# Quantum Monte Carlo Calculation of the Fermi Liquid Parameters of the 2D Homogeneous Electron Gas

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# Two-Dimensional Homogeneous Electron Gas

- 2D homogeneous electron gas (HEG): set of electrons moving in 2D in a uniform, inert, neutralising background. *Archetypal 2D metallic system.*

- Hamiltonian (for finite system):

$$\hat{H} = \sum_i -\frac{1}{2}\nabla_i^2 + \sum_{j>i} v_E(\mathbf{r}_{ij}) + \frac{N v_M}{2}.$$

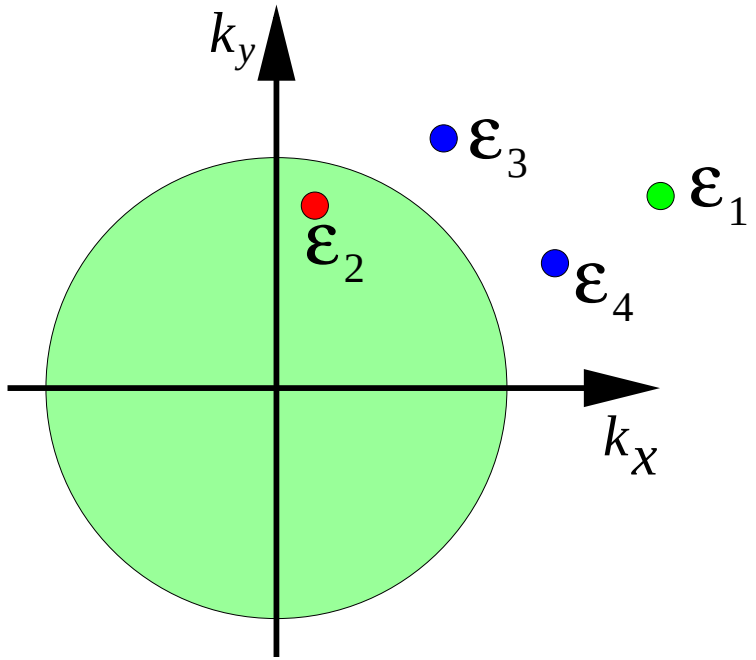
  Infinite-system ground-state energy per particle depends only on the **density** (specified by radius $r_s$ of circle containing one electron on average) and **spin polarisation** [$\zeta = (N_\uparrow - N_\downarrow)/N$].

- Physical realisations:
  - *Electrons on metal surfaces.* E.g. Cu [111].
  - *Electrons on droplets of liquid He.* Held in place by image charges.
  - *Inversion layers in MOS devices.* Can easily tune density. Electrons far from dopants; fewer complications due to disorder; technologically important.

# Fermi Liquid Theory

- Fermi liquid theory[1]: *low-energy excitations in a fluid of interacting electrons can be treated as excitations of* quasiparticles *occupying plane-wave states.*

- Justification: Pauli exclusion principle. Scattering rate of quasiparticles between plane waves is low (vanishes at Fermi surface). Single-particle momenta are approximately good quantum numbers.




[1] L. D. Landau, JETP **3**, 920 (1957); L. D. Landau, JETP **5**, 101 (1957); L. D. Landau, JETP **8**, 70 (1959).

# Landau Energy Functional

- Total energy $E$:

$$E = E_0 + \sum_{\mathbf{k},\sigma} \mathcal{E}_\sigma(\mathbf{k}) \delta N_{\mathbf{k},\sigma} + \frac{1}{2} \sum_{\mathbf{k},\sigma} \sum_{\mathbf{k}',\sigma'} f_{\sigma\sigma'}(\mathbf{k},\mathbf{k}') \delta N_{\mathbf{k},\sigma} \delta N_{\mathbf{k}',\sigma'},$$

  where $E_0$ is the ground-state energy and $\delta N_{\mathbf{k},\sigma}$ is the change in quasiparticle occupancy relative to the ground state.

- Quasiparticle energy band: $\mathcal{E}_\sigma(\mathbf{k})$ is the energy of an isolated quasiparticle.
  - Linear approximation: near the Fermi surface, $\mathcal{E}_\sigma(\mathbf{k}) = \mathcal{E}_F + (k_F/m^*)(k - k_F)$, where $\mathcal{E}_F$ is the Fermi energy and $m^*$ is the quasiparticle effective mass.

- Landau interaction function: $f_{\sigma\sigma'}(\mathbf{k},\mathbf{k}')$ describes quasiparticle interactions.
  - Near the Fermi surface, $f_{\sigma\sigma'}$ only depends on the angle $\theta_{\mathbf{k}\mathbf{k}'}$ between $\mathbf{k}$ and $\mathbf{k}'$.

# Quasiparticle Effective Mass of the 2D HEG

- The effective mass ($m^*$) of a paramagnetic 2D HEG has been the subject of great controversy in recent years:
  - Some experiments[2] found a large enhancement of $m^*$ at low density; other experiments[3] have contradicted this.
  - $GW$ calculations give a range of possible results depending on the choice of effective interaction.[4]
  - Previous QMC studies have predicted (i) much less[5] and (ii) much more[6] enhancement of $m^*$ than found in recent experiments.

- Experiment[3] and theory[7] suggest that $m^*$ in paramagnetic and ferromagnetic HEGs behaves quite differently as a function of density.

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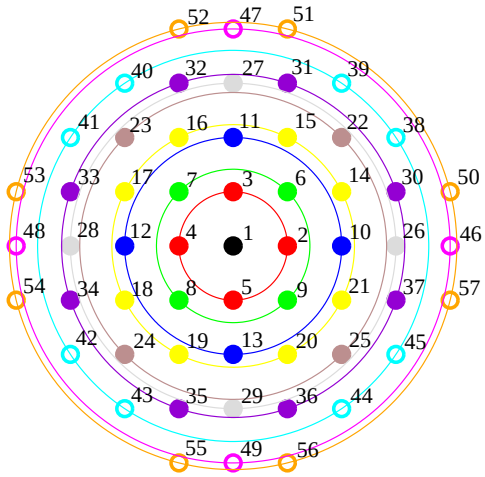
[2] J. L. Smith and P. J. Stiles, Phys. Rev. Lett. **29**, 102 (1972); V. M. Pudalov *et al.*, Phys. Rev. Lett. **88**, 196404 (2002).
[3] Y.-W. Tan *et al.*, Phys. Rev. Lett. **94**, 016405 (2005); M. Padmanabhan *et al.*, Phys. Rev. Lett. **101**, 026402 (2008).
[4] G. F. Giuliani and G. Vignale, *Quantum Theory of the Electron Liquid*, CUP, Cambridge (2005).
[5] Y. Kwon, D. M. Ceperley, and R. M. Martin, Phys. Rev. B **50**, 1684 (1994).
[6] M. Holzmann, B. Bernu, V. Olevano and D. M. Ceperley, Phys. Rev. B **79**, 041308(R) (2009).
[7] Y. Zhang and S. Das Sarma, Phys. Rev. Lett. **95**, 256603 (2005).

# Calculating the Effective Mass and Landau Interaction Functions

- To calculate the quasiparticle effective mass:
  - The DMC energy band $\mathcal{E}(k)$ was determined at a range of $k$ by taking the energy difference when an electron is added to or removed from a closed-shell ground-state.
  - A quadratic $\mathcal{E}(k) = \alpha_0 + \alpha_2 k^2 + \alpha_4 k^4$ was fitted to the energy band values.
  - The effective mass was then calculated as $m^* = k_F/(d\mathcal{E}/dk)_{k_F}$.

- To calculate the Landau interaction functions and hence Fermi liquid parameters:
  - Electrons were promoted from $(\sigma, \mathbf{k})$ just below the Fermi edge to $(\sigma', \mathbf{k}')$ just above it, to obtain the energy difference $\Delta E_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}')$ relative to the ground state.
  - The single-particle contribution was subtracted from the excitation energy, to give $-f_{\sigma\sigma'}(\theta_{\mathbf{k}\mathbf{k}'}) = \Delta E_{\sigma\sigma'}(\mathbf{k}, \mathbf{k}') - [\mathcal{E}(\mathbf{k}') - \mathcal{E}(\mathbf{k})]$.
  - The first few Fourier components of $f_{\sigma\sigma'}(\theta)$ were found by numerical integration in order to obtain the *Fermi liquid parameters*.



# Fermi Liquid Parameters

- Fermi liquid parameters:

$$F_l^{s,a} = \frac{Am^*}{4\pi^2} \int \left[ f_{\uparrow\uparrow}(\theta_{\mathbf{kk}'}) \pm f_{\uparrow\downarrow}(\theta_{\mathbf{kk}'}) \right] \cos(l\theta)\, d\theta,$$

  where $A = \pi r_s^2 N$ is the area of the simulation cell.

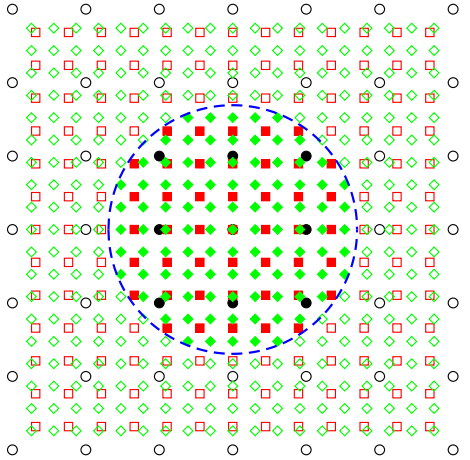
- For a ferromagnetic HEG, the Fermi liquid parameters $\{F_l\}$ are given by the expression above with $f_{\uparrow\downarrow} = 0$.

- *We need to obtain a description of the interaction parameters according to a well-defined prescription for energy differences in a finite cell, then extrapolate the Fermi liquid parameters to the thermodynamic limit.*

- Armed with the effective mass and the Fermi liquid parameters, nearly all thermodynamic and transport properties of the fully interacting electron gas can be calculated.

# Finite-Size Errors

- The calculations were performed in finite cells subject to periodic boundary conditions.
- Major source of error and uncertainty in the QMC results: finite size effects.
- Momentum quantisation:
  - In our finite simulation cell subject to (twisted) periodic boundary conditions, the available momentum states fall on the (offset) grid of reciprocal lattice points.
  - This restricts the $\mathbf{k}$ values we can consider.

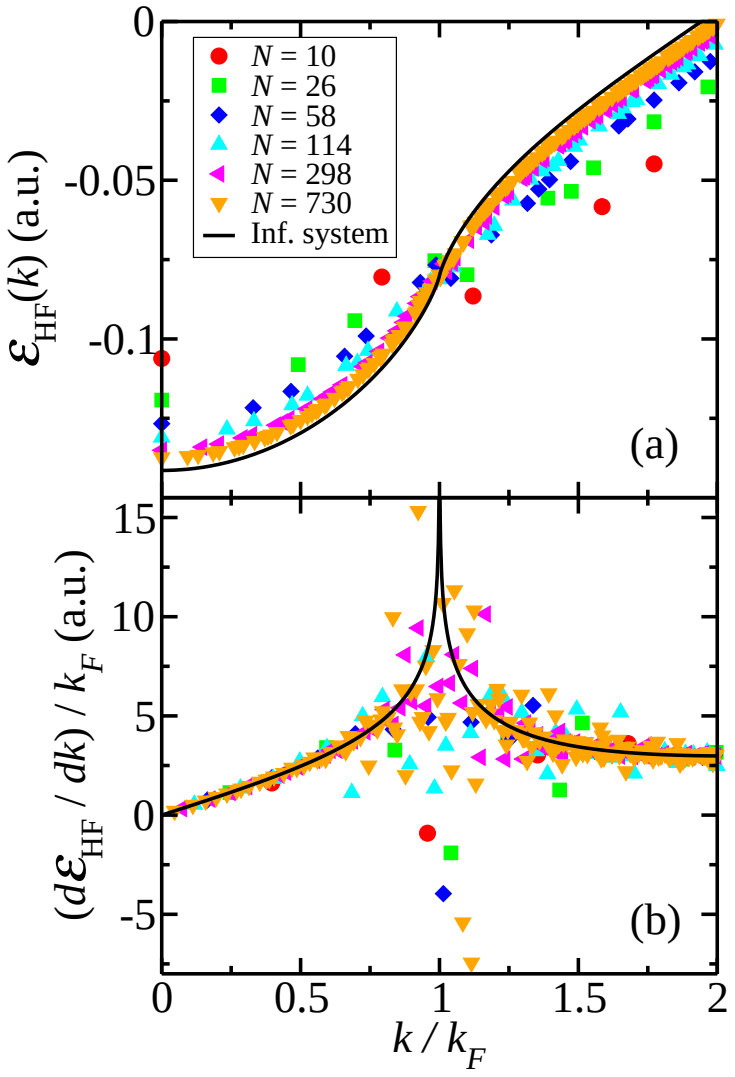


- There are also finite size errors in the excitation energies due to the neglect of long-range interactions and correlations in a finite cell.
  - These errors have been shown to fall off slowly, as $N^{-1/4}$, near the Fermi surface.[8]
  - We use this scaling to extrapolate the Fermi liquid parameters to the thermodynamic limit. The extrapolation process is quite error-prone, however.

[8] M. Holzmann, B. Bernu, V. Olevano and D. M. Ceperley, Phys. Rev. B **79**, 041308(R) (2009).

# Pathological Behaviour at the Fermi Surface (I)

- Fermi liquid theory is only valid near the Fermi surface.
- Energy band is defined by Landau energy functional at all $\mathbf{k}$, but does not correspond to quasiparticle band except near Fermi surface.
- In the infinite-system limit, the exact energy band is smooth and well-behaved everywhere, including the Fermi surface.
- The Hartree–Fock band is pathological.
  - In the infinite-system limit it has a logarithmic divergence at the Fermi surface.
  - In finite systems it behaves very badly.



# Pathological Behaviour at the Fermi Surface (II)

- *DMC may take you 99% of the way from HF to reality, but this does not get rid of the pathological behaviour from HF theory.*

- Hence we need to consider excitations **away from the Fermi surface** in order to obtain the gradient of the energy band at $k_F$.

- Hartree–Fock theory: the Landau interaction functions are $f_{\uparrow\uparrow}(\mathbf{k},\mathbf{k}') = 2\pi/|\mathbf{k}-\mathbf{k}'|$ and $f_{\uparrow\downarrow}(\mathbf{k},\mathbf{k}') = 0$.

- There are no finite-size errors or pathological behaviour in the Hartree–Fock Landau interaction functions (although the integrals for the Fermi liquid parameters diverge).
  - Hence, unlike the energy band, there does not appear to be any reason to consider only excitations in the vicinity of the Fermi surface in DMC.

- However, correlation effects result in significant finite-size errors in the Fermi liquid parameters.[9]

[9] M. Holzmann, B. Bernu, V. Olevano and D. M. Ceperley, Phys. Rev. B **79**, 041308(R) (2009).

# Assessing the Accuracy of our DMC Calculations (I)

- Occupied bandwidth: $\Delta\mathcal{E} = \mathcal{E}(k_F) - \mathcal{E}(0) = E_-(0) - E_-(k_F)$.

- DMC BW is expected to be an upper bound: assuming DMC retrieves the same fraction of the correlation energy in the ground and excited states, the BW will lie between the Hartree-Fock value $E_-^{\rm HF}(0) - E_-^{\rm HF}(k_F)$, which is too large, and the exact result $E_-^{\rm exact}(0) - E_-^{\rm exact}(k_F)$.

- Likewise, Slater-Jastrow DMC BWs are expected to be greater than Slater-Jastrow-backflow DMC BWs.

- *To obtain an accurate BW, it is essential to retrieve a very large fraction of the correlation energy in the DMC calculations, which explains why the inclusion of backflow is so important.*

- The extent to which the BW is overestimated in HF theory grows with $r_s$ so that, assuming DMC retrieves a constant fraction of the correlation energy, the DMC bands become less accurate at low density.

# Assessing the Accuracy of our DMC Calculations (II)

- Extrapolating the VMC energy with different trial wave functions to zero variance suggests that our DMC calculations retrieve more than 99% of the correlation energy, and that the fraction retrieved is similar in both the ground and excited states.

- The free-electron BW is greater than or approximately equal to the exact BW. Hence the error in the HF BW is less than or approximately equal to $\Delta\mathcal{E}^{\rm HF} - \Delta\mathcal{E}^{\rm free} = k_F(1-2/\pi)$.

- So the error in the DMC BW is less than $0.01k_F(1-2/\pi) \approx 0.007/r_s$ for a ferromagnetic HEG and less than about $0.01k_F(1-2/\pi) \approx 0.005/r_s$ for a paramagnetic HEG.
  - Since the BW falls off as $r_s^{-2}$, the error is more significant at large $r_s$.
  - In the worst case (the paramagnetic HEG at $r_s = 10$) this argument suggests that DMC overestimates the BW by $\sim 9\%$. In the next-worse case (paramagnetic, $r_s = 5$), the BW is overestimated by $\sim 4\%$.
  - It is reasonable to assume that DMC underestimates $m^*$ by a similar amount.

# To Reoptimise or Not To Reoptimise

- We optimise the trial wave function in the ground state and then continue to use the same Jastrow factor and backflow function in our excited-state calculations.

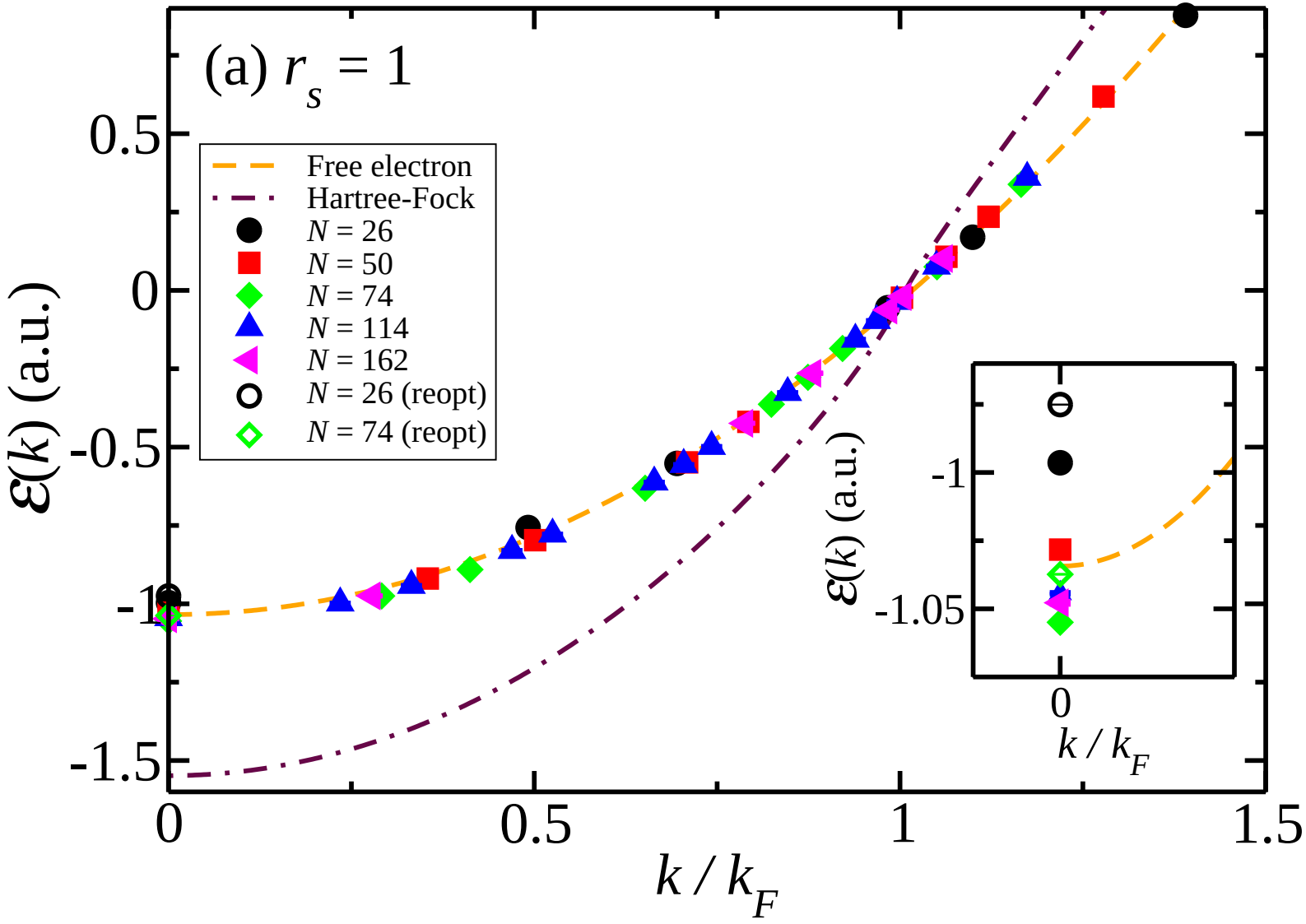
- The excitation of a single electron has no effect on the optimal Jastrow factor or backflow function in the thermodynamic limit.
  - Hence the fact that the Jastrow factor and backflow function can be re-optimised in an excited state in a finite cell[10] is simply a finite-size effect.
  - More finite-size bias is introduced into the energy band by re-optimising the Jastrow factor and backflow function in each excited state considered.

- It is essential not to re-optimise the wave function when an electron is promoted, to maximise the cancellation of errors that occurs when the single-particle contribution is subtracted out from a difference in total energy.

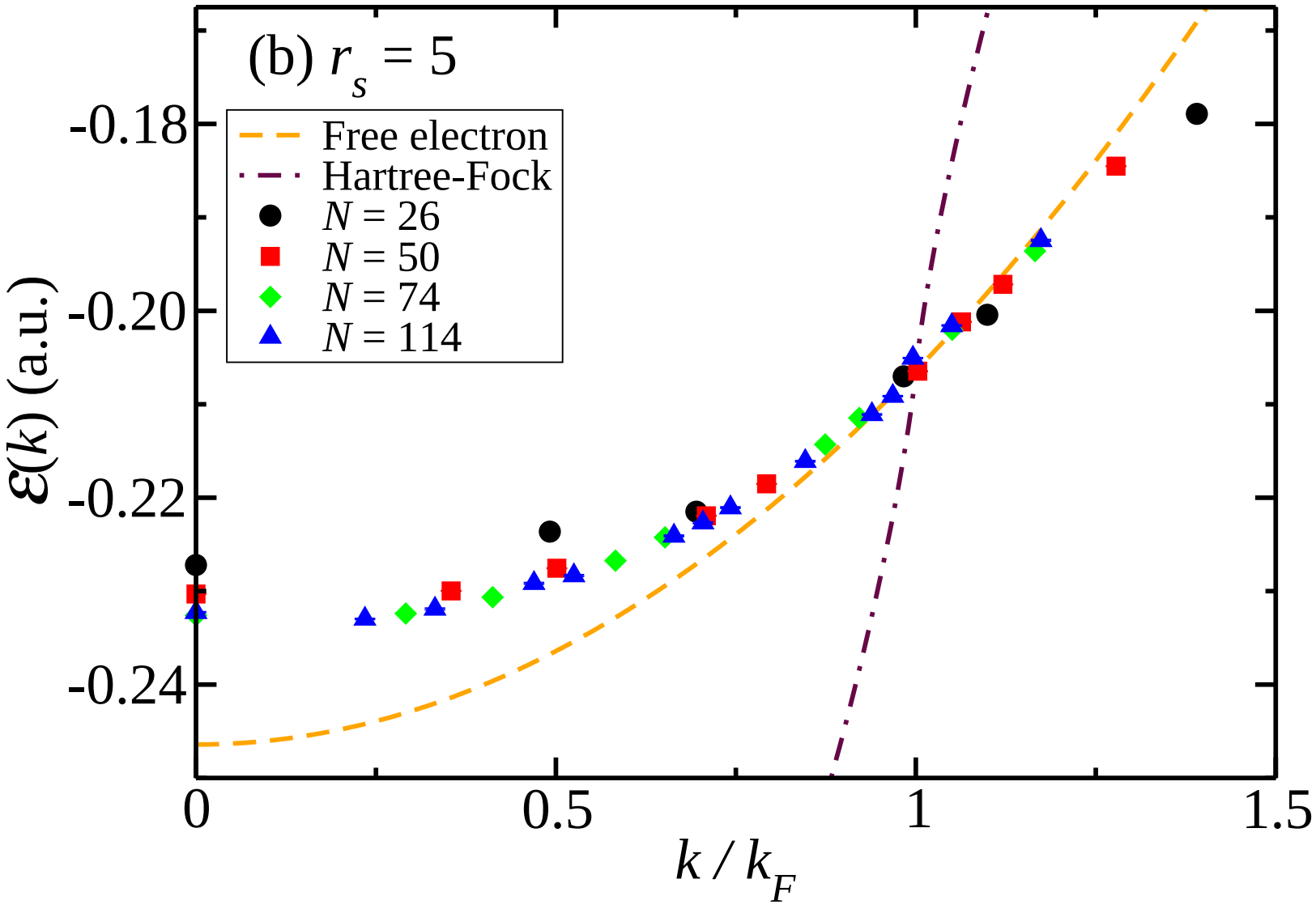
- Promoting an electron results in smaller finite-size errors than adding two electrons, since the latter modifies the density of the finite system.

[10] For example, re-optimising the wave function when an electron is subtracted from $\mathbf{k} = \mathbf{0}$ in a 74-electron HEG at $r_s = 1$ lowers the DMC energy by $0.000241(4)$ a.u.

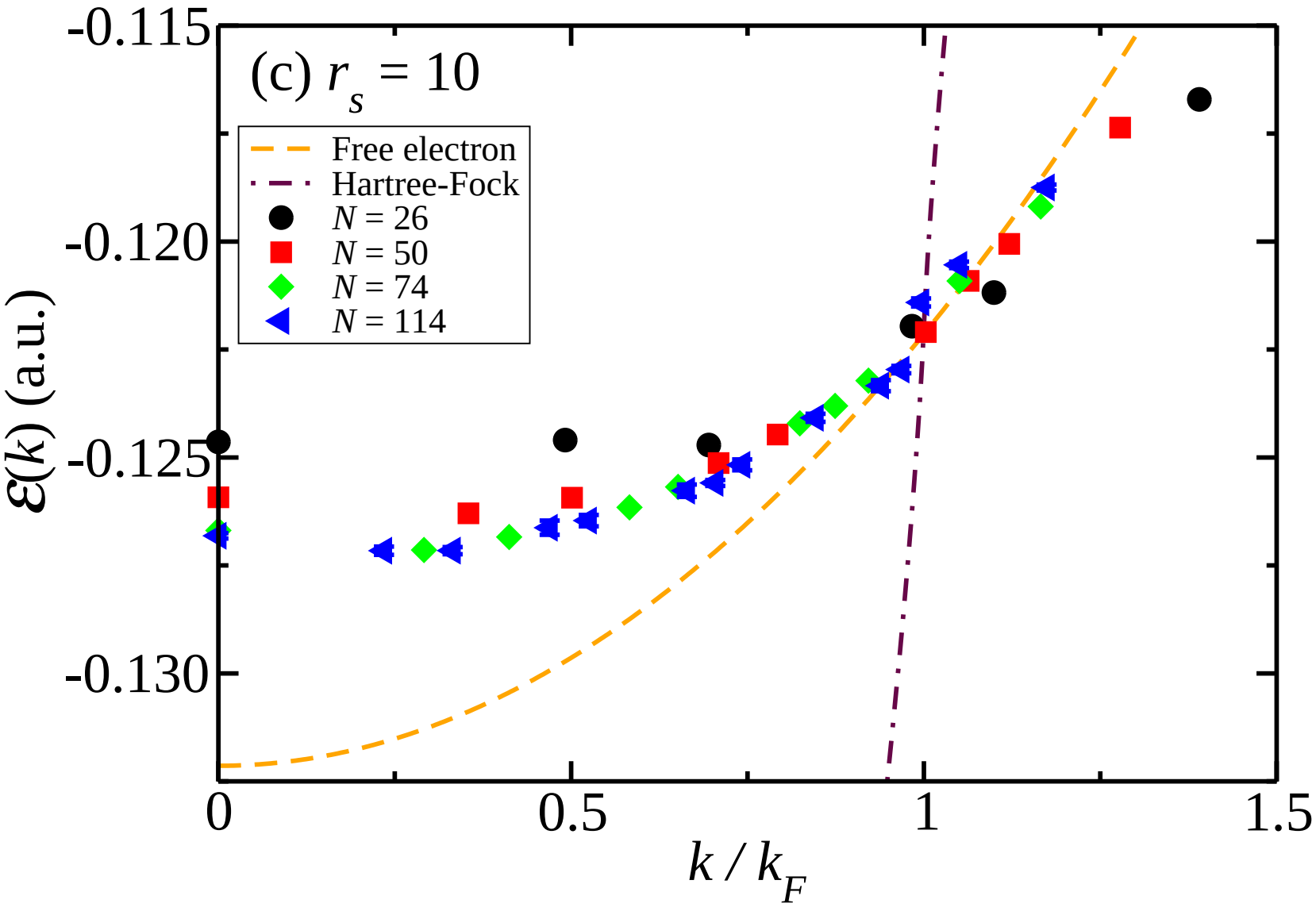
# Paramagnetic Single-Particle Energy Band: $r_s = 1$



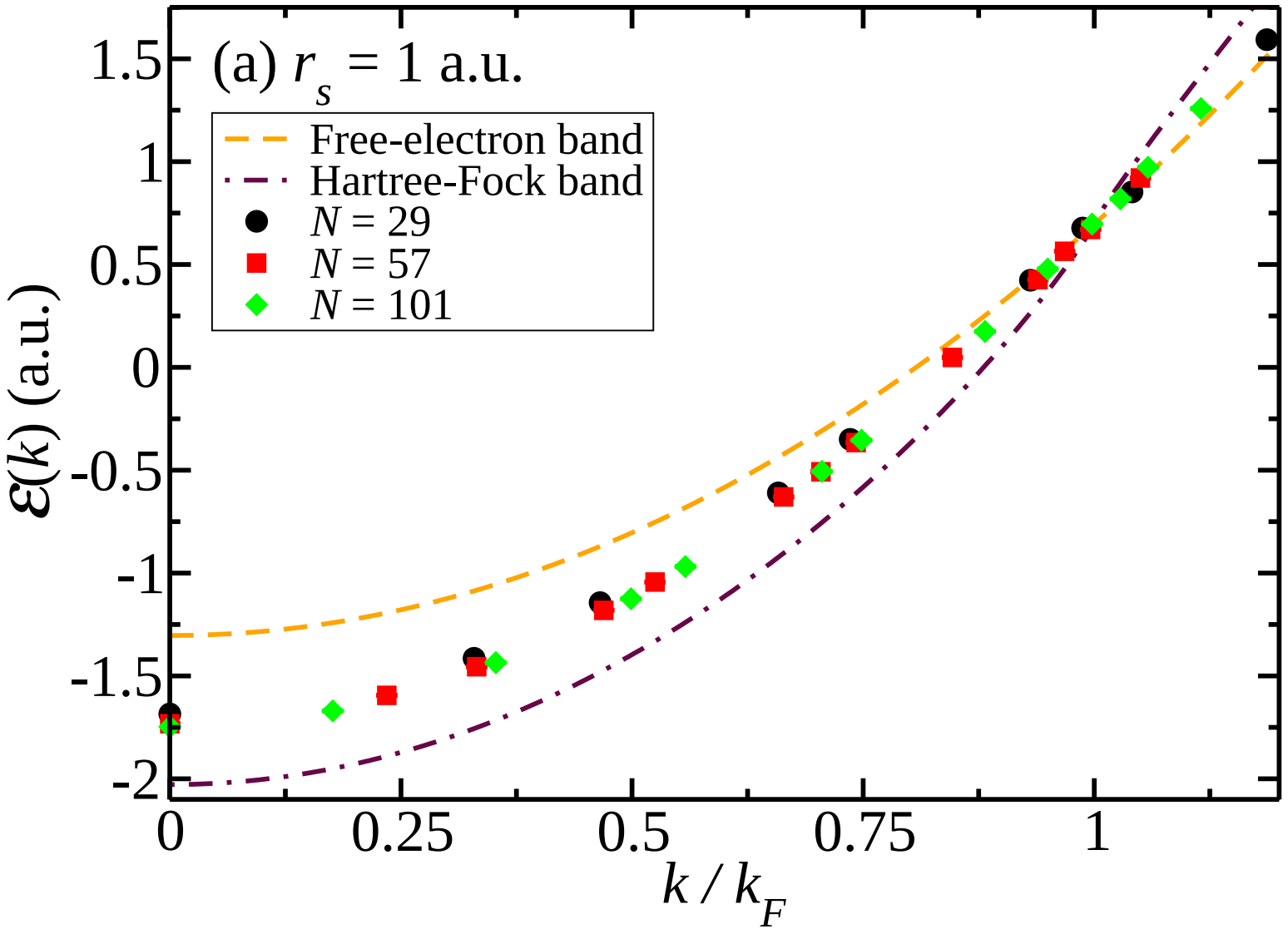
# Paramagnetic Single-Particle Energy Band: $r_s = 5$



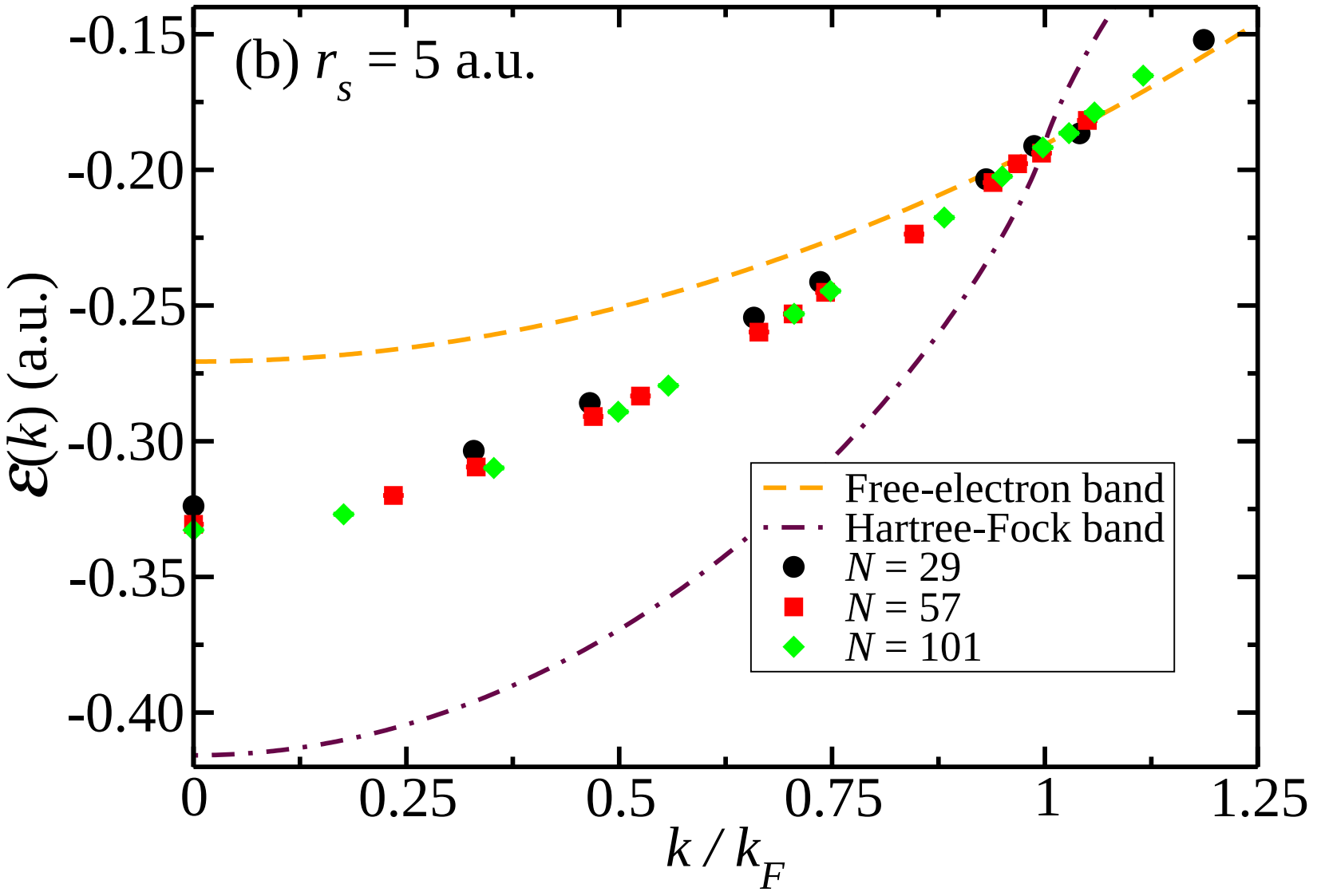
# Paramagnetic Single-Particle Energy Band: $r_s = 10$



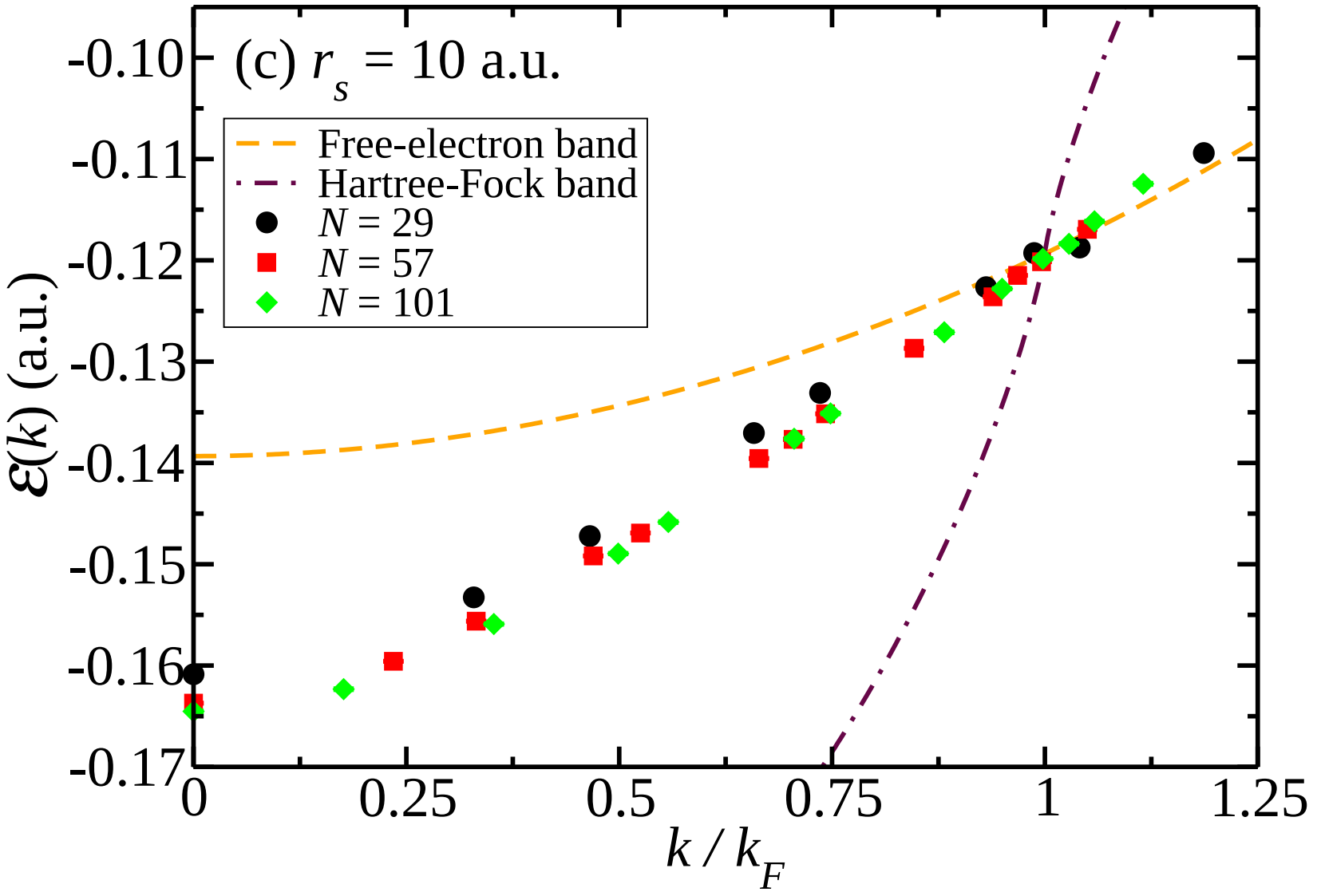
# Ferromagnetic Single-Particle Energy Band: $r_s = 1$



# Ferromagnetic Single-Particle Energy Band: $r_s = 5$

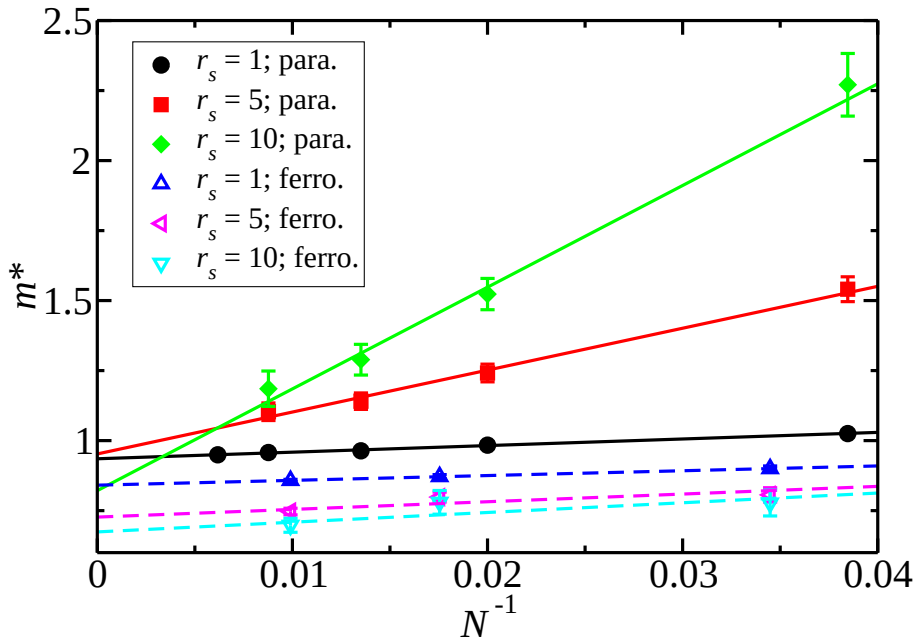


# Ferromagnetic Single-Particle Energy Band: $r_s = 10$



# Extrapolation of the Effective Mass to the Thermodynamic Limit

- Effective mass against system size:



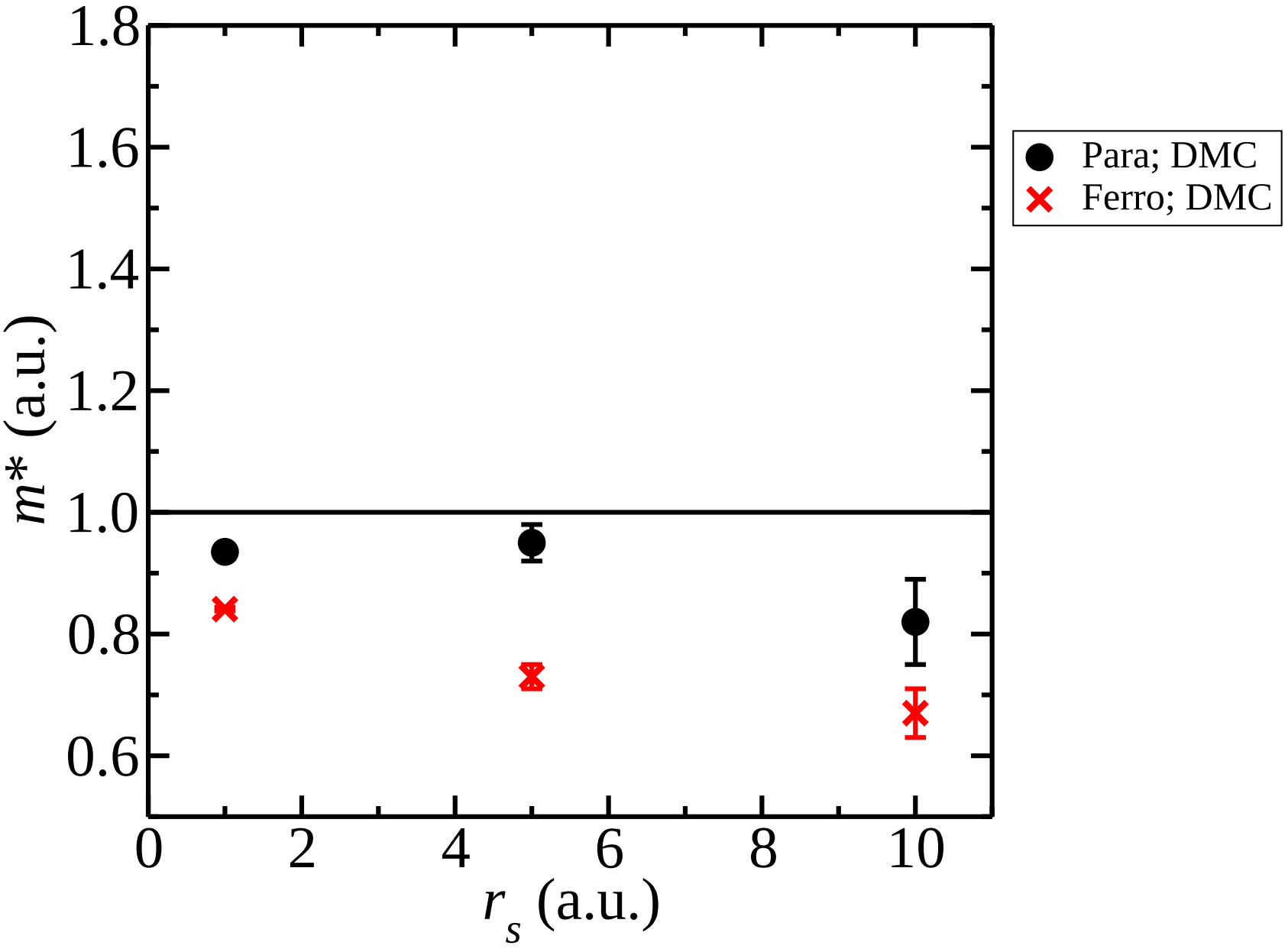

- Scaling is not the $N^{-1/4}$ predicted by Holzmann *et al.* near the Fermi surface. (Because we have fitted to the entire band.)
  - Assume an $N^{-1}$ scaling of the finite-size error.
  - To-do: fit a Padé function rather than a quartic to the energy bands.

# Quasiparticle Effective Masses (I)

- Quasiparticle effective mass results:

| Fluid phase | $r_s$ | $m^*$ (a.u.) |
|---|---|---|
| Paramagnetic | 1 | $0.935(4)$ |
| Paramagnetic | 5 | $0.95(3)$ |
| Paramagnetic | 10 | $0.82(7)$ |
| Ferromagnetic | 1 | $0.841(3)$ |
| Ferromagnetic | 5 | $0.73(2)$ |
| Ferromagnetic | 10 | $0.67(4)$ |

# Quasiparticle Effective Masses (II)

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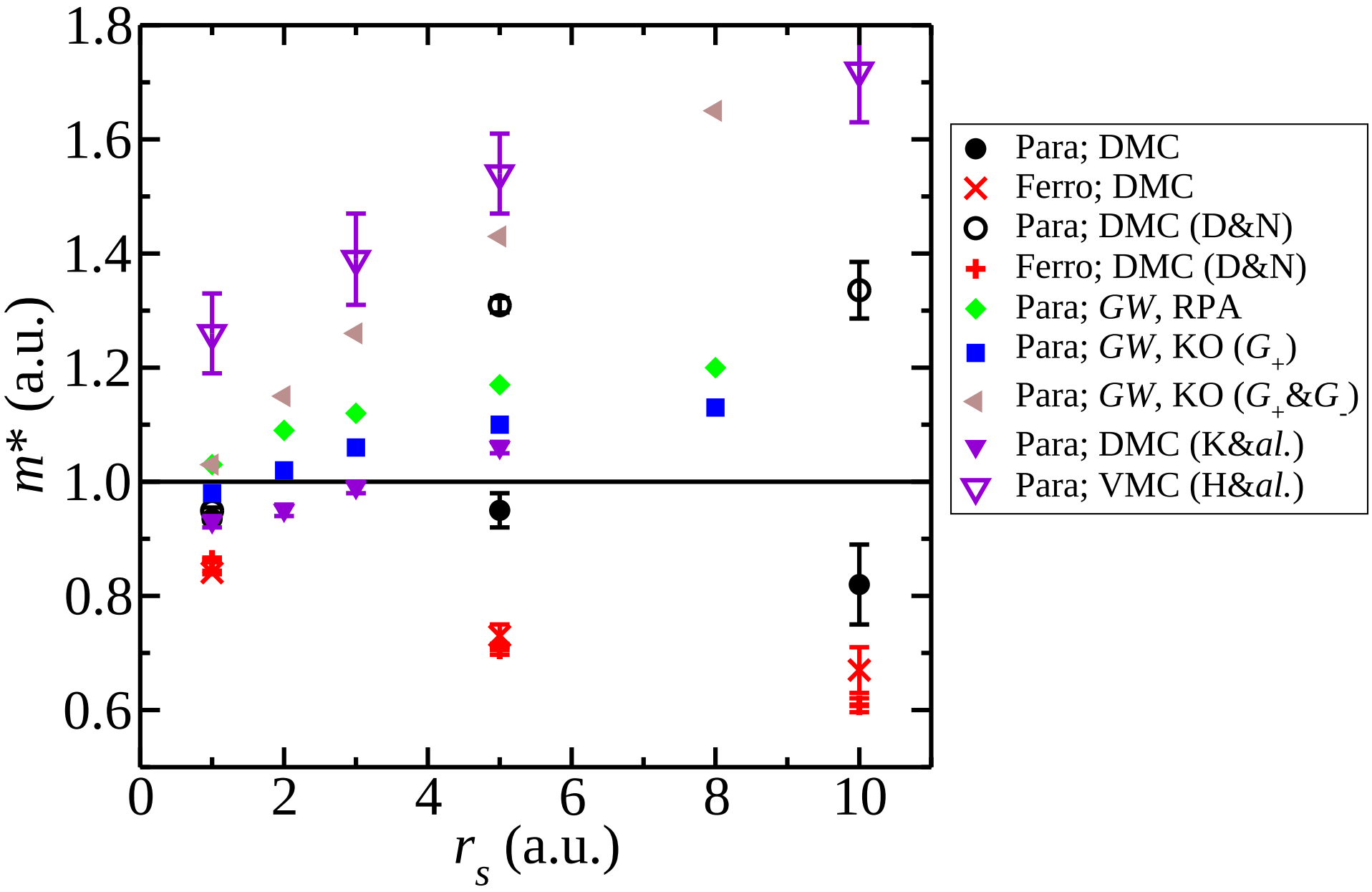
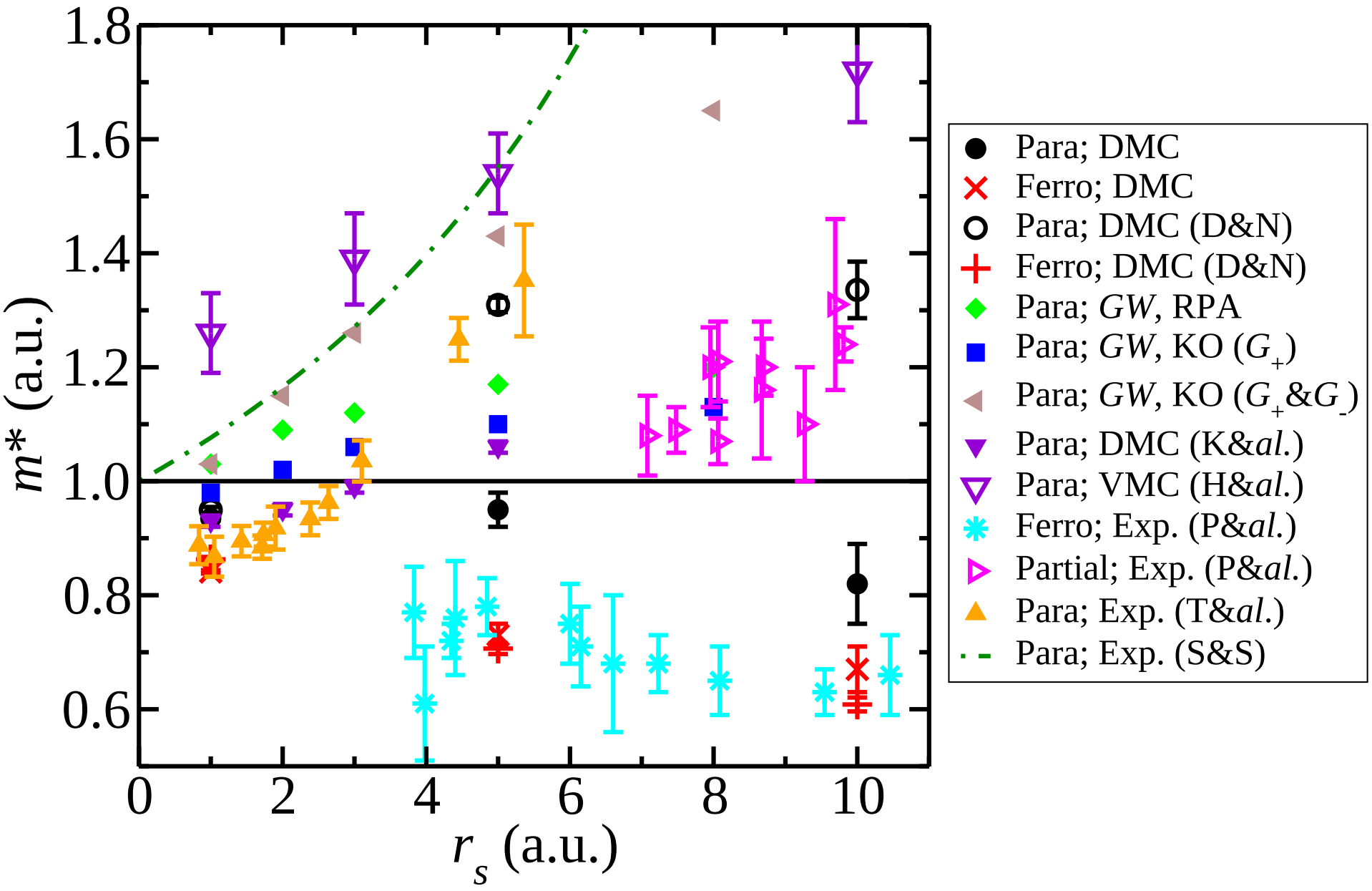
# Quasiparticle Effective Masses (II)



# Quasiparticle Effective Masses (II)

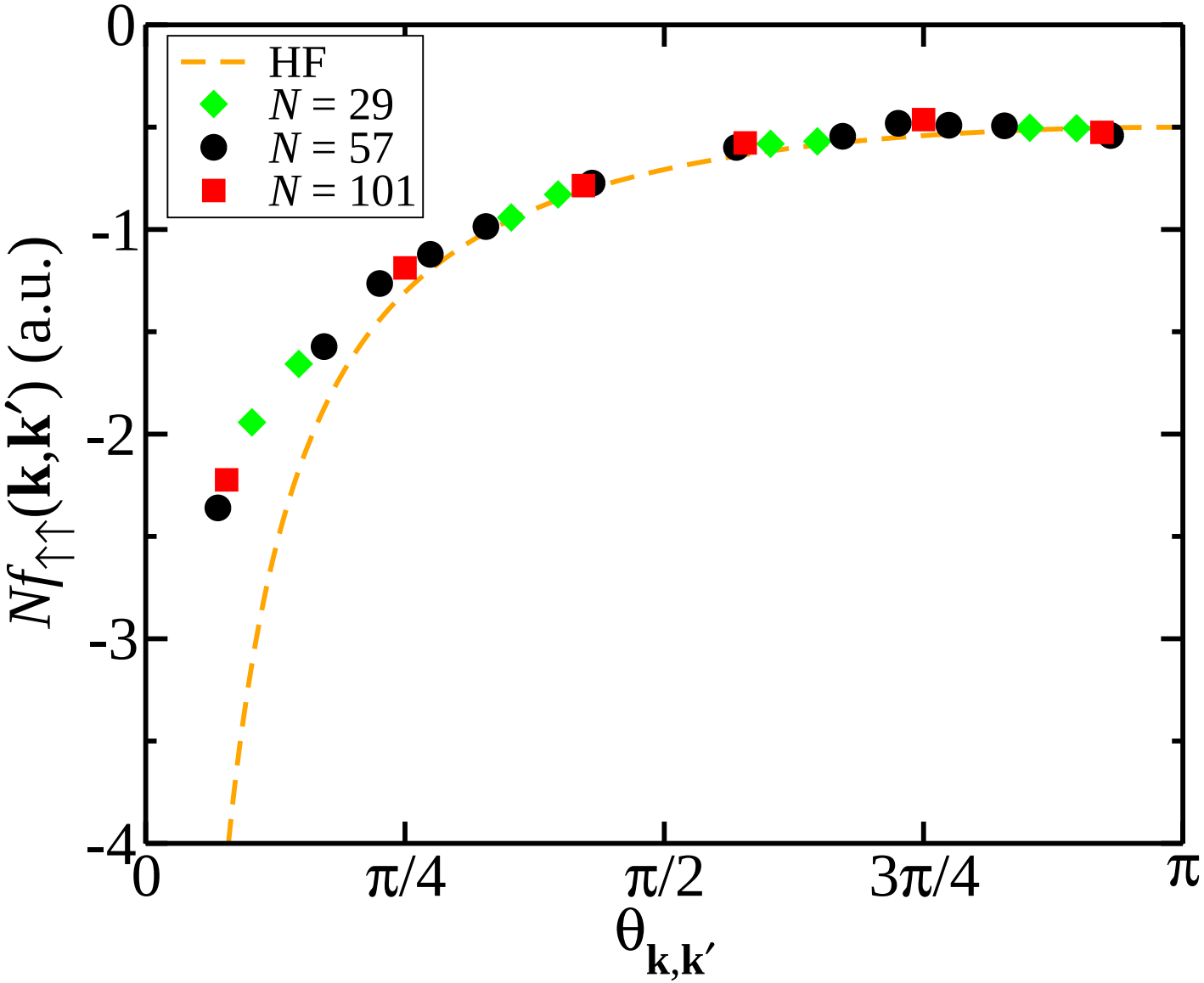


# Quasiparticle Effective Masses (III)

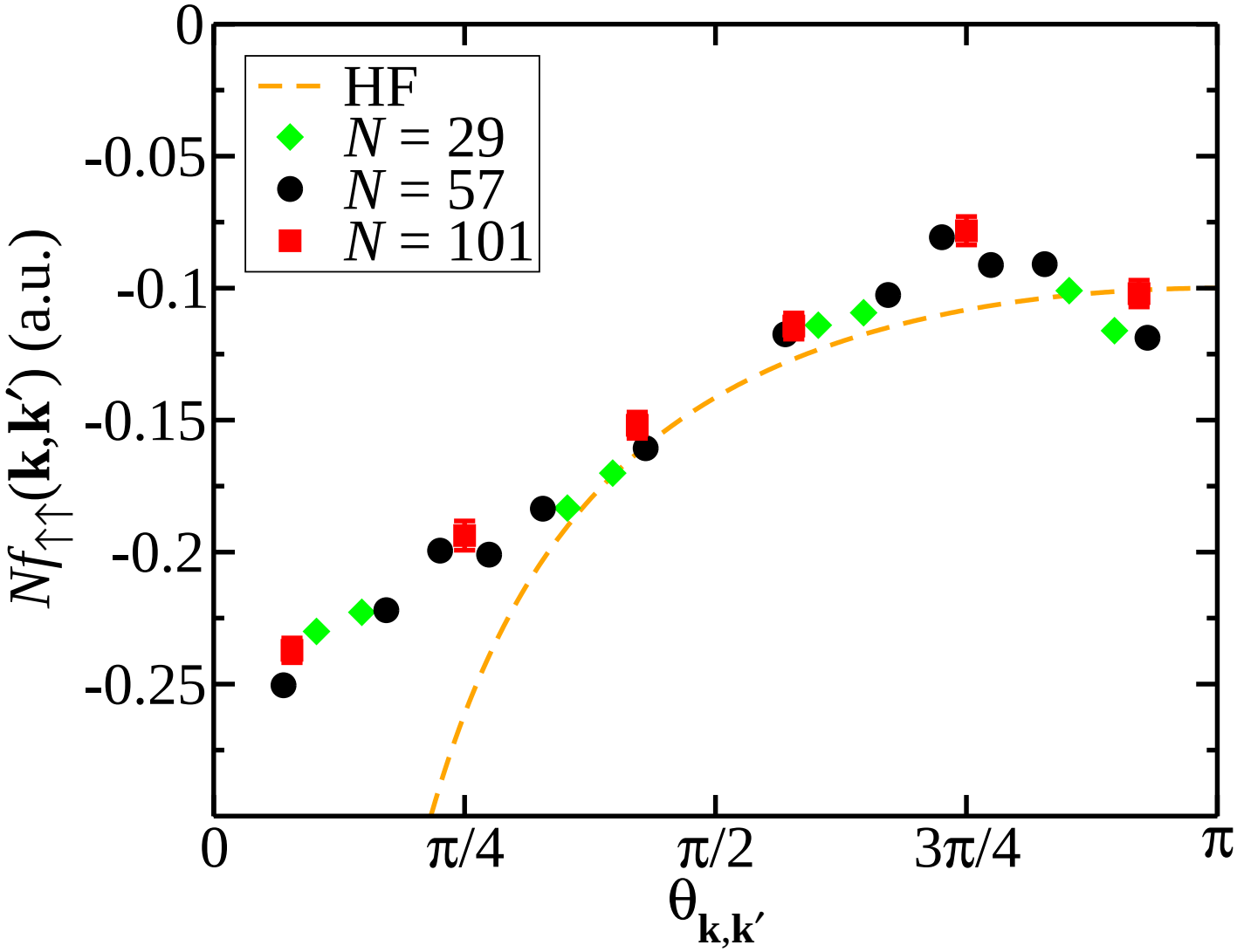
- Paramagnetic HEG: effective mass remains close to 1.
- Ferromagnetic HEG: $m^*$ *decreases* when the density is lowered.
- Our results therefore support the qualitative conclusions of Padmanabhan *et al.*
- Our results suggest that $m^*$ in paramagnetic 2D HEGs does not continue to grow rapidly when the density is reduced beyond $r_s \simeq 5$.
- Disagree with a recent VMC study.[11]
  - Different treatment of finite-size errors, but applying finite-size extrapolation scheme of Holzmann *et al.* (i) would not fit our data, (ii) would further reduce our extrapolated effective mass, moving our results further from Holzmann's, and (iii) the scheme is not necessarily appropriate because we do not just look at excitations near the Fermi surface.
  - Different level of theory: we use DMC rather than VMC.

[11] M. Holzmann, B. Bernu, V. Olevano and D. M. Ceperley, Phys. Rev. B **79**, 041308(R) (2009).

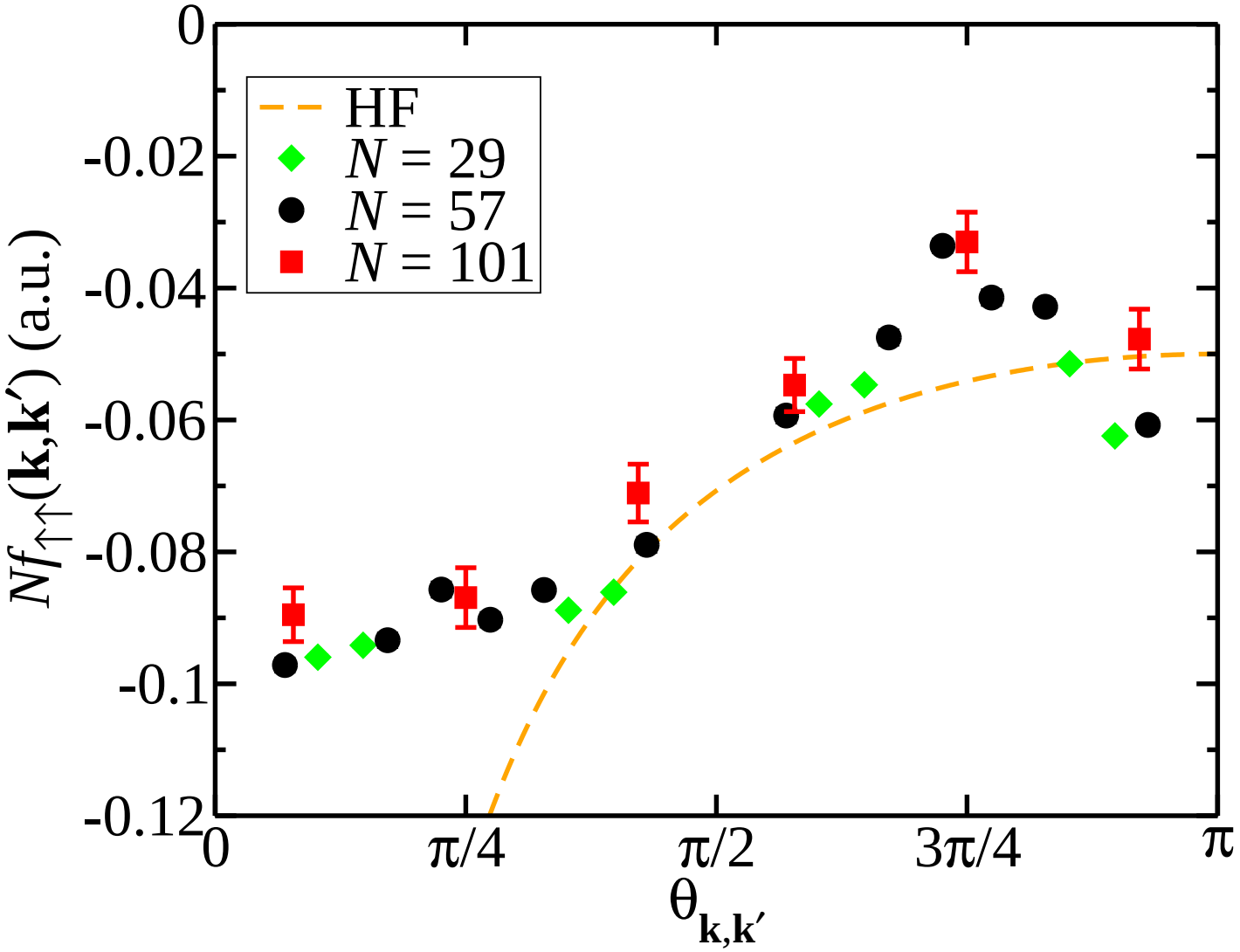
# Ferromagnetic Interaction Functions at $r_s = 1$



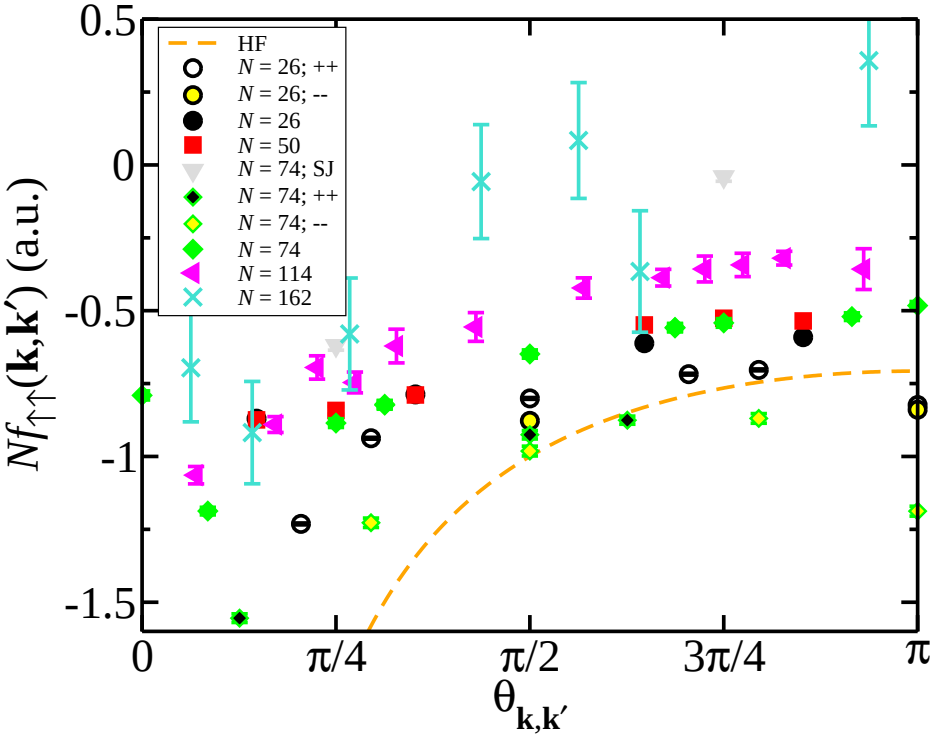
# Ferromagnetic Interaction Functions at $r_s = 5$

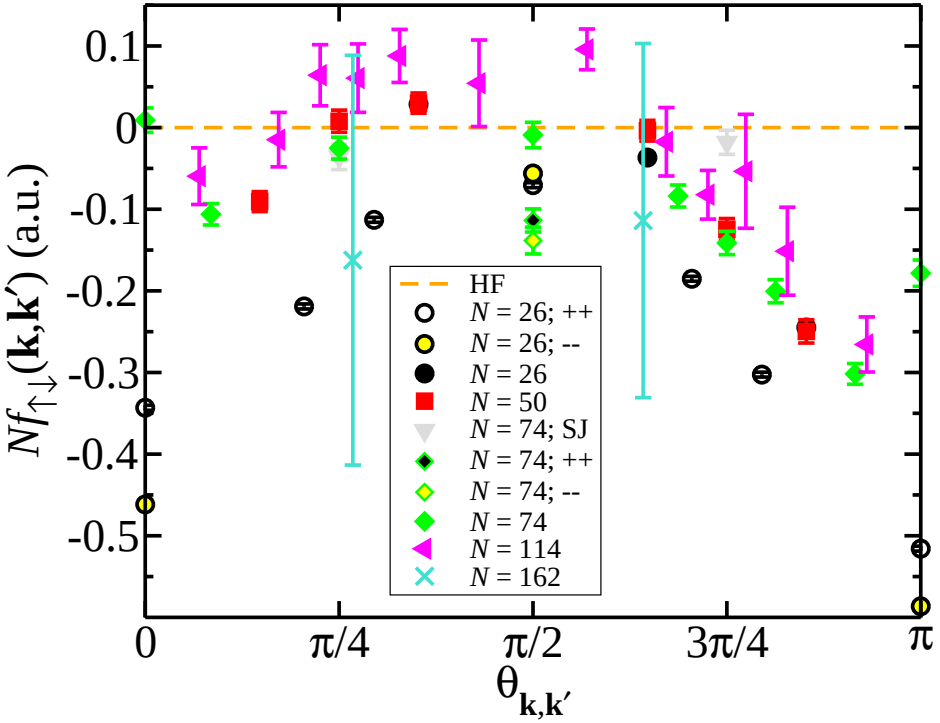


# Ferromagnetic Interaction Functions at $r_s = 10$

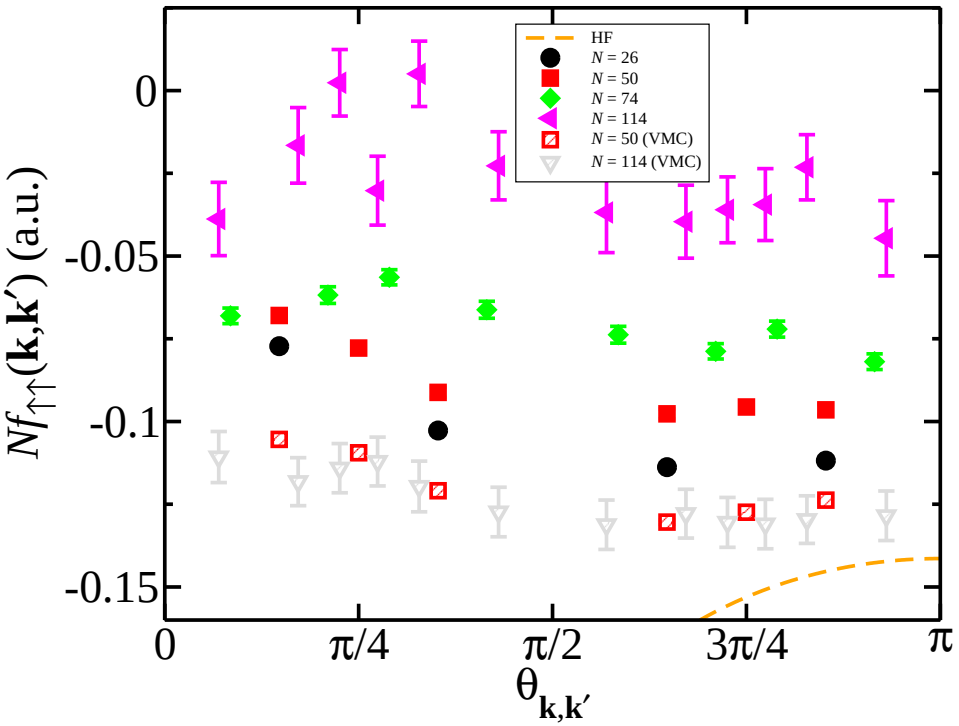


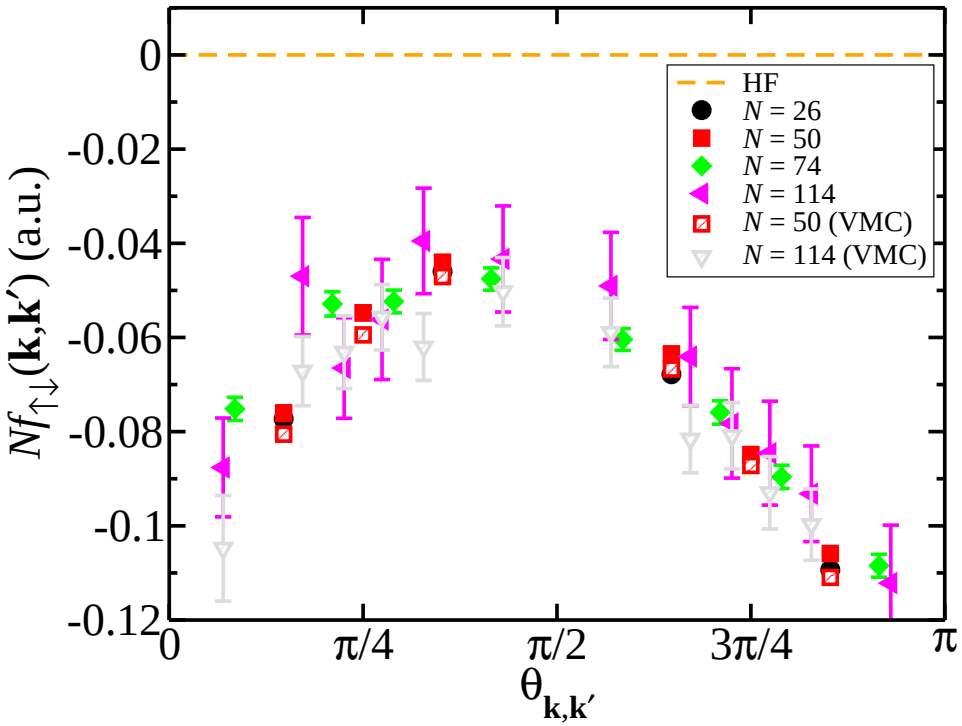
# Paramagnetic Interaction Functions at $r_s = 1$



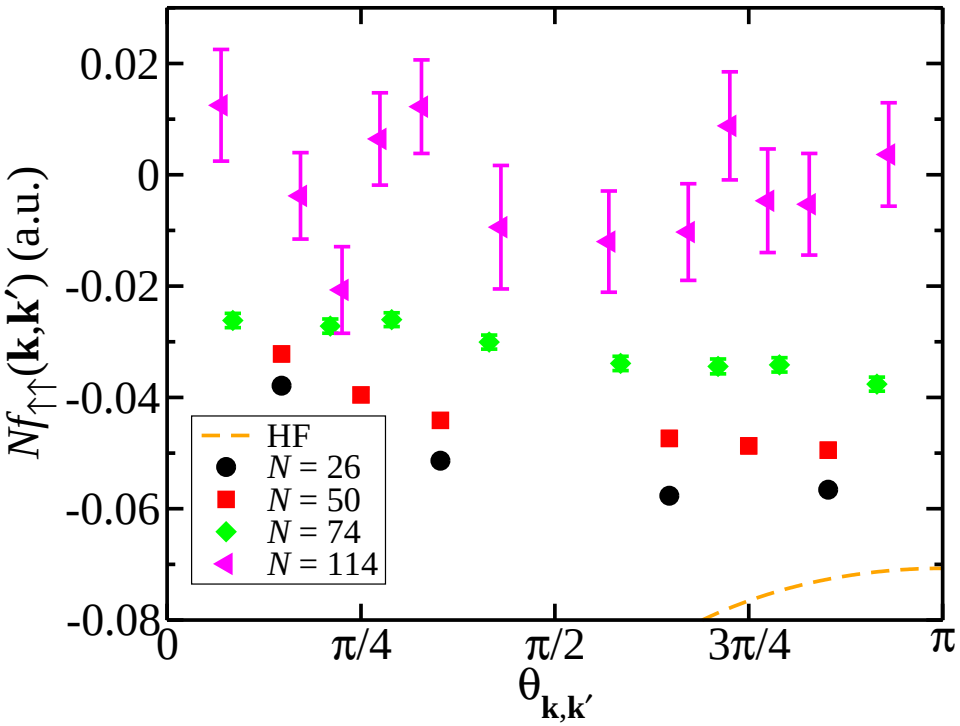



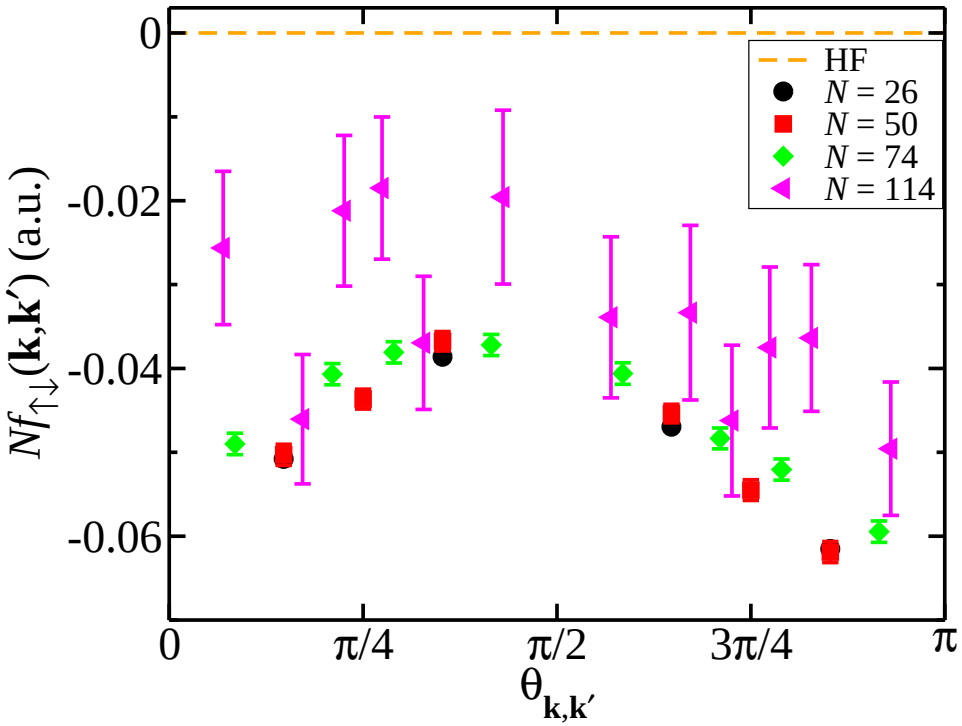
# Paramagnetic Interaction Functions at $r_s = 5$



# Paramagnetic Interaction Functions at $r_s = 10$



# Interaction Functions and Fermi Liquid Parameters

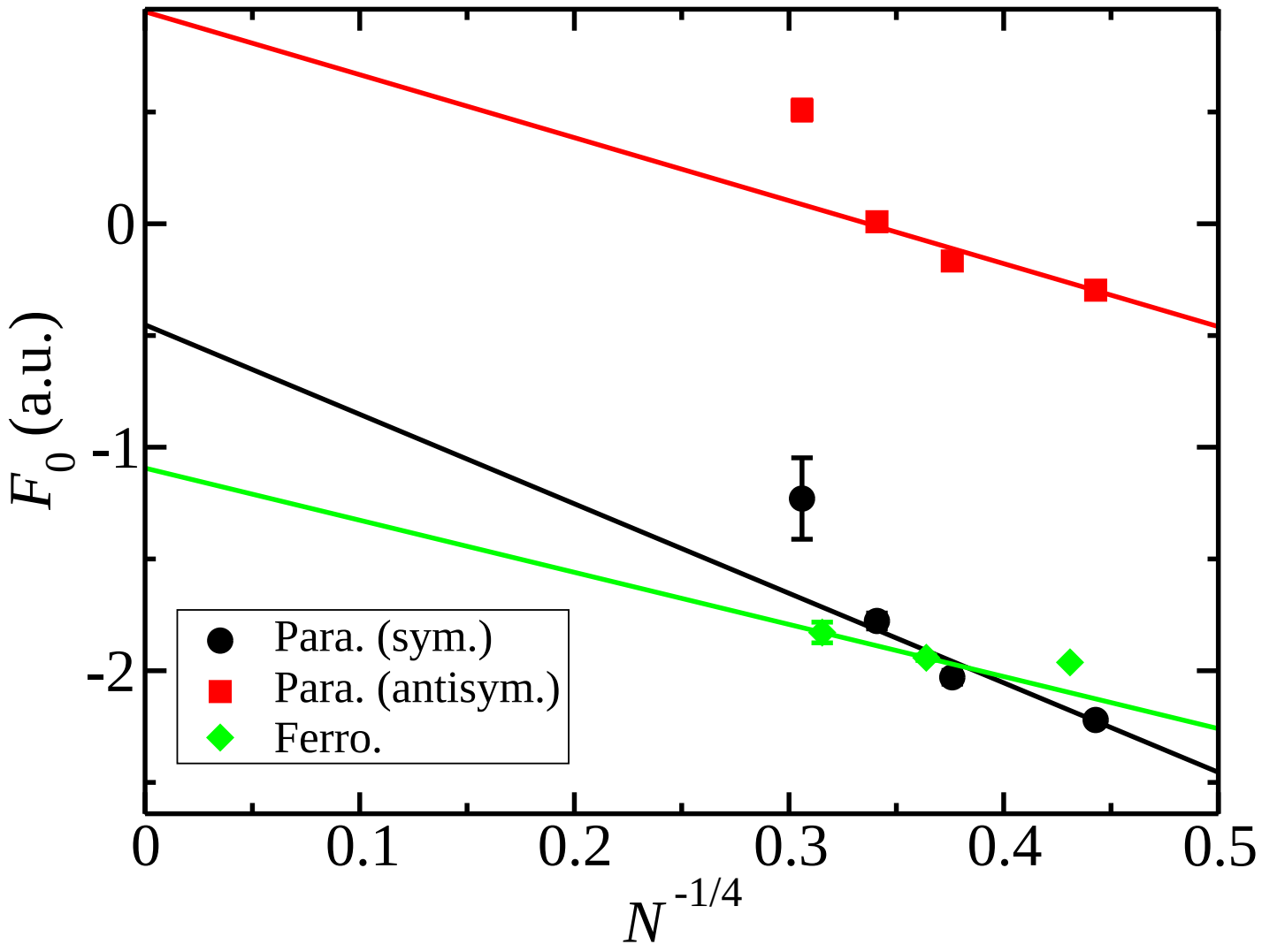
- Difference between the Slater–Jastrow and Slater–Jastrow–backflow results is very significant.
  - **We are working at the limit of current QMC technology.**
  - *Let's hope the Slater–Jastrow–backflow results are sufficiently accurate.*

- There is a significant difference between the quasiparticle interaction functions obtained using promotions and double additions or subtractions.
  - This is indicative of finite-size errors, which are expected to be more severe for double additions or subtractions than for promotions.

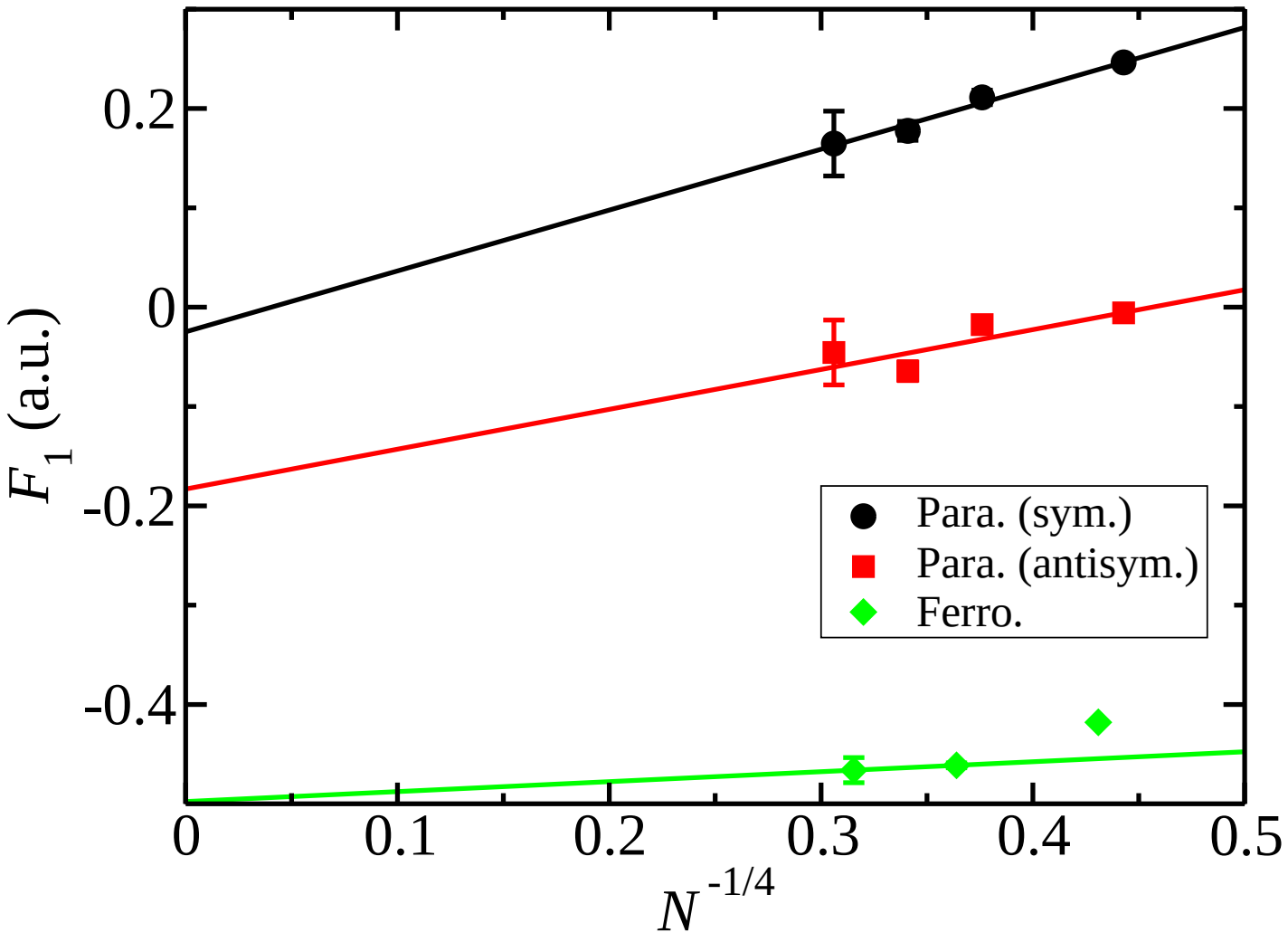
- We have evaluated the Fermi liquid parameters by numerical integration of the Landau interaction functions.

- Since we have considered only excitations in the vicinity of the Fermi surface, we use the $N^{-1/4}$ finite-size scaling proposed by Holzmann *et al.*

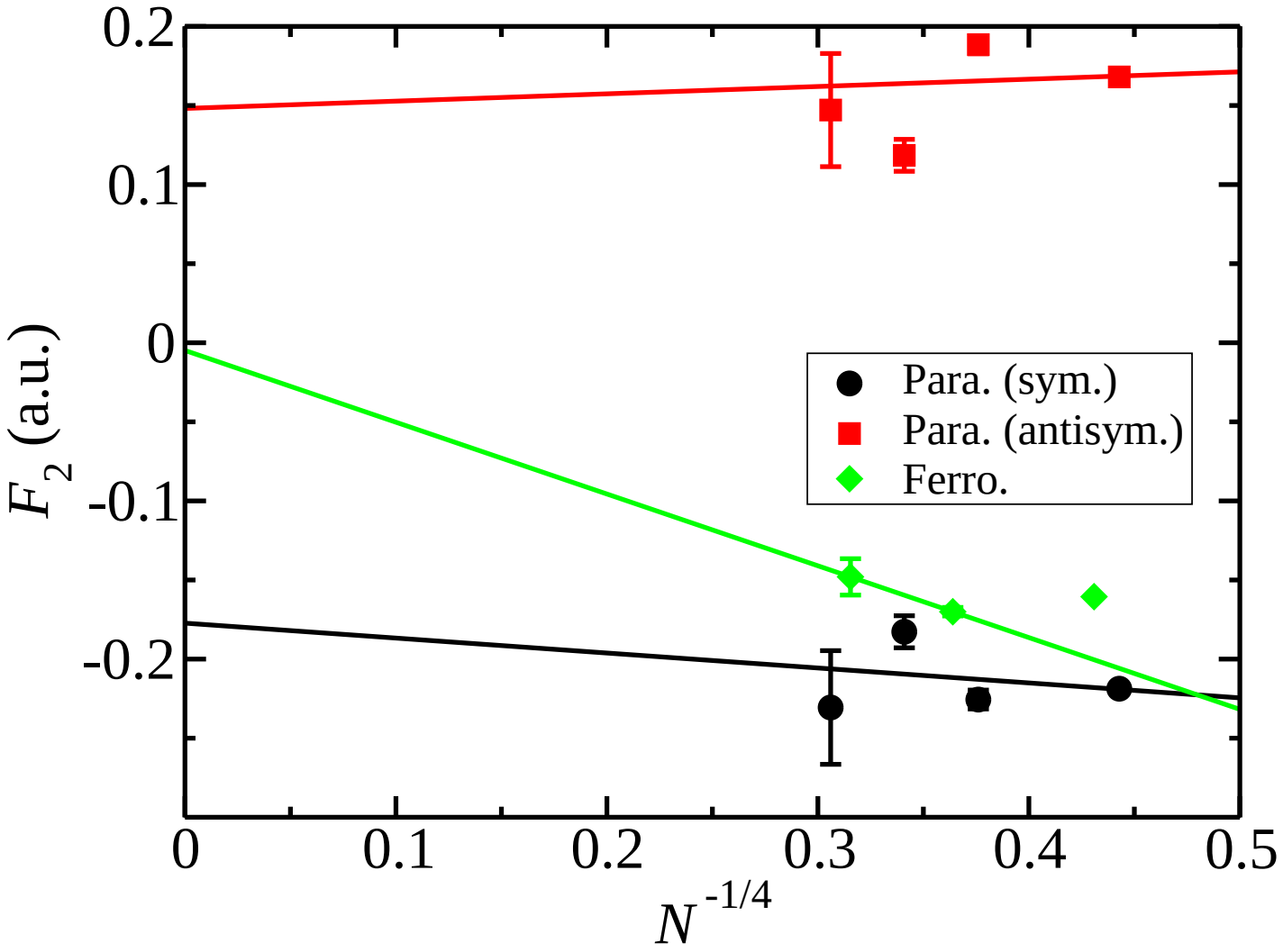
# Extrapolation of the Fermi Liquid Parameters ($r_s = 5$): $F_0$



# Extrapolation of the Fermi Liquid Parameters ($r_s = 5$): $F_1$



# Extrapolation of the Fermi Liquid Parameters ($r_s = 5$): $F_2$



# Fermi Liquid Parameters

- First three paramagnetic Fermi liquid parameters (symmetric and antisymmetric):

| $r_s$ | $F_0^s/m^*$ | $F_0^a/m^*$ | $F_1^s/m^*$ | $F_1^a/m^*$ | $F_2^s/m^*$ | $F_2^a/m^*$ |
|---|---|---|---|---|---|---|
| 1 | $-0.43(3)$ | $-0.225(10)$ | $-0.207(6)$ | $-0.167(6)$ | $-0.11(1)$ | $-0.002(7)$ |
| 5 | $-0.45(13)$ | $0.95(4)$ | $-0.02(3)$ | $-0.18(3)$ | $-0.18(3)$ | $0.15(3)$ |
| 10 | $-0.7(4)$ | $3.11(8)$ | $-0.07(6)$ | $-0.32(6)$ | $-0.08(6)$ | $0.10(5)$ |

- First three ferromagnetic Fermi liquid parameters:

| $r_s$ | $F_0/m^*$ | $F_1/m^*$ | $F_2/m^*$ |
|---|---|---|---|
| 1 | $-0.41(5)$ | $-0.172(9)$ | $-0.09(1)$ |
| 5 | $-1.1(4)$ | $-0.5(1)$ | $0.00(9)$ |
| 10 | $-1(1)$ | $-1.0(3)$ | $0.23(3)$ |

# Checking the Effective Mass

- Galilean invariance: the Fermi liquid parameter $F_1^s$ is related to the effective mass via $m^* = 1 + F_1^s$.

| Phase | Density parameter $r_s$ | Effective mass $m^*$ | |
|---|---|---|---|
| | | $k_F/(\partial\mathcal{E}/\partial k)_{k_F}$ | $1 + F_1^s$ |
| Paramagnetic | 1 | 0.935(4) | 0.829(4) |
| Paramagnetic | 5 | 0.95(3) | 0.98(3) |
| Paramagnetic | 10 | 0.82(7) | 0.93(5) |
| Ferromagnetic | 1 | 0.841(3) | 0.853(7) |
| Ferromagnetic | 5 | 0.73(2) | 0.67(4) |
| Ferromagnetic | 10 | 0.67(4) | 0.50(8) |

- Direct calculation of the effective mass from the band $[m^* = k_F/(\partial\mathcal{E}/\partial k)_{k_F}]$ is more reliable?

# Conclusions

- Our data confirm that the effective mass of the ferromagnetic HEG decreases when the density is lowered, unlike the paramagnetic HEG.
  - The agreement with experiment is reasonable.
- We have obtained preliminary results for the interaction Fermi liquid parameters.
  - The effective mass obtained from the Fermi liquid parameter $F_1^s$ is not wildly different from the effective mass obtained directly from the energy band.
- To-do: compare the expressions for the compressivity and the spin susceptibility within Fermi liquid theory with DMC total energy calculations in the literature.

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