

$$\sum_{\mathbf{R}} \phi(\mathbf{r} - \mathbf{R}) = \frac{1}{\Omega} \sum_{\mathbf{G}} \tilde{\phi}(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}}.$$

## Sampling Theorem

If  $\phi(\mathbf{r})$  dies off rapidly enough as  $r$  increases, we can reconstruct it exactly from the discrete samples  $\tilde{\phi}(\mathbf{G})$  of its Fourier transform.

$$\sum_{\mathbf{R}} \phi(\mathbf{r} - \mathbf{R}) = \frac{1}{\Omega} \sum_{\mathbf{G}} \tilde{\phi}(\mathbf{G}) e^{i\mathbf{G} \cdot \mathbf{r}}$$

## Poisson summation formula

Setting  $\mathbf{r} = 0$  and noting that  $\phi(\mathbf{0}) = \int \tilde{\phi}(\mathbf{k}) \frac{d\mathbf{k}}{(2\pi)^3}$  gives

$$\int \tilde{\phi}(\mathbf{k}) \frac{d\mathbf{k}}{(2\pi)^2} = \frac{1}{\Omega} \sum_{\mathbf{G}} \tilde{\phi}(\mathbf{G}) - \sum_{\mathbf{R}(\neq 0)} \phi(\mathbf{R}).$$

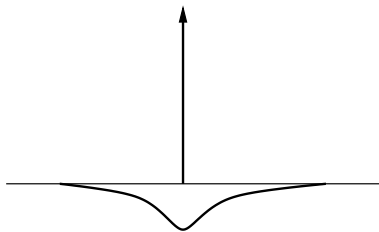
If  $\phi(\mathbf{R}) = 0$  for all  $\mathbf{R} \neq 0$ , the discrete quadrature is exact!

Once the “missing”  $\mathbf{G} = \mathbf{0}$  term has been included, the reciprocal-space expression for the XC energy is:

$$E_{\text{xc}} = \frac{1}{2\Omega} \sum_{\mathbf{G}} \frac{4\pi \tilde{S}(\mathbf{G}) e^{-\epsilon^2 G^2}}{G^2} - \frac{1}{2} \int \frac{4\pi e^{-\epsilon^2 G^2}}{G^2} \frac{d\mathbf{G}}{(2\pi)^3}$$

- The quadrature is exact if the inverse FT of  $4\pi \tilde{S}(\mathbf{k})/k^2$  dies off to zero within radius  $|\mathbf{R}|$ .
- $\tilde{S}(\mathbf{k}) = \tilde{n}_{\text{xc}}^{\text{Av}}(\mathbf{k}) + 1 \Rightarrow S(\mathbf{r}) = n_{\text{xc}}^{\text{Av}}(\mathbf{r}) + \delta(\mathbf{r})$ .
- The inverse FT of  $4\pi \tilde{S}(\mathbf{k})/k^2$  is the Coulomb potential due to the charge density  $S(\mathbf{r})$ .

The reciprocal-space approach is exact if the potential of the charge distribution  $n_{xc}^{Av}(\mathbf{r}) + \delta(\mathbf{r})$



dies away to zero before  $|\mathbf{r}|$  reaches  $|\mathbf{R}|$ .



# Strengths and weaknesses revisited

- The real-space approach is exact if
  - ▶ The shape of the XC hole is correct.
  - ▶ The XC hole “fits in” to the simulation cell.
- The reciprocal-space approach is exact if
  - ▶ The shape of the XC hole is correct.
  - ▶ The potential of the charge distribution  $n_{XC}^{Av}(\mathbf{r}) + \delta(\mathbf{r})$  dies away to zero before  $|\mathbf{r}|$  reaches  $|\mathbf{R}|$ .
- If the second moment of the sampled XC hole is inaccurate, *both* methods can be improved by using RPA values.

Which method is better? Little to choose between them.

## KE errors

Chiesa also points out that an RPA Jastrow factor

$$\exp \left[ - \sum_{i>j} u(r_{ij}) \right],$$

with  $u(r) \sim 1/r$  at large  $r$  (and hence  $\tilde{u}(k) \sim 1/k^2$  at small  $k$ ), contributes

$$-\frac{1}{4\Omega} \sum_{\mathbf{G}(\neq 0)} G^2 \tilde{u}(\mathbf{G}) [\tilde{S}(\mathbf{G}) - 1]$$

to the KE expectation value

$$\left\langle -\frac{1}{2} \sum_i \nabla_i^2 \ln |\Psi| \right\rangle$$

This term shows an analogous  $1/N$  error.

- Louisa Fraser and I did not see this KE error. But we were doing VMC with short-range Jastrow factors.
- The RPA Jastrow factor ought to be accurate at large  $r$ , so the KE error should be visible in DMC, regardless of the choice of trial function.

# Summary

- The two approaches to finite-size errors in simulations of Coulombic systems are almost equivalent.
- Chiesa's identification of the long-range KE errors is useful.
- A simple reciprocal-space finite-size correction works well in HF calculations.