First-Principles Study of a Positron Immersed in an Electron Gas

Neil Drummond, Pablo López Ríos, Chris Pickard and Richard Needs

TCM Group, Cavendish Laboratory, University of Cambridge

TTI, Tuscany, Italy

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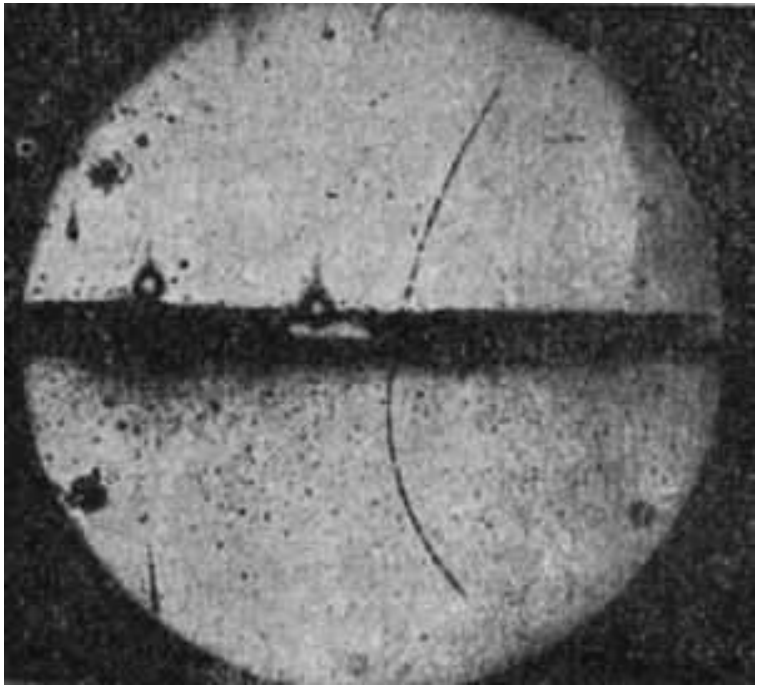
Positrons and Positronium Atoms

Positrons are **anti-electrons**.

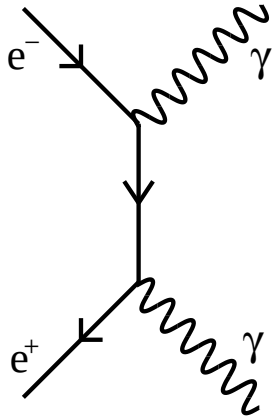


Positrons are produced in β^+ decays of proton-rich nuclei.

A positron may bind with an electron to form a *positronium atom*.

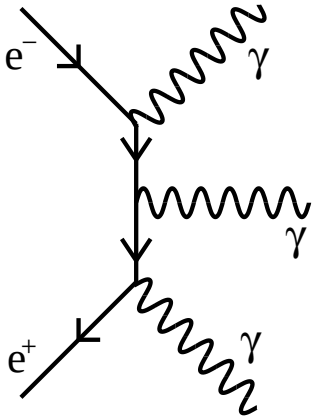
The ground-state energy of positronium is $-1/4$ a.u. (Like a hydrogen atom, but the reduced mass is $1/2$ a.u.)

Positron Annihilation



Annihilation of an **antiparallel**-spin electron–positron pair is a 2nd-order process, producing two 0.511 MeV photons.

Annihilation of a **parallel**-spin electron–positron pair is a 3rd-order process (need to conserve angular momentum), producing three photons.



Only two-photon annihilation events are considered here because they are (a) much more frequent and (b) much more useful.

The low-velocity two-photon annihilation cross-section is $\sigma_{2\gamma} = \pi/(vc^3)$, where v is the positron velocity and c is the speed of light.[1]

Positron annihilation is widely used to study material properties.

Usual source of positrons in experiments: ${}^{22}_{11}\mathrm{Na}_{11} \rightarrow {}^{22}_{10}\mathrm{Ne}_{12} + \beta^+ + \nu + \gamma$.

Energy of photon emitted at birth of positron: 1.274 MeV.

[1] P. A. M. Dirac, Proc. Cam. Phil. Soc. **26**, 361 (1930).

Positron Spectroscopies (I)

Suppose a positron is injected into a sample of material. Positrons tend to settle in negatively charged defects, particularly voids. Lifetime is typically a few nanoseconds.

POLIS: measure the time difference between the positron birth (one 1.274 MeV photon emitted) and annihilation (two 0.511 MeV photons emitted).

The annihilation rate is characteristic of the defects at which positrons settle.

Conservation of momentum: total momentum of annihilation γ-rays is equal to the momentum of the **annihilating electron–positron pair**.

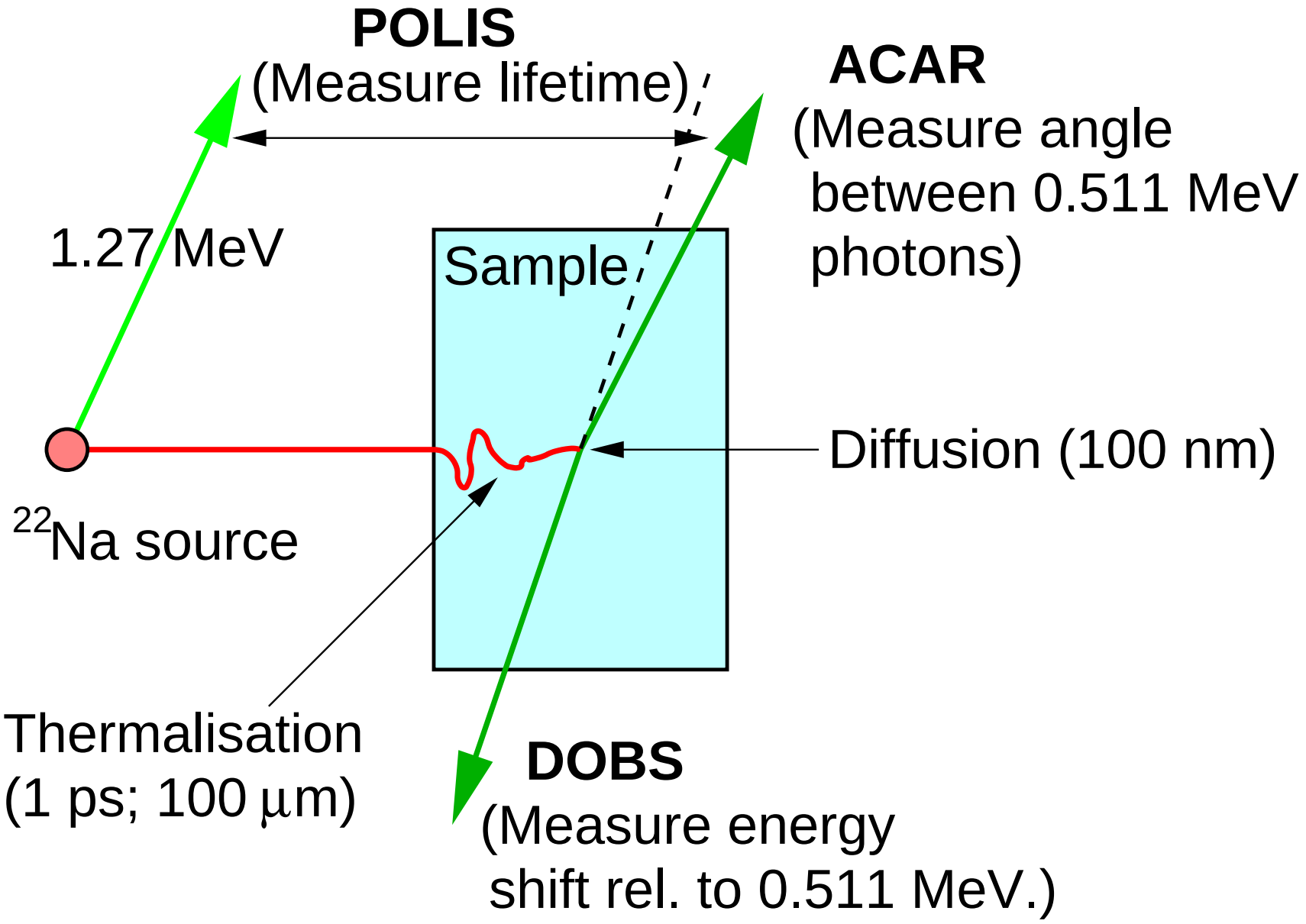
Measure the distribution of momenta of the 0.511 MeV annihilation radiation to find out about the distribution of electron momenta at the defects at which positrons settle.

Angular correlation of annihilation radiation (ACAR) spectroscopy and *Doppler-broadening spectroscopy* (DOBS) are powerful methods for identifying defects and measuring Fermi surfaces.

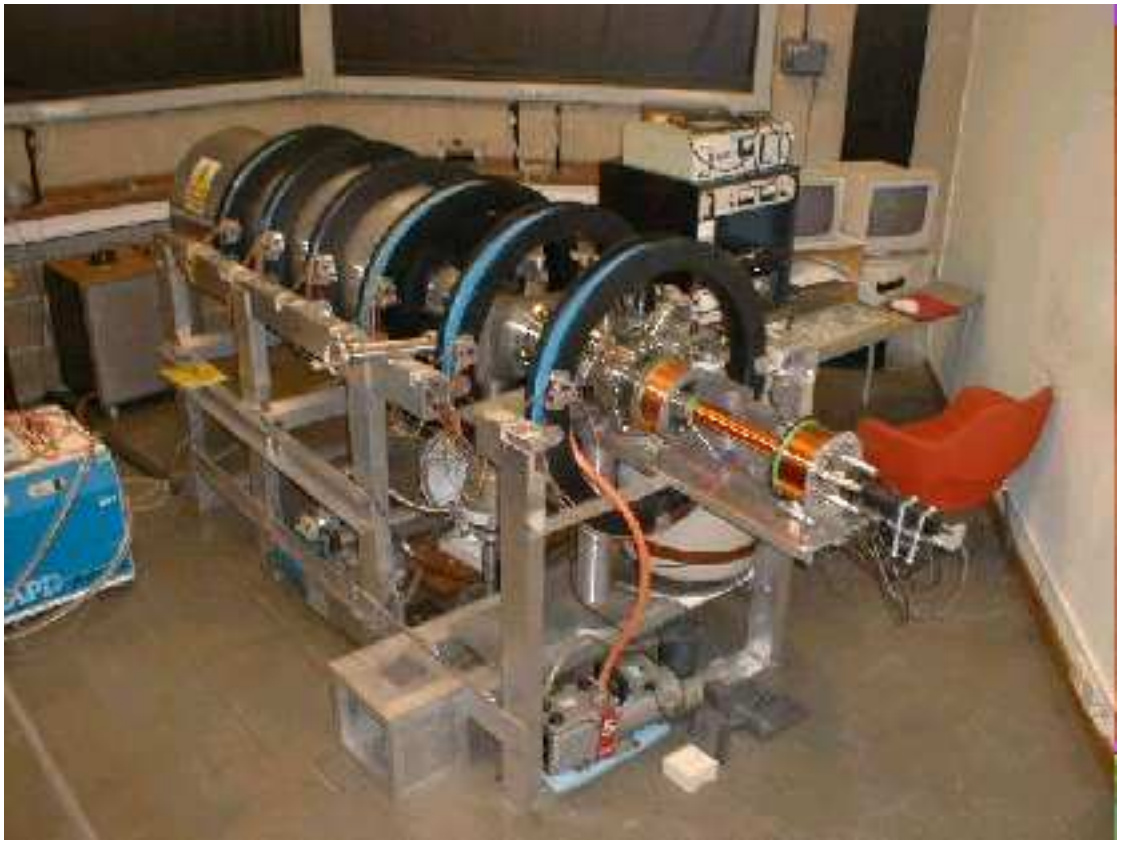
Sensitive, nondestructive techniques allowing simultaneous measurement of type and quantity of defects in metals and semiconductors.[2]

[2] R. Krause-Rehberg and H. S. Leipner, *Positron Annihilation in Semiconductors*, Springer–Verlag (1999).

Positron Spectroscopies (II)



Positron Spectroscopies (III)



Magnetically confined positron beam for DOBS experiments at the University of Bath

Challenges for Theory: Positron in a Homogeneous Electron Gas

Problem: *the positron modifies the electron distribution and momentum density.*

Annihilation rate of a positron in a *noninteracting* electron gas of number density n:[3]

$$\lambda = nv\sigma_{2\gamma} = \pi n/c^3.$$

The actual annihilation rate is higher, because the positron attracts electrons to it: *contact-density enhancement*.

The positron causes an increase in the momentum density near the Fermi edge: *Kahana enhancement*.[4]

Ultimately, we want to calculate annihilation rates and annihilating-pair momentum densities for positrons in real materials. First step: *calculate the energy, annihilation rate and momentum density for a positron in a HEG*.

Then use the energy data to construct electron–positron correlation functionals, enabling DFT simulations of positrons in real materials.

[3] P. A. M. Dirac, Proc. Cam. Phil. Soc. **26**, 361 (1930).

[4] S. Kahana, Phys. Rev. **129**, 1622 (1963).

Some of the Better Previous Attempts at this Problem

- **Bethe–Goldstone equation**
  - S. Kahana, Phys. Rev. **129**, 1622 (1963).
- **Tamm–Dancoff approximation**
  - J. Arponen and E. Pajanne, Ann. Phys. **121**, 343 (1979).
- **Fermi and perturbed hypernetted chain approximations**
  - L. J. Lantto, Phys. Rev. B **36**, 5160 (1987).
  - V. Apaja, S. Denk and E. Krotscheck, Phys. Rev. B **68**, 195118 (2003).
  - H. Stachowiak, Phys. Rev. B **41**, 12522 (1990).
  - H. Stachowiak and J. Lach, Phys. Rev. B **48**, 9828 (1993).
  - E. Boroński and H. Stachowiak, Phys. Rev. B **57**, 6215 (1998).
- **Variational quantum Monte Carlo (using plane-wave orbitals)**
  - G. Ortiz, PhD thesis, Swiss Federal Institute of Technology, Lausanne (1992).
  - L. Fraser, PhD thesis, Imperial College, London (1995).

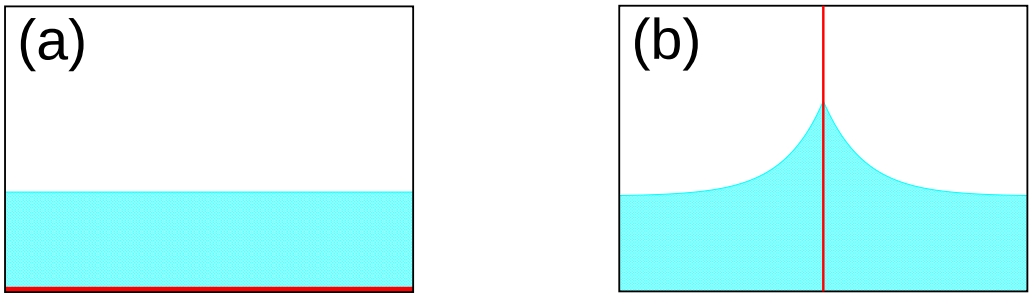
Electron–Positron Hamiltonian (I)

Hamiltonian for a positron in a HEG:

$$\hat{H} = \sum_i \frac{-1}{2}\frac{\partial^2}{\partial \mathbf{r}_i^2} - \frac{1}{2}\frac{\partial^2}{\partial \mathbf{s}^2} - \sum_i \frac{1}{|\mathbf{r}_i - \mathbf{s}|} + \sum_{j>i} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}.$$

Make the coordinate transformation suggested by Leung *et al.*[5]

$$\begin{aligned} \mathbf{X} &= \frac{1}{N+1}\left(\mathbf{s} + \sum_{i=1}^{N} \mathbf{r}_i\right) \\ \mathbf{x}_i &= \mathbf{r}_i - \mathbf{s}. \end{aligned}$$



Electron and positron density in (a) the original and (b) the transformed frame.

[5] C. H. Leung, M. J. Stott and C. O. Almbladh, Phys. Lett. **57A**, 26 (1976).

Electron–Positron Hamiltonian (II)

Then the Hamiltonian is

$$\hat{H} = \frac{-1}{2(N+1)}\frac{\partial^2}{\partial \mathbf{X}^2} - \sum_i \left(\frac{\partial^2}{\partial \mathbf{x}_i^2} + \frac{1}{|\mathbf{x}_i|} \right) + \sum_{j>i} \left(-\frac{\partial^2}{\partial \mathbf{x}_i \partial \mathbf{x}_j} + \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|} \right).$$

The first term on the RHS is the CoM KE operator. May neglect it in the ground state.

Left with a Hamiltonian for N interacting Fermions of mass $1/2$ a.u. and charge -1 a.u. in the presence of a fixed positive charge of magnitude 1 a.u. at the origin.

There is an extra interaction term $\hat{A} = -\sum_{j>i} \partial^2/(\partial \mathbf{x}_i \partial \mathbf{x}_j)$.

This term was neglected by Leung *et al.*, who argued that it has only a small effect on the electron–positron correlation energy.

But the term isn't small. For a HEG without a positron, the expectation of the extra interaction is minus half the KE in the transformed frame.

Extra Interaction in a One-Electron Theory

Suppose Ψ is a product of determinants of **orthonormal** orbitals $\{\phi_i\}$ for spin-up and spin-down electrons. Then the expectation of the extra interaction is

$$\left\langle \Psi \left| \hat{A} \right| \Psi \right\rangle = -\frac{1}{2} \sum_{i,j} \left[\langle \phi_i | \nabla \phi_i \rangle \cdot \langle \phi_j | \nabla \phi_j \rangle - \delta_{s_i,s_j} \langle \phi_i | \nabla \phi_j \rangle \cdot \langle \phi_j | \nabla \phi_i \rangle \right],$$

where s_i is the spin of particle i.

The direct term vanishes if all the orbitals are real or are occupied at both $\mathbf{k}$ and $-\mathbf{k}$. Only closed-shell ground states are considered, so the direct term can be neglected.

The exchange term is only nonzero between bands with the same $\mathbf{k}$ vector, unlike the exchange term for the Coulomb interaction.

Kohn–Sham Equations

Require $\langle\Psi|\hat{T}|\Psi\rangle + \langle\Psi|\hat{A}|\Psi\rangle + E_H[n] + E_{\rm ext}[n] + E_{\rm xc}[n]$ to be stationary with respect to variations in ϕ_i^*:

$$\begin{aligned}\left[-\nabla^2 + V_H(\mathbf{x}) + V_{\rm ext}(\mathbf{x}) + V_{\rm xc}(\mathbf{x})\right]\phi_i(\mathbf{x}) & \\ + \sum_j f_j \delta_{s_i,s_j}\langle\phi_j|\nabla\phi_i\rangle\cdot\nabla\phi_j(\mathbf{x}) &= \mathcal{E}_i\phi_i(\mathbf{x}),\end{aligned}$$

where V_H, $V_{\rm ext}$ and $V_{\rm xc}$ are the Hartree, external (positron) and exchange–correlation potentials, and f_j and $\mathcal{E}_j$ are the occupation number and eigenvalue of state j.

The equations are solved self-consistently by a modified version of the CASTEP[6] plane-wave DFT code: *pCASTEP*.

[6] M. D. Segall, P. J. D. Lindan, M. J. Probert, C. J. Pickard, P. J. Hasnip, S. J. Clark and M. C. Payne, J. Phys. Cond. Matt. **14**, 2717 (2002).

Eigenvalues

Consider a HEG in the transformed coordinate system. The orbitals are $\exp(i\mathbf{G}\cdot\mathbf{x})/\sqrt{V}$. Eigenvalue of one-electron extra interaction operator:

$$\begin{aligned}\exp(-i\mathbf{G}\cdot\mathbf{x})\hat{a}_1\exp(i\mathbf{G}\cdot\mathbf{x}) &= \sum_{\mathbf{G}'}\frac{f_{\mathbf{G}'}}{V}\int\exp[i(\mathbf{G}-\mathbf{G}')\cdot(\mathbf{x}'-\mathbf{x})]i\mathbf{G}\,d\mathbf{x}'\cdot i\mathbf{G}' \\ &= -G^2 f_{\mathbf{G}}.\end{aligned}$$

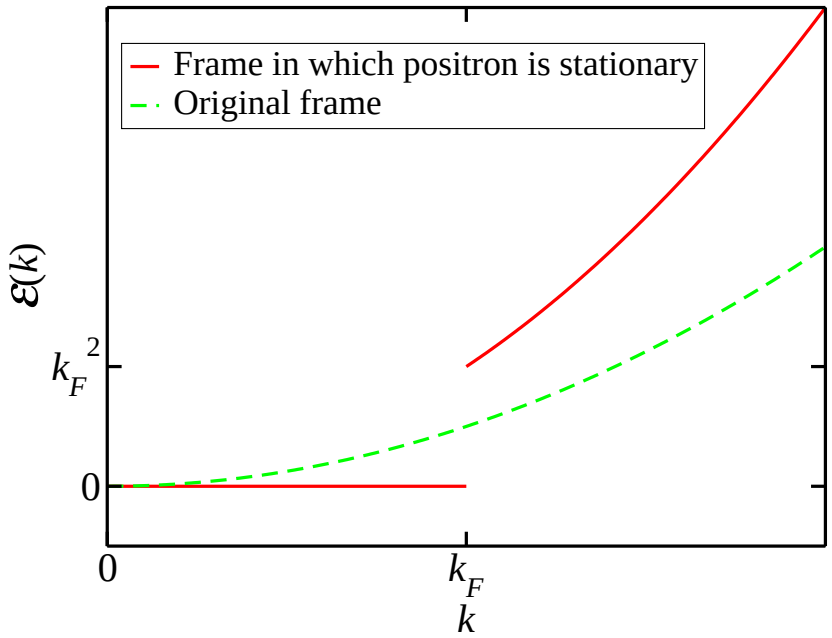
So the Kohn–Sham eigenvalues are $\mathcal{E}_{\mathbf{G}} = G^2(1-f_{\mathbf{G}})$.

Eigenvalues are zero for occupied states and G^2 for unoccupied states.

In the infinite-system limit there is a discontinuity of magnitude k_F^2 in the energy band at k_F.

Adding the positron does not remove the gap.

System is like a metal with a huge band gap!



Getting pCASTEP to Converge

The large gap quickly forces the occupancies to be zero or one. There is a huge energy cost to fractional occupancy. Must ensure the electron number is a magic number for the system with unfolded $\mathbf{k}$ points.

Calculations with multiple $\mathbf{k}$ points often get stuck in excited states because the initial (random) number of occupied states at each $\mathbf{k}$ gets frozen in.

Solution: just work at Γ. (Shell-filling effects mostly cancel out of energy differences and don't affect pair correlation functions very much anyway.)

Successful strategies:

(A) iterate the orbital coefficients to self-consistency every time the density is updated;

(B) converge the orbitals in the absence of the extra interaction, then switch on the extra interaction and re-converge.

Relaxation Energy

If there is no electron–positron correlation then the positron occupies its zero-momentum ground state. *In this case, the energy of the HEG+positron is the same as the energy of the HEG without the positron.*

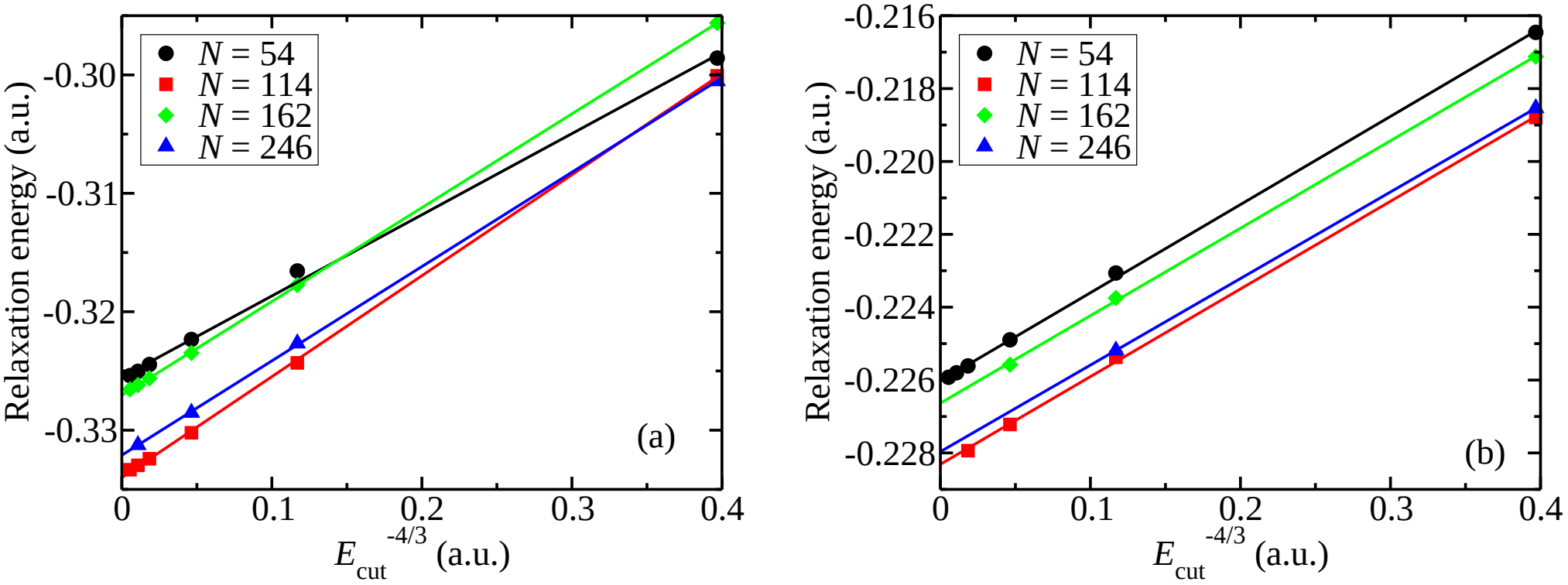
So the electron–positron correlation energy is the difference of the energy of the N-electron HEG+positron and the N-electron HEG.

The electron–positron correlation energy is called the *relaxation energy*.

HEG+positron calculations should be performed in a cell of volume $(4/3)\pi r_s^3(N-1)$, so the electron density at the edge of the cell is the same as that of a HEG of density parameter r_s. This reduces finite-size errors.

Having calculated the relaxation energy, a function of r_s can be fitted to the data, providing an electron–positron correlation functional for use in DFT studies of positrons in real materials.

Finite-Basis Error in the Relaxation Energy

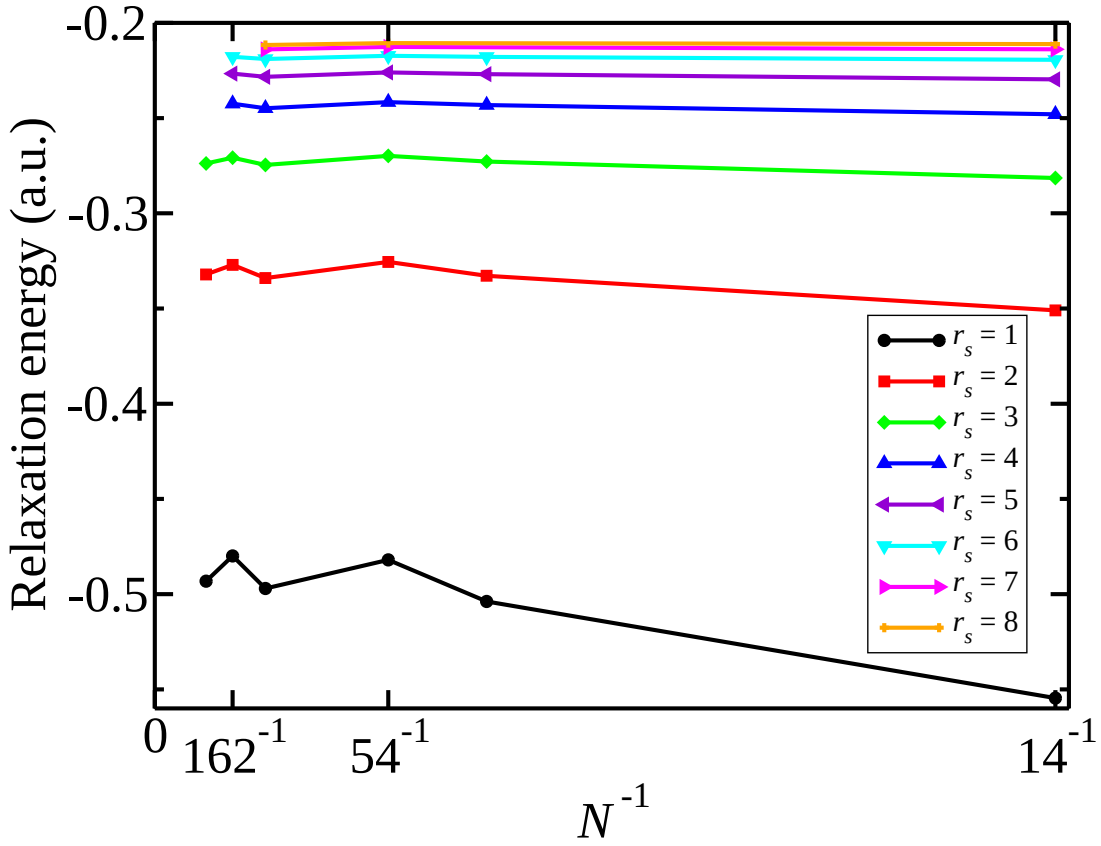


Relaxation energy against plane-wave cutoff energy $E_{\rm cut}$ at $r_s = 2$ and 5.

Extrapolate to basis-set completeness by assuming error goes as $E_{\rm cut}^{-4/3}$.

Still need to deal with finite-size errors.

Finite-Size Error in the Relaxation Energy



Relaxation energy (extrap. to basis-set completeness) against number of electrons N.

For small N, systematic errors due to the interaction of images of the positron are visible, especially at high density.

Above this, only oscillatory shell-filling effects are visible. Average over the relaxation energies at the highest three N available at each density.

Annihilating-Pair Momentum Density (I)

CoM and difference coordinates: $\bar{\mathbf{r}}_i \equiv (\mathbf{r}_i + \mathbf{s})/2$ and $\delta\mathbf{r}_i \equiv \mathbf{r}_i - \mathbf{s}$.

Electron–positron centre-of-mass momentum wave function:

$$\tilde{\Psi}(\bar{\mathbf{p}}_1, \delta\mathbf{r}_1; \mathbf{r}_2, \ldots, \mathbf{r}_N) = \frac{1}{V} \int \exp(-i\bar{\mathbf{p}}_1 \cdot \bar{\mathbf{r}}_1) \Psi(\bar{\mathbf{r}}_1, \delta\mathbf{r}_1; \mathbf{r}_2, \ldots, \mathbf{r}_N)\, d\bar{\mathbf{r}}_1,$$

Distribution of annihilating-pair momenta is the same as the distribution of CoM momenta when the positron coincides with an electron of opposite spin.

Unnormalised distribution of CoM momentum for positron annihilating with electron 1:

$$\int \cdots \int |\tilde{\Psi}(\bar{\mathbf{p}}_1, \mathbf{0}; \mathbf{r}_2, \ldots, \mathbf{r}_N)|^2\, d\mathbf{r}_2 \ldots d\mathbf{r}_N.$$

Annihilating-Pair Momentum Density (II)

Normalise and use antisymmetry of wave function to get momentum density:

$$\rho_\uparrow(\bar{\mathbf{p}}) = \frac{\int \cdots \int \left| \int \exp(-i\bar{\mathbf{p}} \cdot \mathbf{r}_1) \Psi(\mathbf{r}_1; \mathbf{r}_1, \ldots, \mathbf{r}_N)\, d\mathbf{r}_1 \right|^2 d\mathbf{r}_2 \ldots d\mathbf{r}_N}{V \int \cdots \int |\Psi(\mathbf{r}_1; \mathbf{r}_1, \ldots, \mathbf{r}_N)|^2 \, d\mathbf{r}_1 \ldots d\mathbf{r}_N}.$$

Now suppose

$$\begin{aligned} \Psi(\mathbf{s}; \mathbf{r}_1, \ldots, \mathbf{r}_N) \quad = \quad & \frac{1}{\sqrt{N_\uparrow! N_\downarrow!}} \begin{vmatrix} \phi_1^\uparrow(\mathbf{r}_1 - \mathbf{s}) & \cdots & \phi_{N_\uparrow}^\uparrow(\mathbf{r}_1 - \mathbf{s}) \\ \vdots & & \vdots \\ \phi_1^\uparrow(\mathbf{r}_{N_\uparrow} - \mathbf{s}) & \cdots & \phi_{N_\uparrow}^\uparrow(\mathbf{r}_{N_\uparrow} - \mathbf{s}) \end{vmatrix} \\ & \times \begin{vmatrix} \phi_1^\downarrow(\mathbf{r}_{N_\uparrow+1} - \mathbf{s}) & \cdots & \phi_{N_\downarrow}^\downarrow(\mathbf{r}_{N_\uparrow+1} - \mathbf{s}) \\ \vdots & & \vdots \\ \phi_1^\downarrow(\mathbf{r}_N - \mathbf{s}) & \cdots & \phi_{N_\downarrow}^\downarrow(\mathbf{r}_N - \mathbf{s}) \end{vmatrix}. \end{aligned}$$

Annihilating-Pair Momentum Density (III)

The numerator of the momentum density may be shown to be

$$\rho_{\uparrow u}(\bar{\mathbf{p}}) = \int e^{-i\bar{\mathbf{p}}\cdot\mathbf{R}} \int \cdots \int \sum_{i=1}^{N_\uparrow}\sum_{j=1}^{N_\uparrow} (-1)^{i+j} \phi_i^{\uparrow *}(\mathbf{0})\phi_j^{\uparrow}(\mathbf{0}) M_{1i}N_{1j}\, d\mathbf{r}_2 \ldots d\mathbf{r}_{N_\uparrow}$$
$$\times \frac{V}{N_\uparrow!} \begin{vmatrix} \int \phi_1^{\downarrow *}(\mathbf{r})\phi_1^{\downarrow}(\mathbf{r}-\mathbf{R})\, d\mathbf{r} & \cdots & \int \phi_{N_\downarrow}^{\downarrow *}(\mathbf{r})\phi_1^{\downarrow}(\mathbf{r}-\mathbf{R})\, d\mathbf{r} \\ \vdots & & \vdots \\ \int \phi_1^{\downarrow *}(\mathbf{r})\phi_{N_\downarrow}^{\downarrow}(\mathbf{r}-\mathbf{R})\, d\mathbf{r} & \cdots & \int \phi_{N_\downarrow}^{\downarrow *}(\mathbf{r})\phi_{N_\downarrow}^{\downarrow}(\mathbf{r}-\mathbf{R})\, d\mathbf{r} \end{vmatrix} d\mathbf{R},$$

where M_{ij} and N_{ij} are the (i,j)th minors of

$$\begin{vmatrix} \phi_1^{\uparrow *}(\mathbf{0}) & \cdots & \phi_{N_\uparrow}^{\uparrow *}(\mathbf{0}) \\ \phi_1^{\uparrow *}(\mathbf{r_2}) & \cdots & \phi_{N_\uparrow}^{\uparrow *}(\mathbf{r}_2) \\ \vdots & & \vdots \\ \phi_1^{\uparrow *}(\mathbf{r}_{N_\uparrow}) & \cdots & \phi_{N_\uparrow}^{\uparrow *}(\mathbf{r}_{N_\uparrow}) \end{vmatrix} \quad \text{and} \quad \begin{vmatrix} \phi_1^{\uparrow}(\mathbf{0}) & \cdots & \phi_{N_\uparrow}^{\uparrow}(\mathbf{0}) \\ \phi_1^{\uparrow}(\mathbf{r_2}-\mathbf{R}) & \cdots & \phi_{N_\uparrow}^{\uparrow}(\mathbf{r}_2-\mathbf{R}) \\ \vdots & & \vdots \\ \phi_1^{\uparrow}(\mathbf{r}_{N_\uparrow}-\mathbf{R}) & \cdots & \phi_{N_\uparrow}^{\uparrow}(\mathbf{r}_{N_\uparrow}-\mathbf{R}) \end{vmatrix}.$$

Annihilating-Pair Momentum Density (IV)

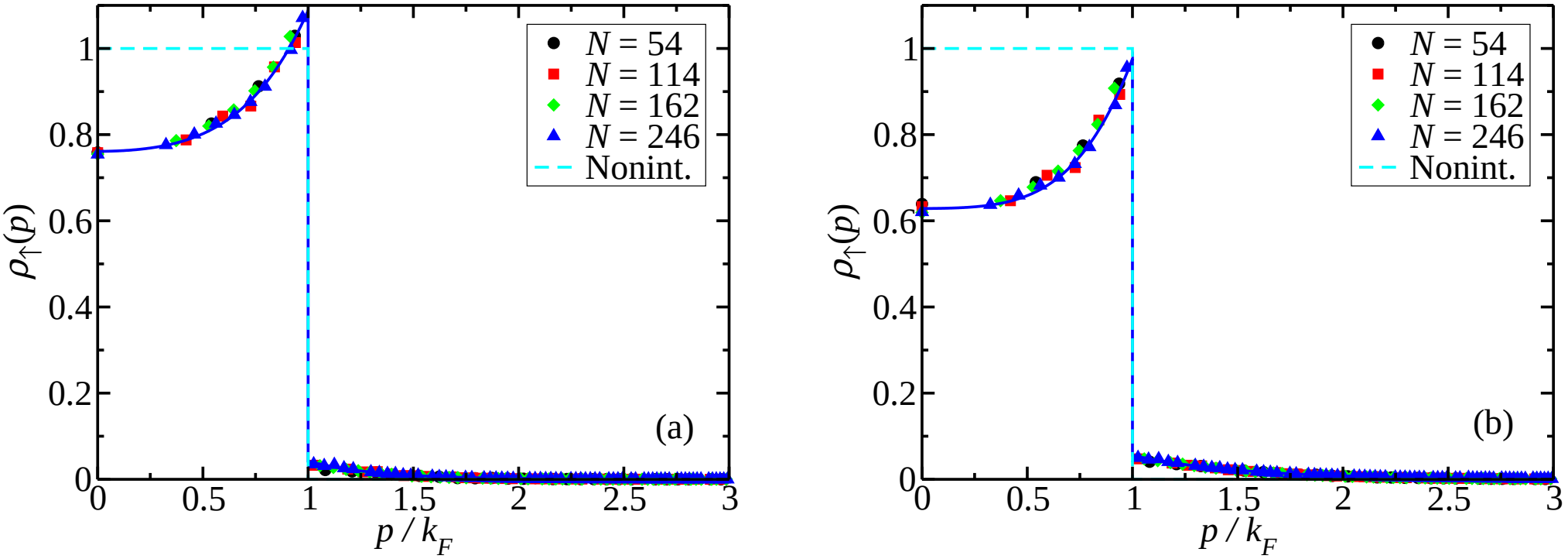
For each $i, j \in \{1, \ldots, N_\uparrow\}$, we can use the overlap integral theorem to determine a $(N_\uparrow - 1) \times (N_\uparrow - 1)$ matrix $B^{\mathbf{R}}(i,j)$ such that

$$\det\left(B^{\mathbf{R}}(i,j)\right) = \frac{1}{(N_\uparrow - 1)!} \int \cdots \int M_{1i} N_{1j}\, d\mathbf{r}_2 \ldots d\mathbf{r}_{N_\uparrow}.$$

So the unnormalised annihilating-pair momentum density is

$$\begin{aligned} \rho_{\uparrow u}(\bar{\mathbf{p}}) &= \int \exp(-i\bar{\mathbf{p}} \cdot \mathbf{R}) \sum_{i=1}^{N_\uparrow} \sum_{j=1}^{N_\uparrow} (-1)^{i+j} \phi_i^{\uparrow *}(\mathbf{0}) \phi_j^{\uparrow}(\mathbf{0}) \det\left(B^{\mathbf{R}}(i,j)\right) \\ &\quad \times \begin{vmatrix} \int \phi_1^{\downarrow *}(\mathbf{r}) \phi_1^{\downarrow}(\mathbf{r} - \mathbf{R})\, d\mathbf{r} & \cdots & \int \phi_{N_\downarrow}^{\downarrow *}(\mathbf{r}) \phi_1^{\downarrow}(\mathbf{r} - \mathbf{R})\, d\mathbf{r} \\ \vdots & & \vdots \\ \int \phi_1^{\downarrow *}(\mathbf{r}) \phi_{N_\downarrow}^{\downarrow}(\mathbf{r} - \mathbf{R})\, d\mathbf{r} & \cdots & \int \phi_{N_\downarrow}^{\downarrow *}(\mathbf{r}) \phi_{N_\downarrow}^{\downarrow}(\mathbf{r} - \mathbf{R})\, d\mathbf{r} \end{vmatrix} d\mathbf{R}. \end{aligned}$$

Finite-Size Error in the Momentum Density



MDs extrapolated to basis-set completeness at $r_s = 2$ and 5.

MDs are reasonably well-converged with respect to N.

Fit model MD to data at largest system size available at each density.

Tail of MD falls off exponentially. (Artifact of DFT.)

Electron–Positron Pair-Correlation Function

Spin-down positron–spin-up electron pair-correlation function:

$$g^{\uparrow}(\mathbf{r},\mathbf{s}) = \frac{\rho_{1p}^{\uparrow}(\mathbf{r},\mathbf{s})}{\rho_{1}^{\uparrow}(\mathbf{r})\rho_{p}(\mathbf{s})} = \frac{V^2}{N_{\uparrow}} \sum_{i} |\phi_{i}^{\uparrow}(\mathbf{r}-\mathbf{s})|^2.$$

The electron–positron PCF is proportional to the electronic charge density in the transformed system (as one would expect).

Contact-Density Enhancement and Annihilation Rate

Effective density of spin-up electrons at the positron:

$$n_{\text{eff}}^{\uparrow} = \frac{N_{\uparrow}}{V} g^{\uparrow}(0).$$

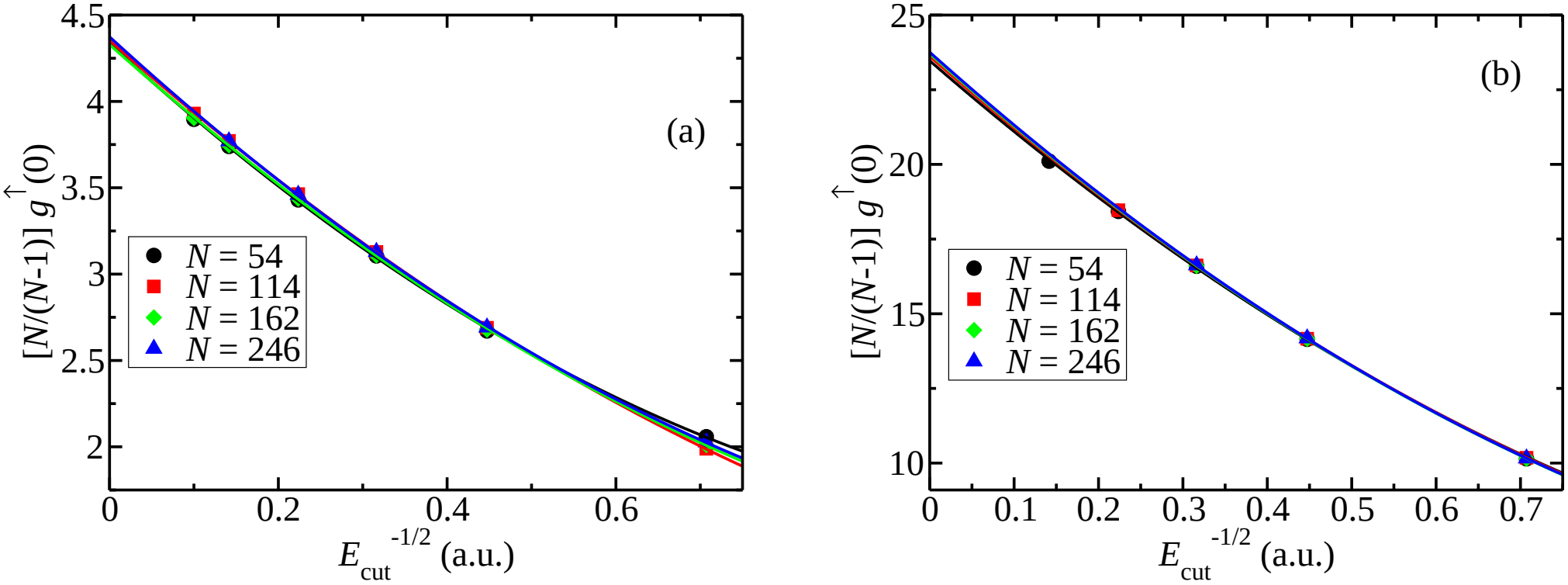
This *contact density* should be used to calculate annihilation rate using the 2-photon annihilation cross-section.

Overall annihilation rate:

$$\lambda = \frac{\pi n g(0)}{c^3} = \frac{3g(0)}{4c^3 r_s^3}.$$

For a paramagnetic HEG (considered here), $g(r) = g^{\uparrow}(r)$.

Finite-Basis and Finite-Size Errors in the Contact PCF



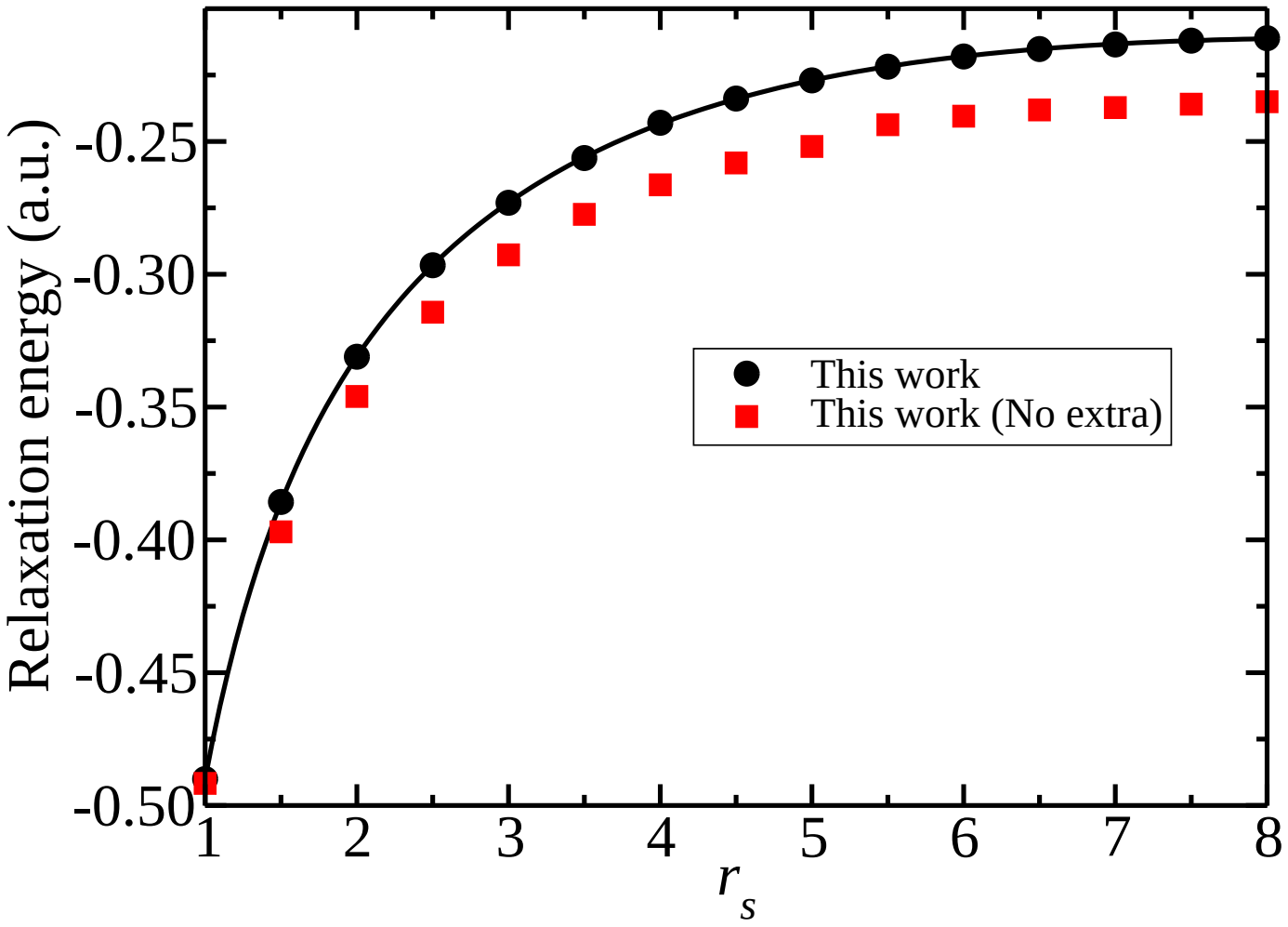
Contact PCFs at $r_s = 2$ and 5.

Large finite-basis errors, because Kimball cusp condition $(\partial \bar{g}^{\uparrow}/\partial r)_0 = -g^{\uparrow}(0)$ is violated.

Extrapolate $g^{\uparrow}(0)$ to basis-set completeness assuming error goes as $aE_{\mathrm{cut}}^{-1/2} + bE_{\mathrm{cut}}^{-1}$.

Multiply by $N/(N-1)$ to make PCF go to 1 at edge of cell and average data with $N > 100$.

Results (I): Relaxation Energy



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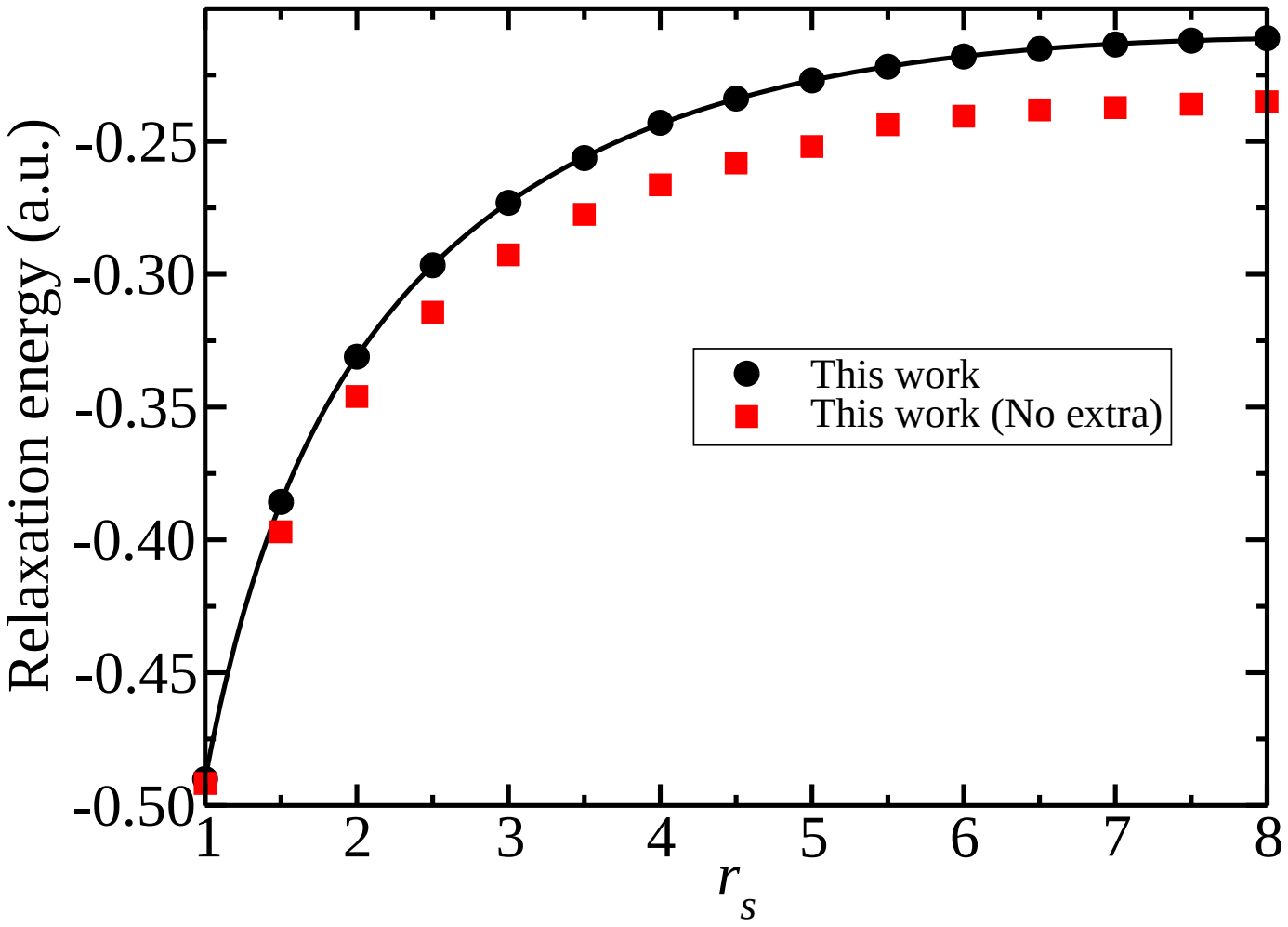

- *Extra interaction makes a small but significant difference to the relaxation energy.*

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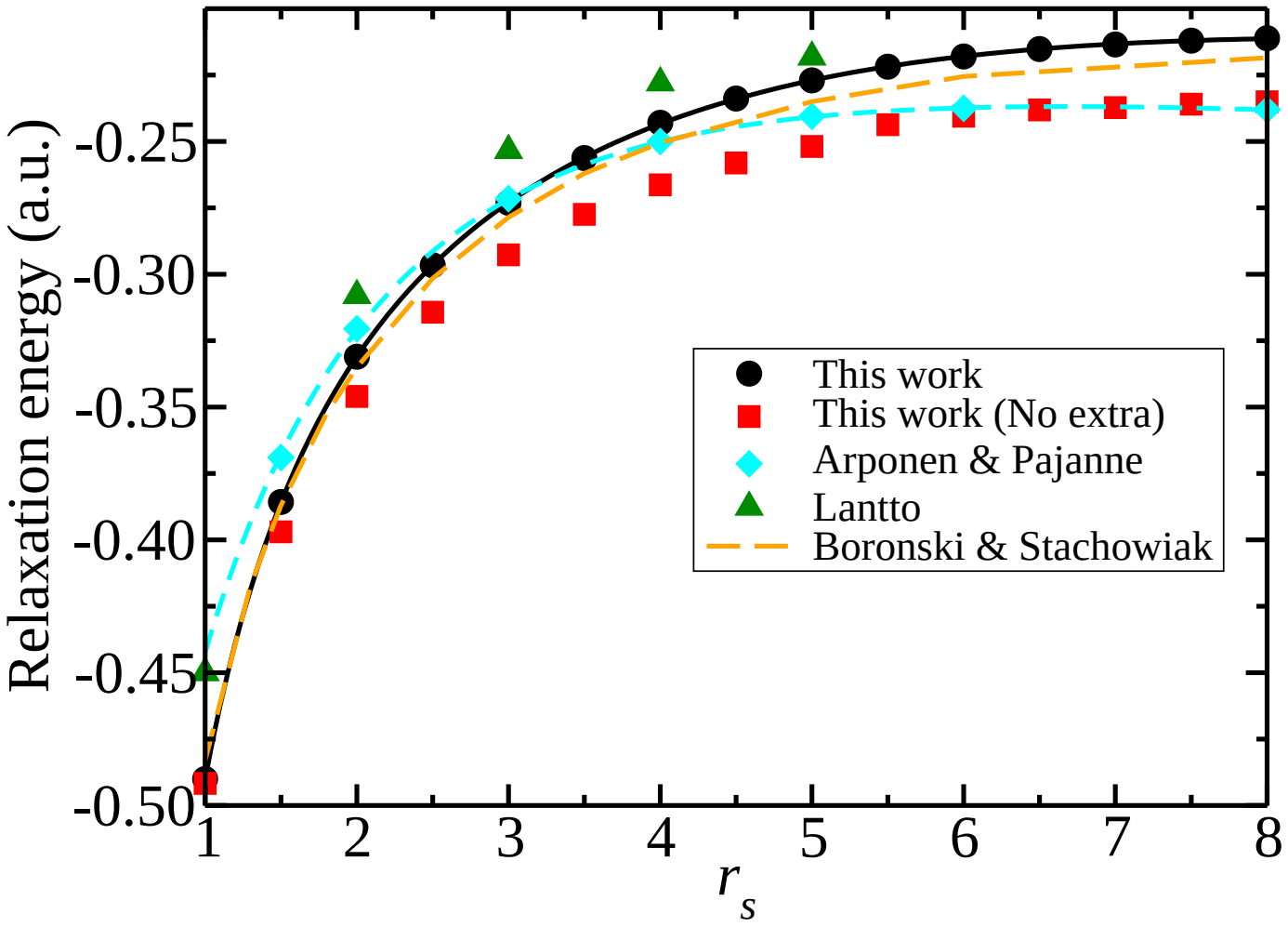

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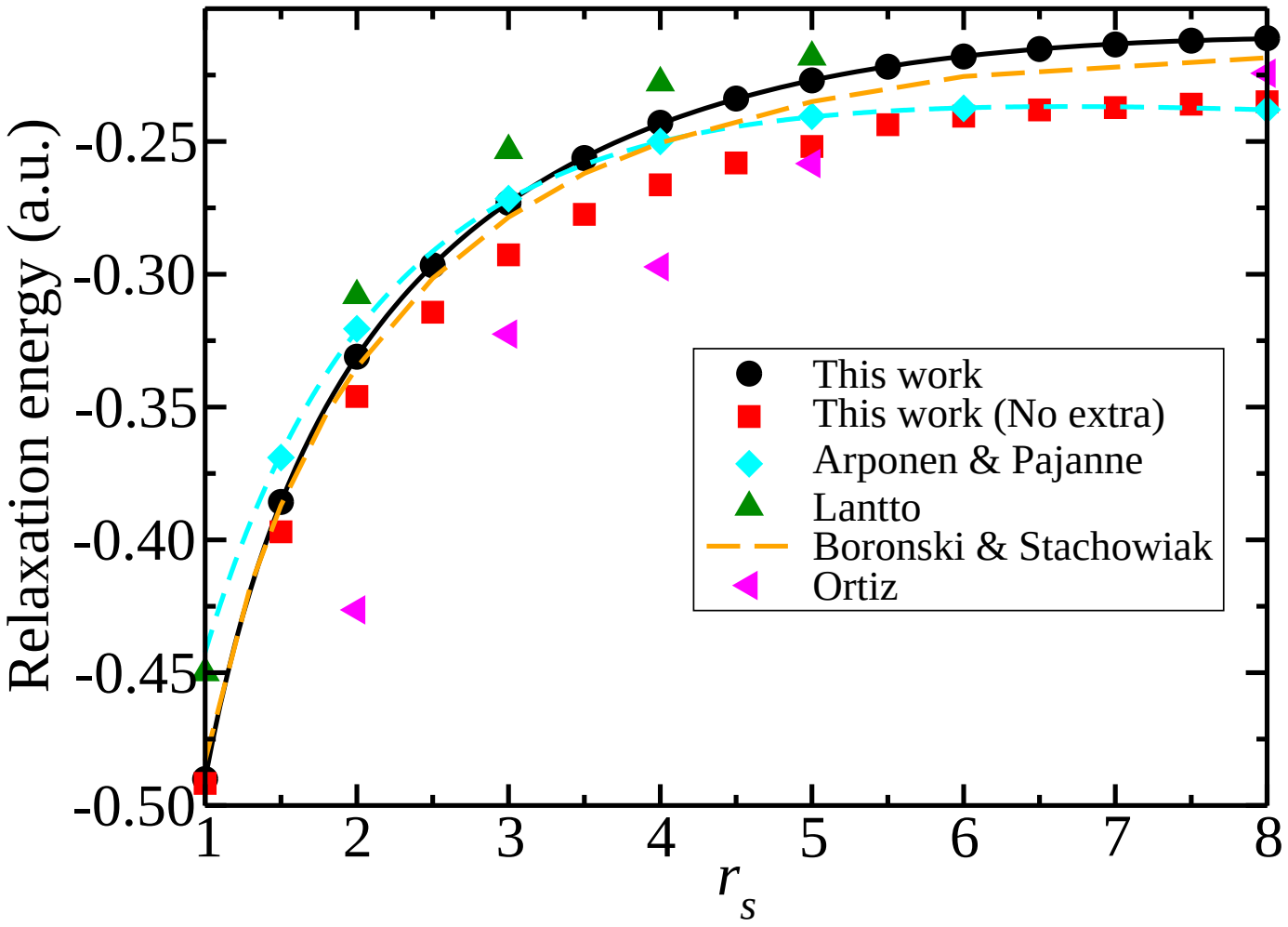

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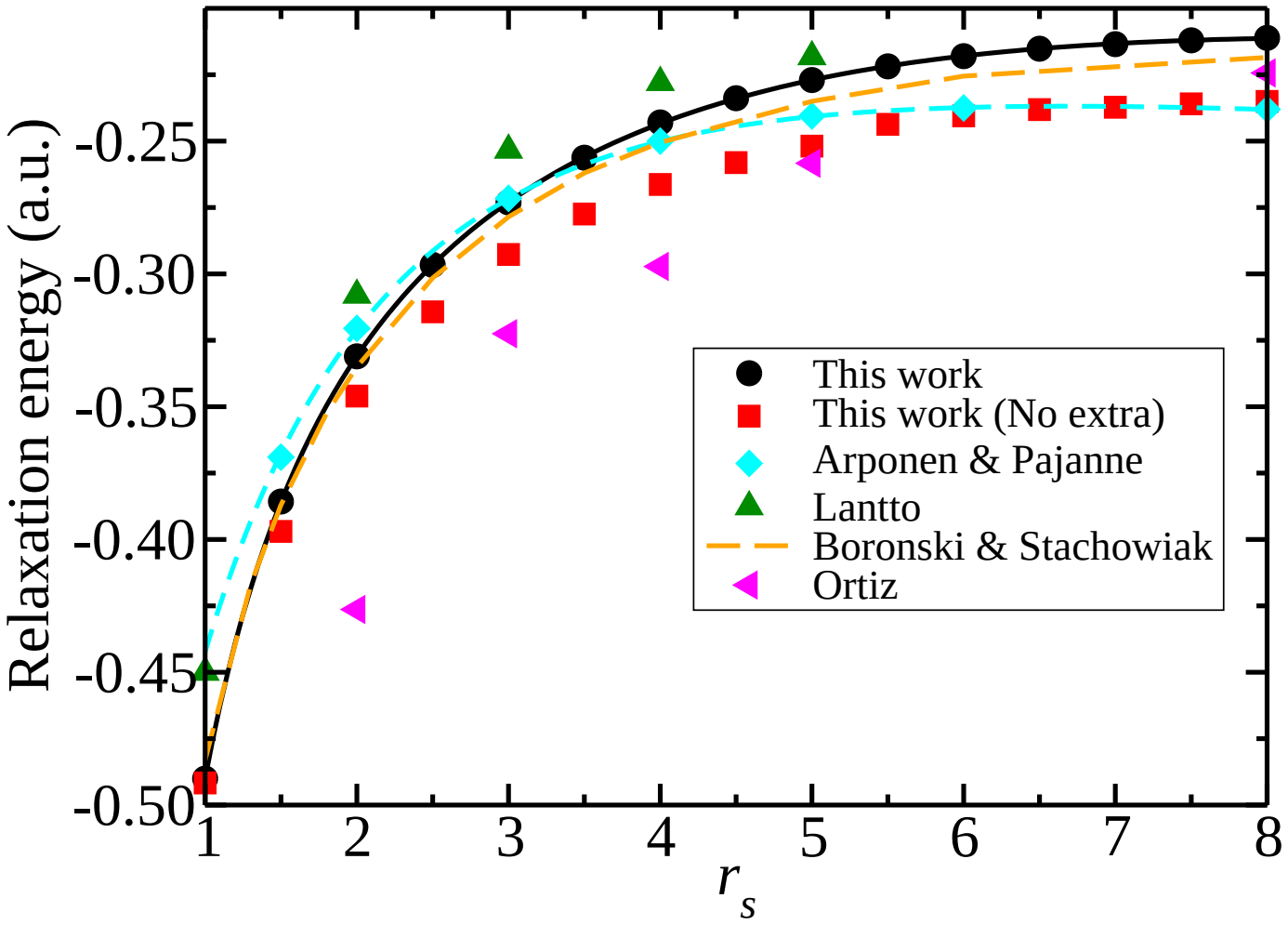
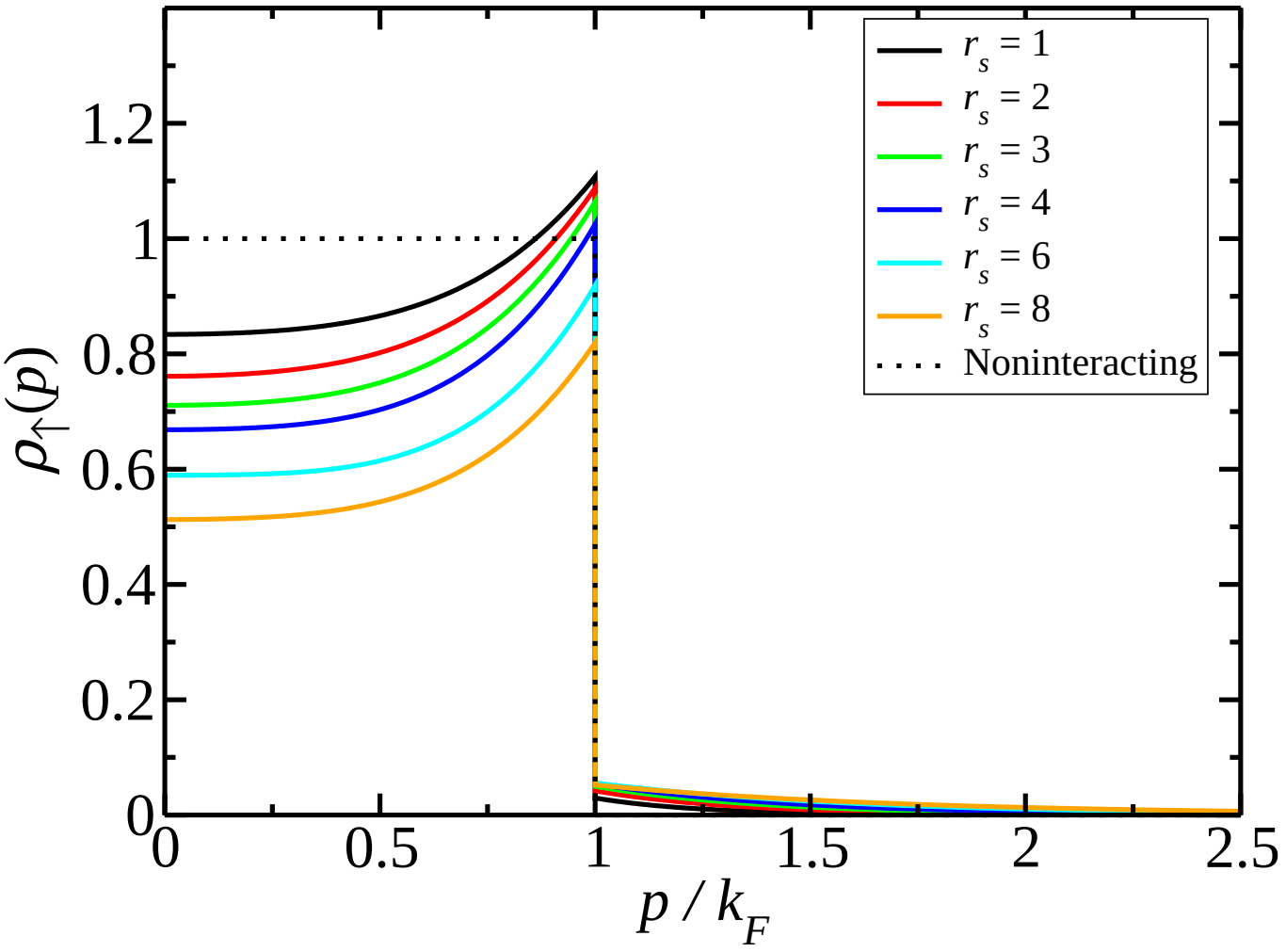
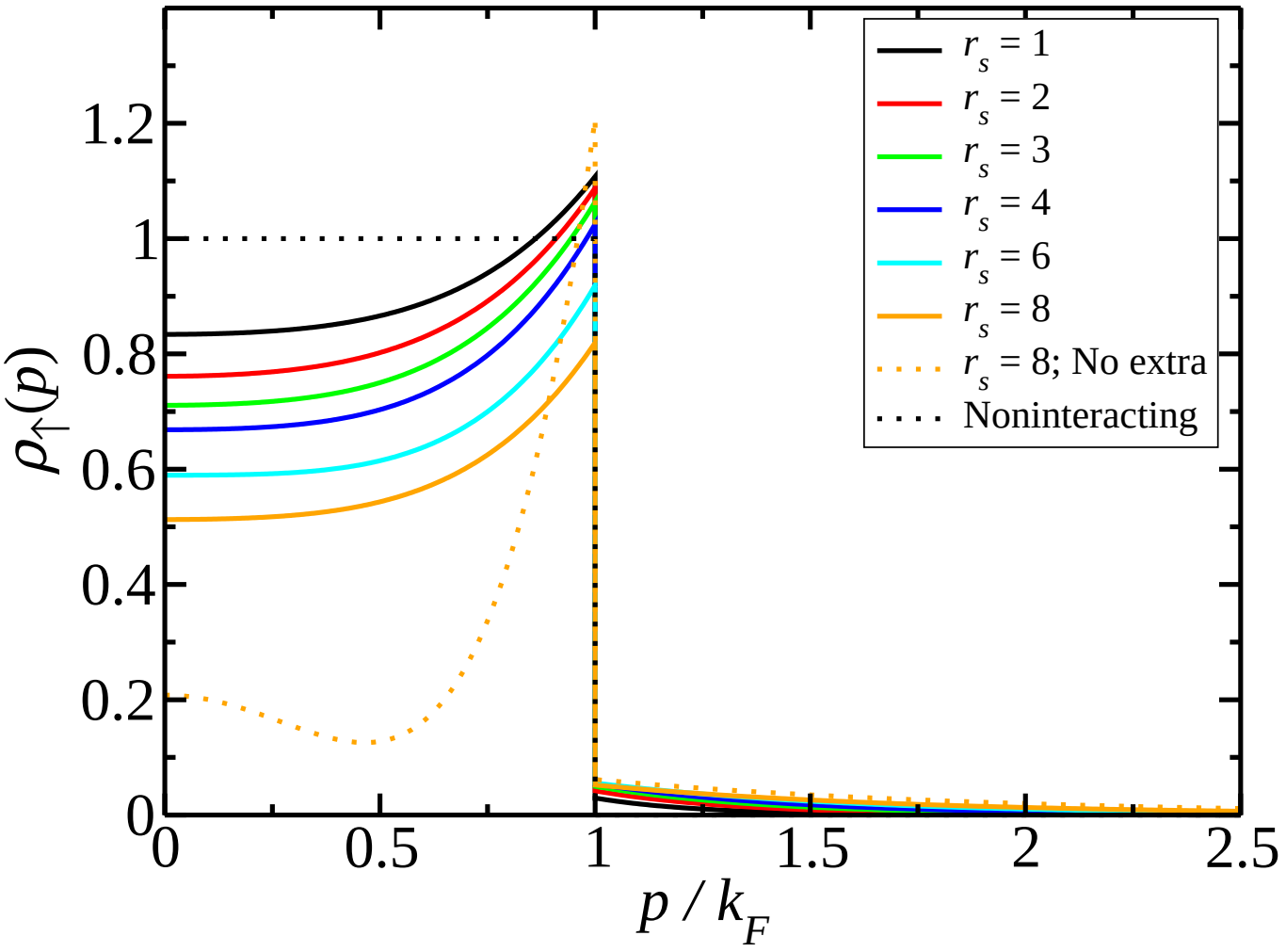


- *Extra interaction makes a small but significant difference to the relaxation energy.*
- *My results are in reasonable agreement with Boroński and Stachowiak.*

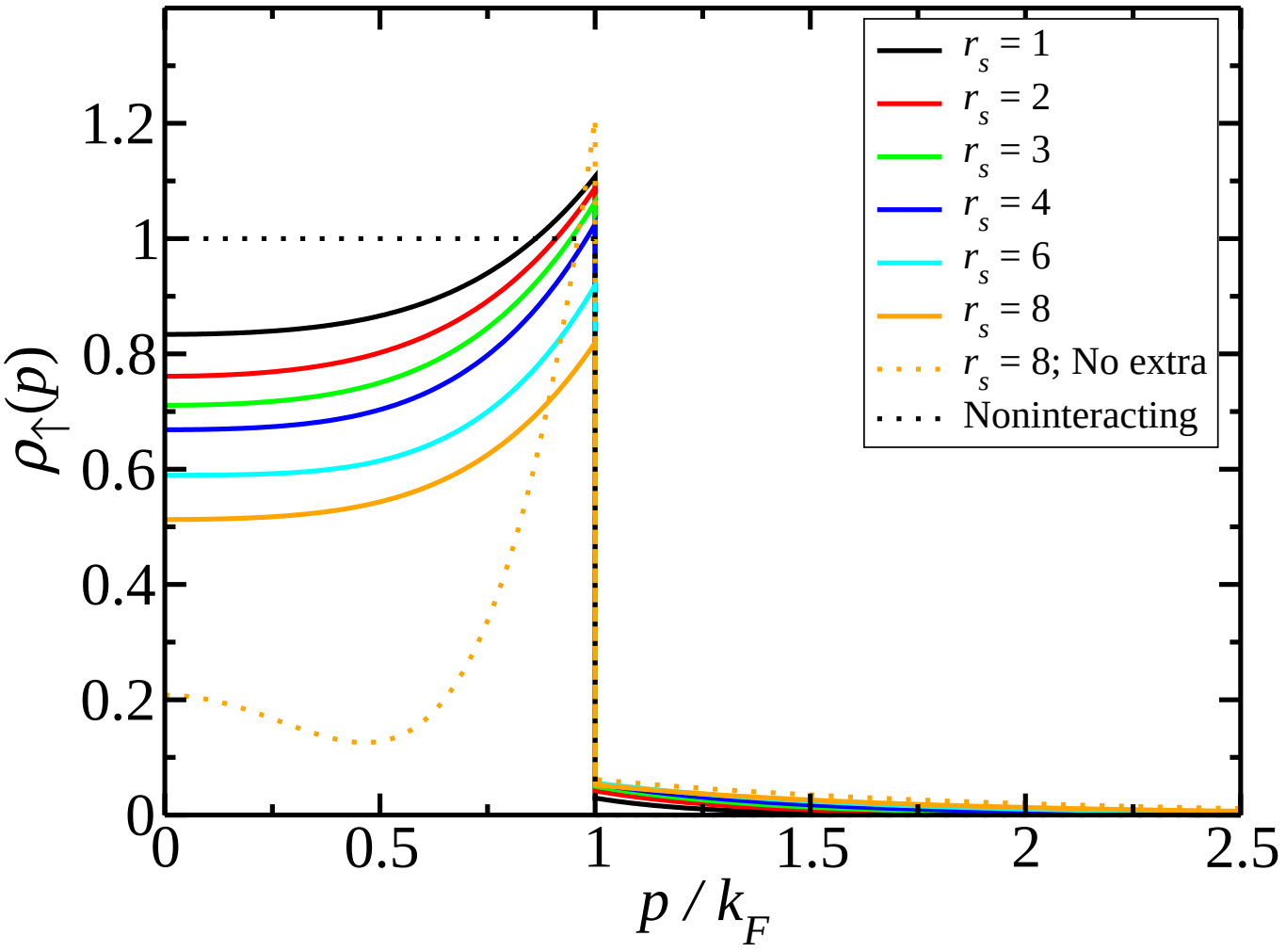
Results (II): Annihilating-Pair Momentum Density



Results (II): Annihilating-Pair Momentum Density

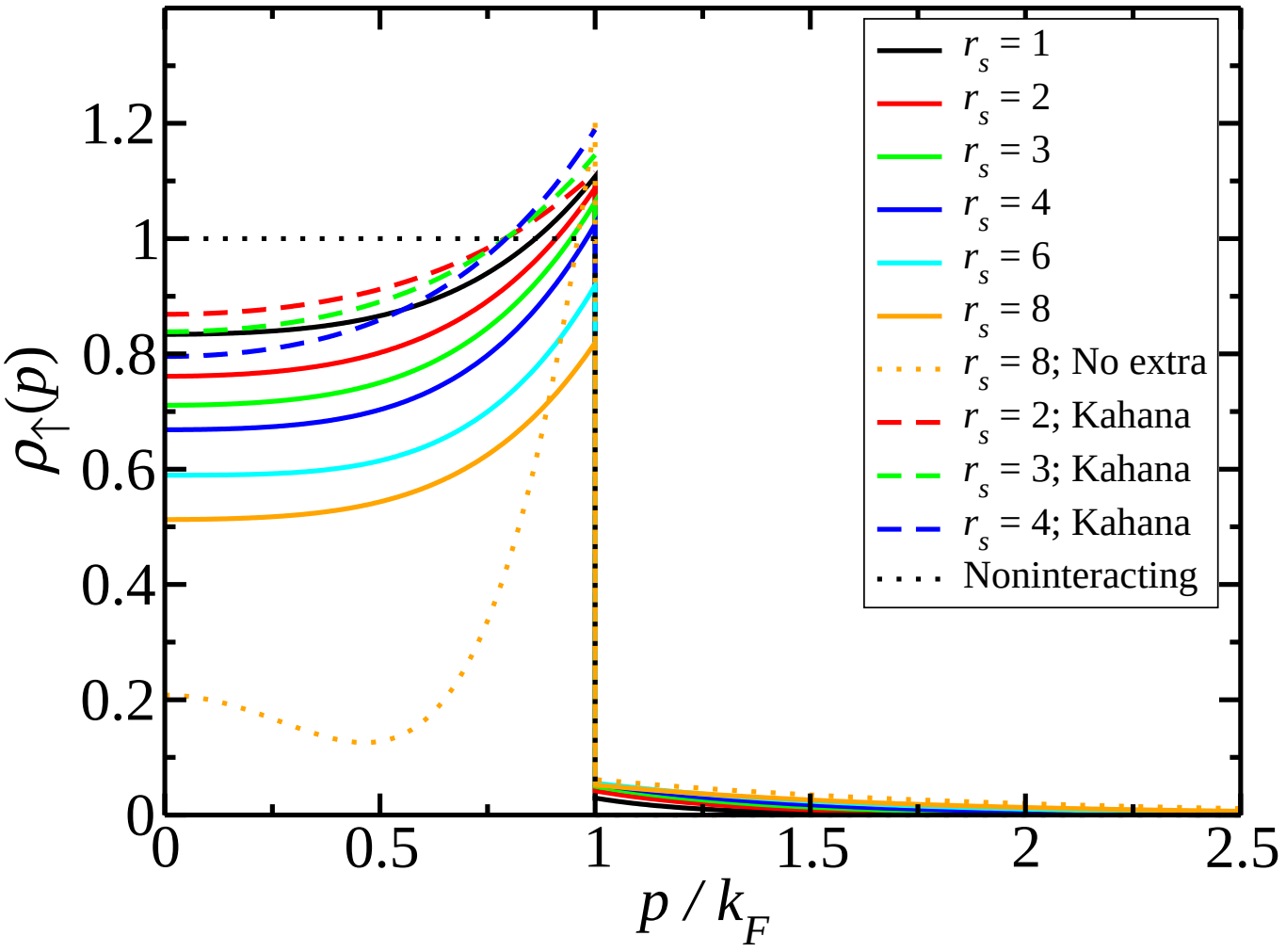


Results (II): Annihilating-Pair Momentum Density



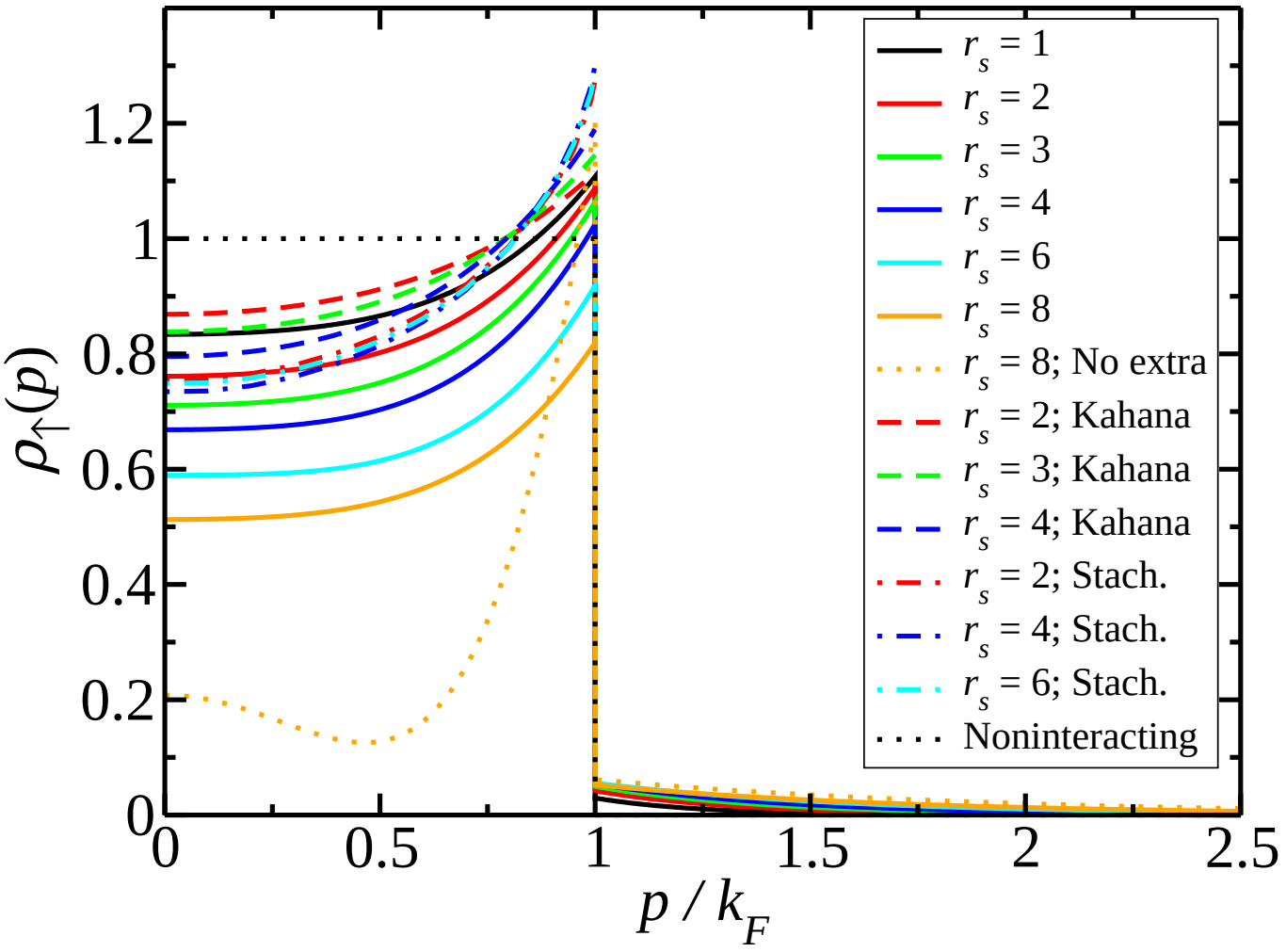
- *The extra interaction is clearly needed when calculating the MD.*

Results (II): Annihilating-Pair Momentum Density



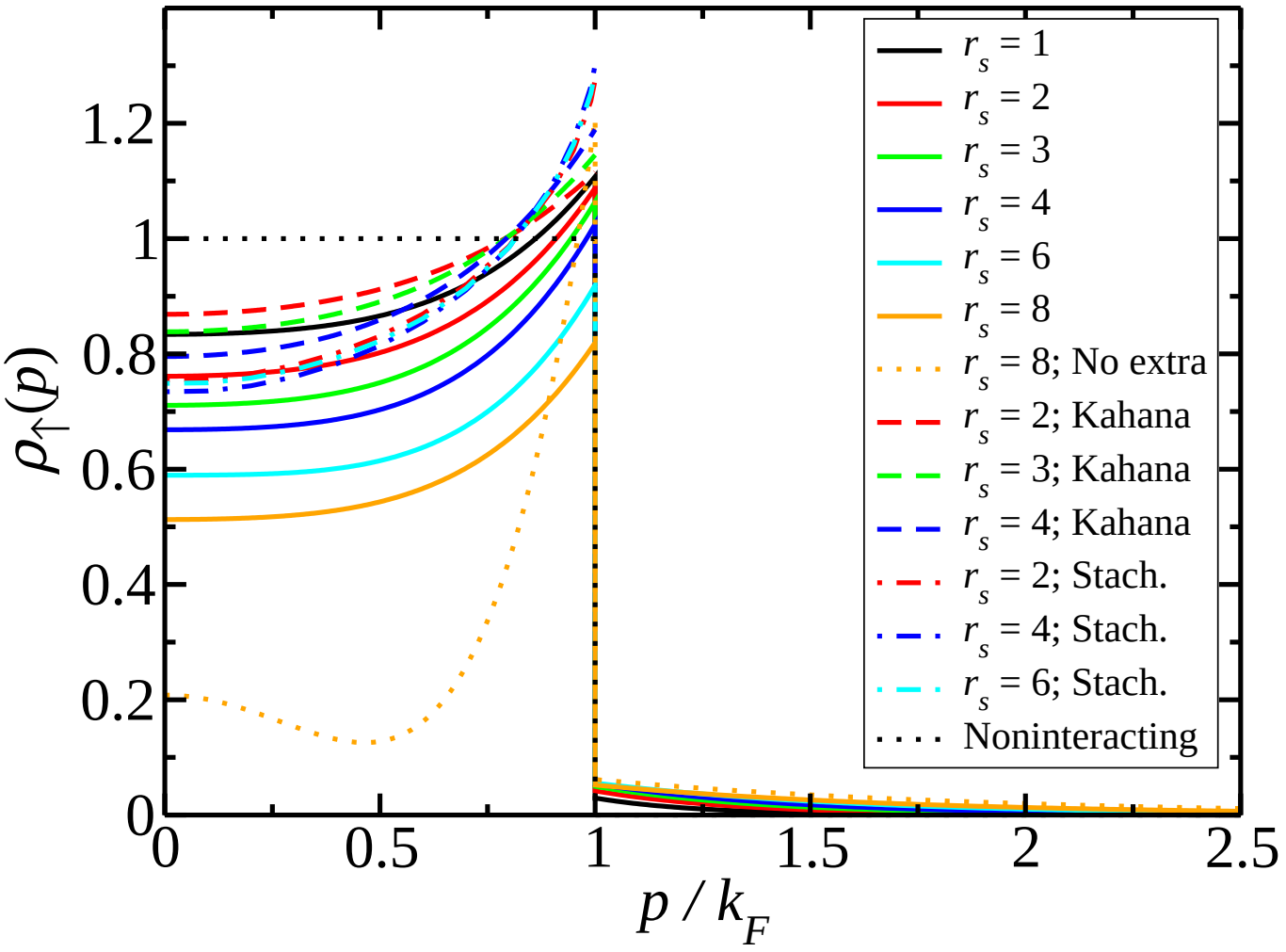
- *The extra interaction is clearly needed when calculating the MD.*

Results (II): Annihilating-Pair Momentum Density



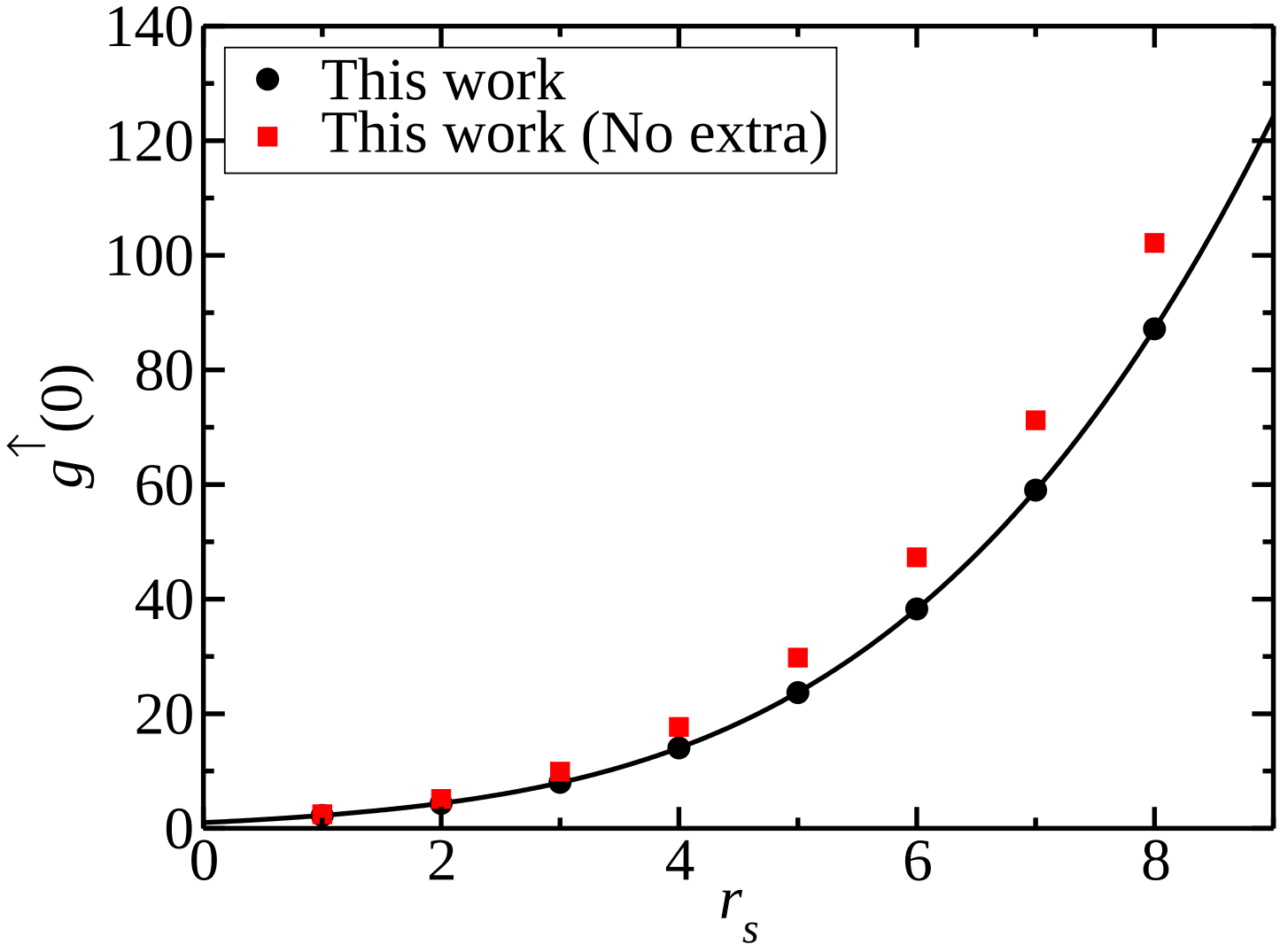
- *The extra interaction is clearly needed when calculating the MD.*

Results (II): Annihilating-Pair Momentum Density

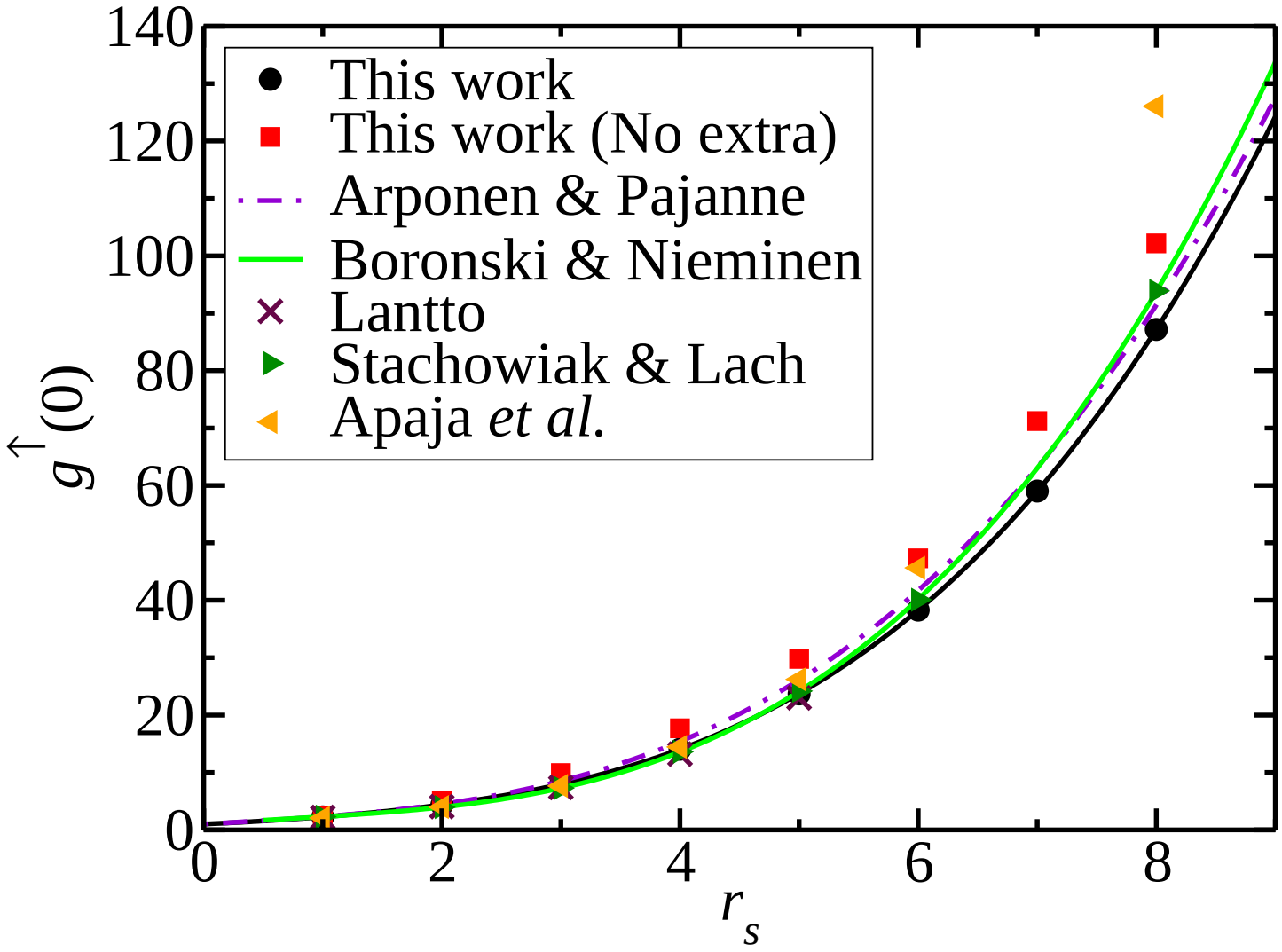


- *The extra interaction is clearly needed when calculating the MD.*
- *Previous results (i) lack the post-edge tail; (ii) disagree with each other and with me.*

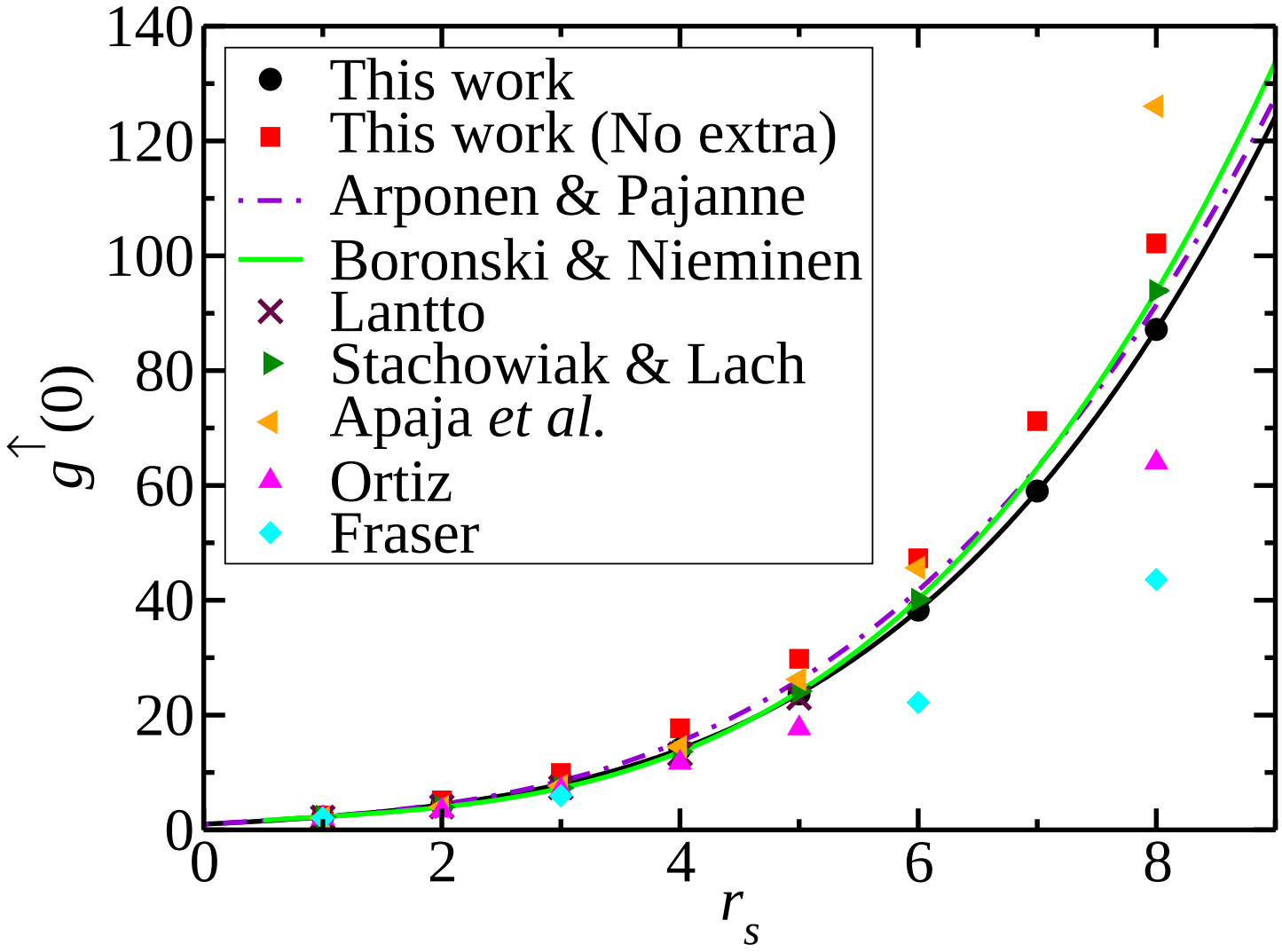
Results (III): Contact-Density Enhancement Factor



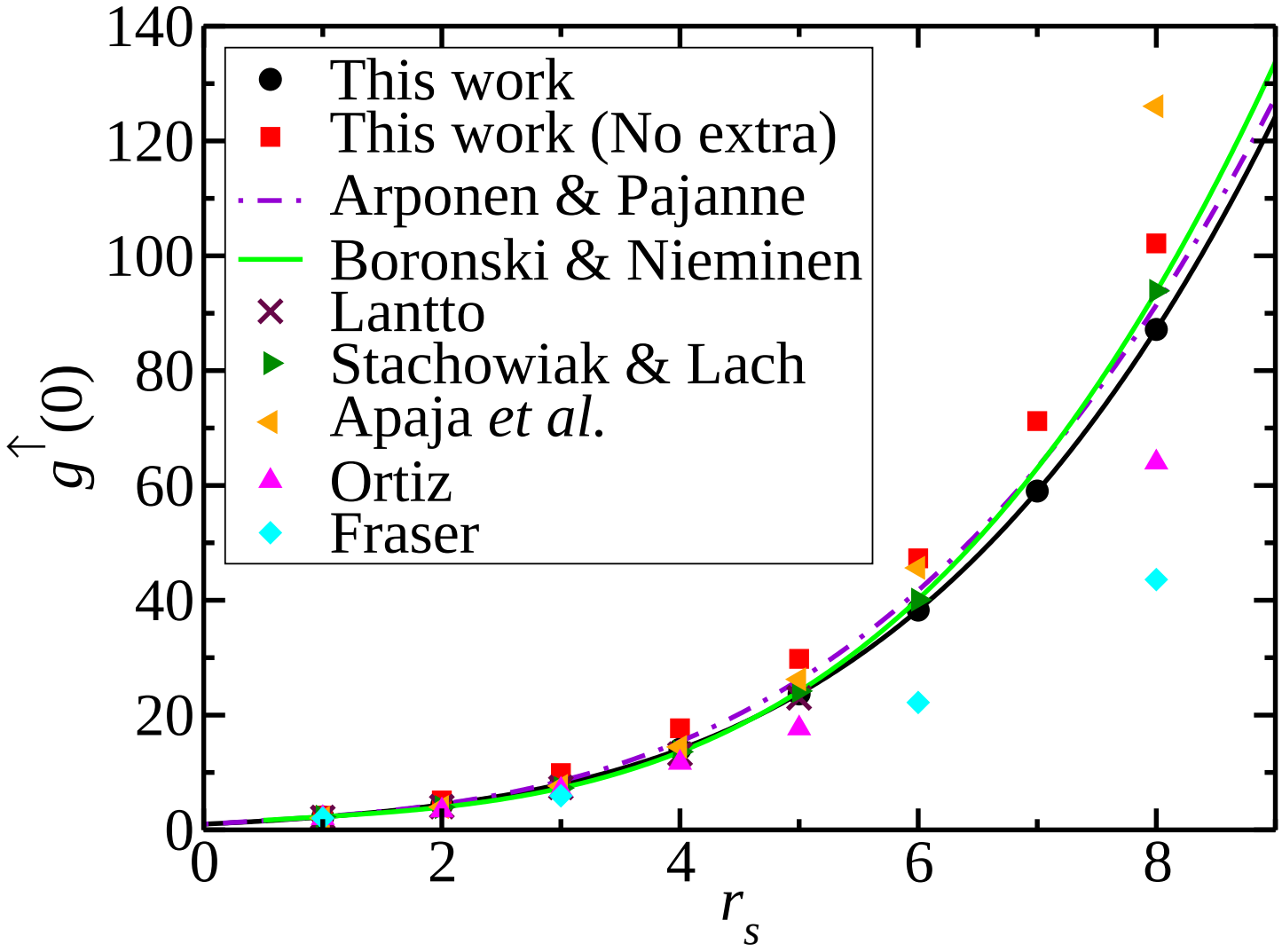
Results (III): Contact-Density Enhancement Factor



Results (III): Contact-Density Enhancement Factor



Results (III): Contact-Density Enhancement Factor



- *My results are in reasonable agreement with Arponen and Pajanne.*

Quantum Monte Carlo Studies of Positrons in Electron Gases

Previous QMC studies of positrons in HEGs have used plane-wave orbitals for both the electrons and the positron.

But at low densities the positron binds with a single electron to form a positronium atom. *Plane-wave orbitals are therefore completely inappropriate at low density.*

But pCASTEP can now be used to generate pairing orbitals for use in QMC and it has no difficulty describing positronium.

QMC will provide definitive data for the behaviour of positrons in electron gases.

This will pave the way for DFT studies of positrons in real materials, which in turn will extend our ability to interpret the results of positron-annihilation experiments.

A General Approach for Studying Quantum Impurity Problems

The methodology described here can be applied straightforwardly to many other impurity situations, such as **muons** in electron gases or **Mahan excitons** (single holes immersed in electron gases or *vice versa*[7]).

As far as the calculations are concerned, the only difference from the positron-in-HEG problem is that the impurity mass is not equal to 1 a.u.

I plan to study Mahan excitons (with isotropic masses) in the near future.

More generally, the approach can be used to study any single quantum impurity immersed in a homogeneous fluid of host particles, provided a suitable mean-field description of the host is available and the form of the impurity–host interaction is known.

For example, one could use the approach to study an impurity **atom** in a Bose–Einstein condensate of ultracold **atoms**, using the Gross–Pitaevskii equation[8] to describe the behaviour of the condensate.

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[7] G. D. Mahan, Phys. Rev. **153**, 882 (1966).

[8] E. P. Gross, Nuovo Cimento **20**, 454 (1961); L. P. Pitaevskii, Sov. Phys. JETP **13**, 451 (1961).

Acknowledgements

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Jesus College
University of Cambridge