Quasiparticle Effective Mass of the Two-Dimensional Homogeneous Electron Gas

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Two-Dimensional Homogeneous Electron Gas (I)

- 2D HEG: set of electrons moving in 2D in a uniform, inert, neutralising background.

- 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** [$\zeta = (N_\uparrow - N_\downarrow)/N$].

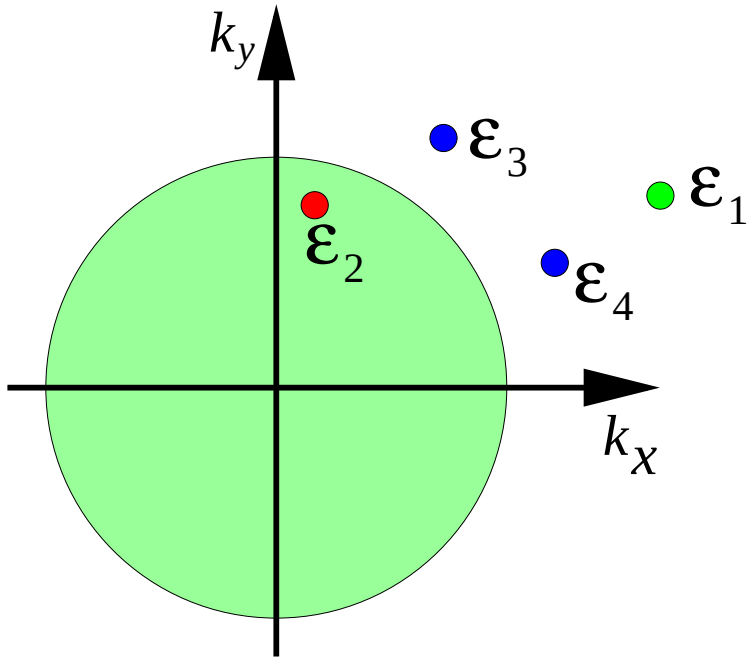
- Physical realisations:

  - *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 independent* quasiparticles *occupying plane-wave states.*

Justification: scattering rate of quasiparticles between plane-wave states is low (and vanishes at Fermi surface) because of Pauli exclusion principle. Hence single-particle momentum states are approximately good quantum numbers near Fermi surface.



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

Renormalisation of the Electron Mass

Quasiparticle energy–momentum relationship $\mathcal{E}(\mathbf{k})$ generally differs from that of free electrons.

The description of most metallic properties, e.g. response functions, involves the excitation of a few particles close to the Fermi surface.

For excitations close to the Fermi surface, the main effect of the modification to the band is a change in the gradient (offsets to the energy band are not significant).

In this region, excitations are like those of **free** particles with a *quasiparticle effective mass* (EM) such that the free-particle band has the same gradient as the quasiparticle band at the Fermi surface.

The EM is

$$m^* = \frac{k_F}{(\partial\mathcal{E}/\partial k)_{k_F}}.$$

Landau Energy Functional

As in Hartree–Fock theory, total energy is not simply the sum of single-particle energies. Quasiparticle energies depend on distribution of other quasiparticles.

We may write the *Landau energy functional*, which gives the dependence of the total energy on changes to the quasiparticle occupation numbers $\delta N_{\mathbf{k},\sigma}$ from the Fermi–Dirac distribution at $T = 0$, as

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

where E_0 is the ground-state energy.

- $\mathcal{E}_\sigma(\mathbf{k})$ is the energy of an isolated quasiparticle. Near the Fermi surface, $\mathcal{E}_\sigma(\mathbf{k}) = \mu + (k_F/m^*)(k - k_F)$, where μ is the chemical potential.

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

Fermi Liquid Parameters

The *local quasiparticle energy*

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

plays the role of the free-particle energy in thermodynamic calculations.

In most cases of interest, the quasiparticle occupation number only changes near the Fermi surface. In this case we may assume that $f_{\sigma,\sigma'}(\mathbf{k},\mathbf{k}')$ only depends on the angle between $\mathbf{k}$ and $\mathbf{k}'$ and that $\mathcal{E}(\mathbf{k})$ is free-particle-like (with mass m^*).

For calculations of many quantities of interest, the quasiparticle number is approximately conserved, i.e., $\sum_{\mathbf{k},\sigma} \delta N_{\mathbf{k},\sigma} = 0$. If $\delta N_{\mathbf{k},\sigma}$ is also spherically symmetric then the second term in the local quasiparticle energy vanishes. Hence one can calculate e.g. the heat capacity as the heat capacity of a gas of noninteracting Fermions of mass m^*.

For calculations which involve changes to the number of quasiparticles, e.g. a calculation of the compressibility, or for calculations involving an anisotropic change in the quasiparticle distribution, angular integrals over $f_{\sigma,\sigma'}(\mathbf{k},\mathbf{k}')$ at the Fermi surface are required. These are called the *Fermi liquid parameters*.

Quasiparticle Effective Mass of the 2D HEG

Surprisingly, the EM of a paramagnetic 2D HEG has been the subject of great controversy in recent years.

Early experiments[2] found a large enhancement of the EM at low density; more recent experiments[3] have contradicted this.

On the theoretical side, GW calculations give a range of possible results depending on the choice of effective interaction, while previous QMC studies[4] have suggested that there is much less enhancement of the EM than found in any of the experiments.

Finally, the recent experiments of Padmanabhan *et al.* have shown that the EMs in paramagnetic and ferromagnetic HEGs behave quite differently as a function of density, as had been predicted by theorists.[5]

Understanding the magnetic behaviour of the 2D HEG at low density will play an important role in the design of **spintronic** devices.

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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] Y. Kwon, D. M. Ceperley, and R. M. Martin, Phys. Rev. B **50**, 1684 (1994).

[5] Y. Zhang and S. Das Sarma, Phys. Rev. Lett. **95**, 256603 (2005).

Electronic Energy Band

The *electronic energy band* $\mathcal{E}(\mathbf{k})$ is defined in terms of the total energy difference when an electron is added to or subtracted from a HEG at a constant cell volume:

- Occupied $\mathbf{k}$: $\mathcal{E}(\mathbf{k})$ is the difference between the total closed-shell GS energy and the energy of an $(N-1)$-electron system with an electron removed from $\mathbf{k}$.

- Unoccupied $\mathbf{k}$: $\mathcal{E}(\mathbf{k})$ is the difference between the energy of the $(N+1)$-electron system in which $\mathbf{k}$ is occupied and the closed-shell GS energy.

It follows from the discussion above that within Fermi liquid theory the **electronic** energy band agrees with the **quasiparticle** band in the vicinity of the Fermi surface (but does not include finite-lifetime effects away from the Fermi surface).

So we can differentiate the electronic band to find the EM.

QMC Calculations (I)

We have performed the first complete DMC calculation of the 2D HEG electronic energy band, enabling us to predict the EM.[6]

Kwon *et al.* attempted to calculate the EM by promoting electrons from just below the Fermi edge to just above it, then fitting the EM and other Fermi liquid parameters to the energy differences evaluated within QMC.

This allows the Fermi liquid parameters to be determined at the same time as the EM, but noise and finite-size errors make determining the EM difficult. Different variants of Kwon's method give different results.

By adding or removing electrons, we avoid the need to consider the effect of the electron–hole interaction. We can therefore calculate the EM with relative ease.

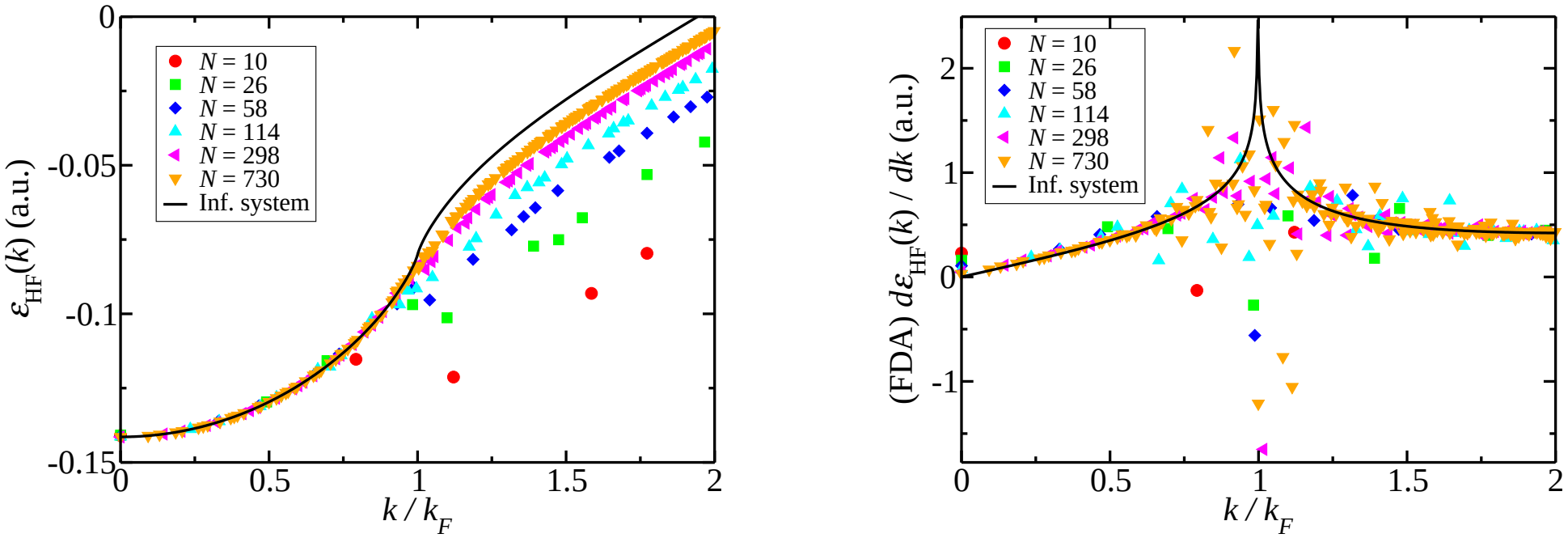
Once the EM has been determined, obtaining the other Fermi liquid parameters using the method of Kwon *et al.* should be relatively straightforward (especially as we have better wave functions and can study larger systems). Will do this soon.

[6] N. D. Drummond and R. J. Needs, submitted to Phys. Rev. Lett. (2009).

QMC Calculations (II)

DMC takes one $\sim 99\%$ of the way from the HF band to the real band.

Hence the pathological behaviour of the HF band is also present in the DMC band.



HF band and its derivative for a paramagnetic 2D HEG at $r_s = 10$ a.u.

Avoid pathology at Fermi surface by fitting to DMC band over a wide range of k.

QMC Calculations (III)

In our finite simulation cell subject to (twisted) periodic boundary conditions, the available momentum states fall on the (offset) grid of reciprocal lattice points.

We have confirmed that finite-size biases are small by carrying out simulations in different cell sizes. But see later. . .

Having determined the energy band at a series of k values, we performed a least-squares fit of a quartic function $\mathcal{E}(k) = \alpha_0 + \alpha_2 k^2 + \alpha_4 k^4$ to our data.

We used "magic" numbers of electrons N in each of our ground-state calculations, corresponding to closed-shell configurations. Hence a real, single-determinant wave function is appropriate, facilitating the optimisation of the wave function.

This also minimises angular effects in the excited-state calculations.

We verified that our DMC results are converged with respect to time step.

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 each case, the BW will lie between the HF 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 $\Delta\mathcal{E}^{\mathrm{HF}} - \Delta\mathcal{E}^{\mathrm{free}} = k_F(1-2/\pi)$.

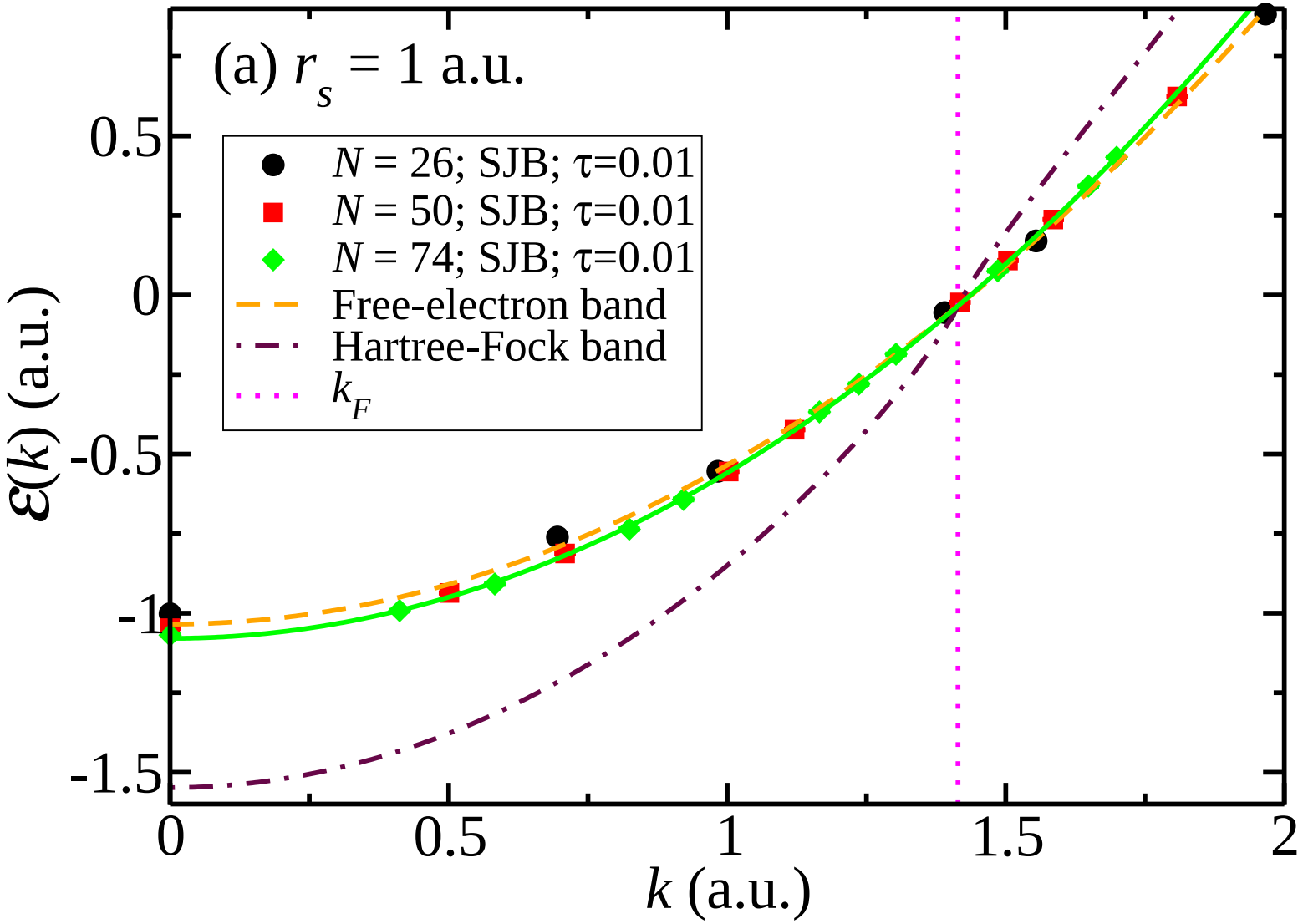
So the error in the DMC BW is less than $0.01k_F(1-2/\pi) \approx 0.007/r_s$ for a ferromagnetic HEG and less than about $0.01k_F(1-2/\pi) \approx 0.005/r_s$ for a paramagnetic HEG.

Since the BW falls off as r_s^{-2}, the error is more significant at large r_s.

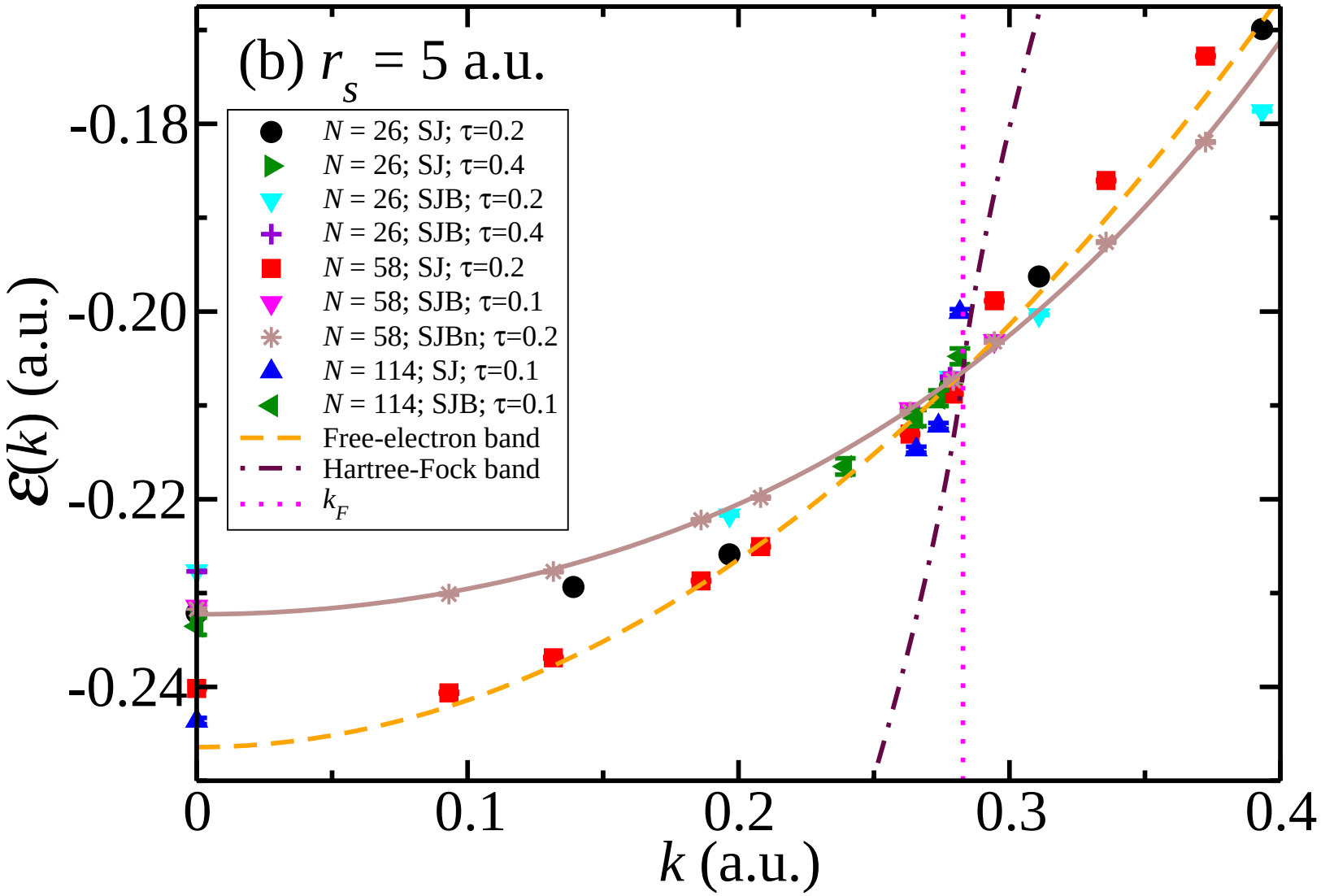
In the worst case (the paramagnetic HEG at $r_s = 10$ a.u.) this argument suggests that DMC overestimates the BW by $\sim 9\%$. In the next-worse case (paramagnetic, $r_s = 5$ a.u.), the BW is overestimated by $\sim 4\%$.

It is reasonable to assume that DMC underestimates the EM by a similar amount.

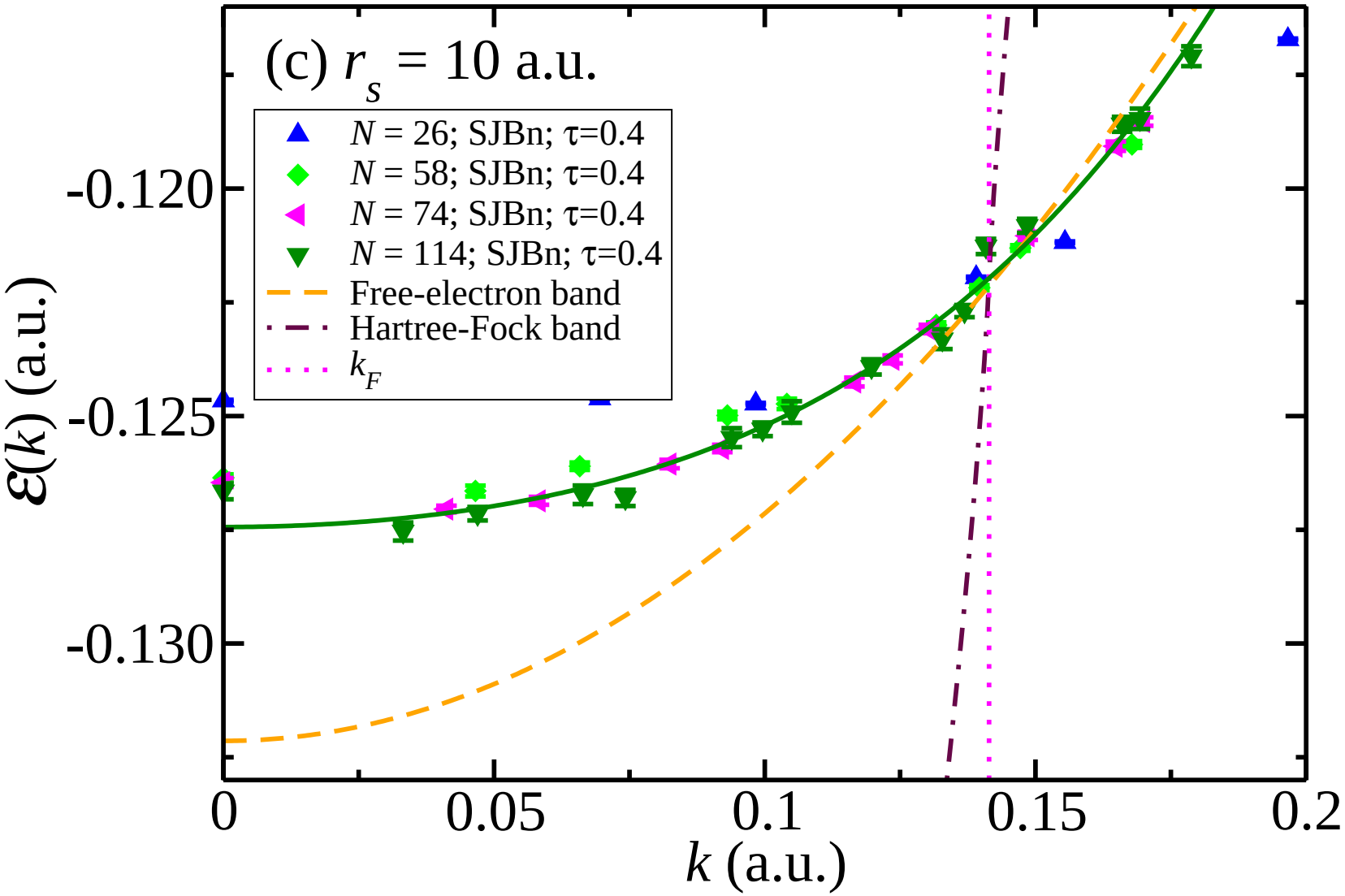
Paramagnetic Electronic Energy Band: $r_s = 1$ a.u.



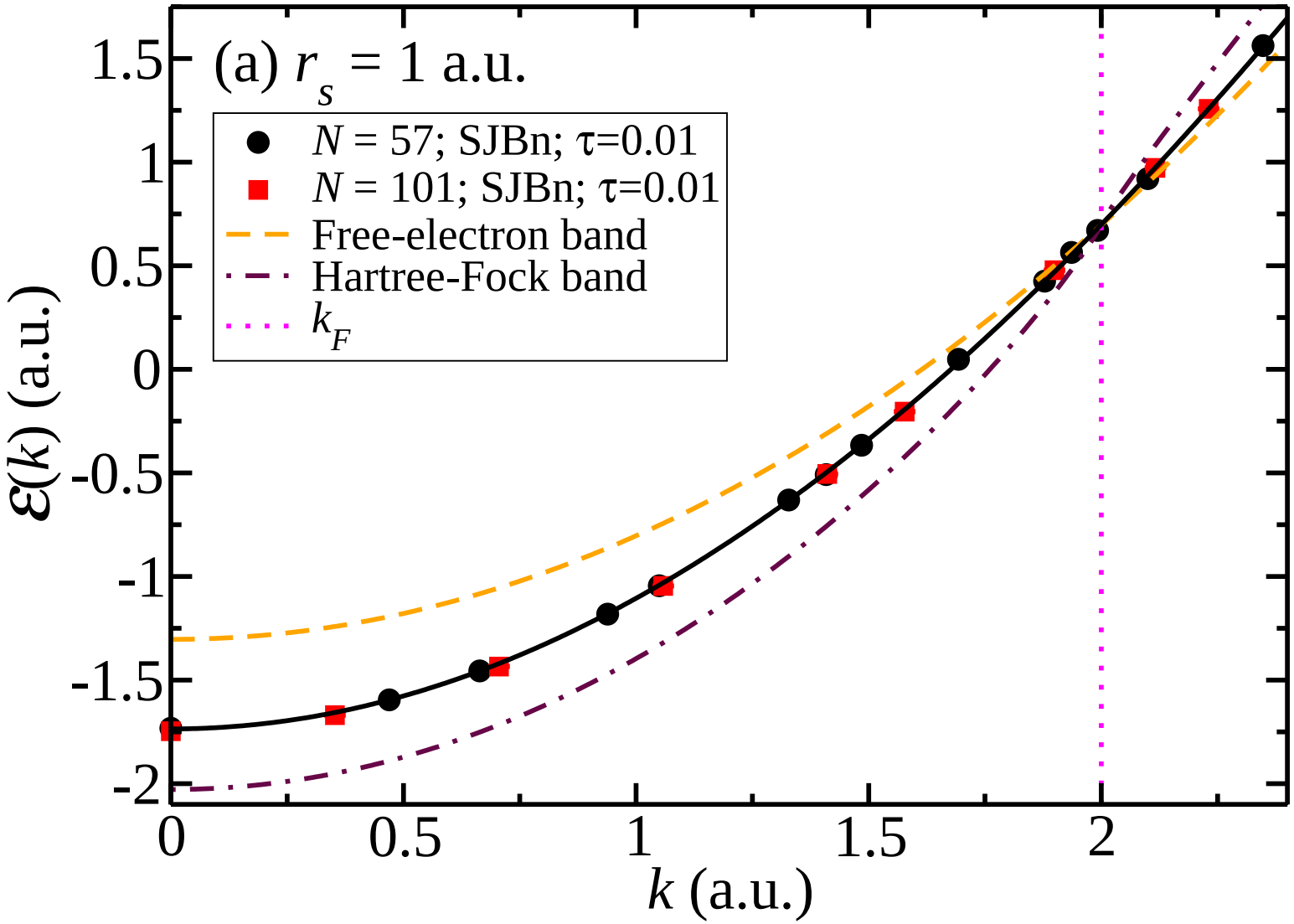
Paramagnetic Electronic Energy Band: $r_s = 5$ a.u.



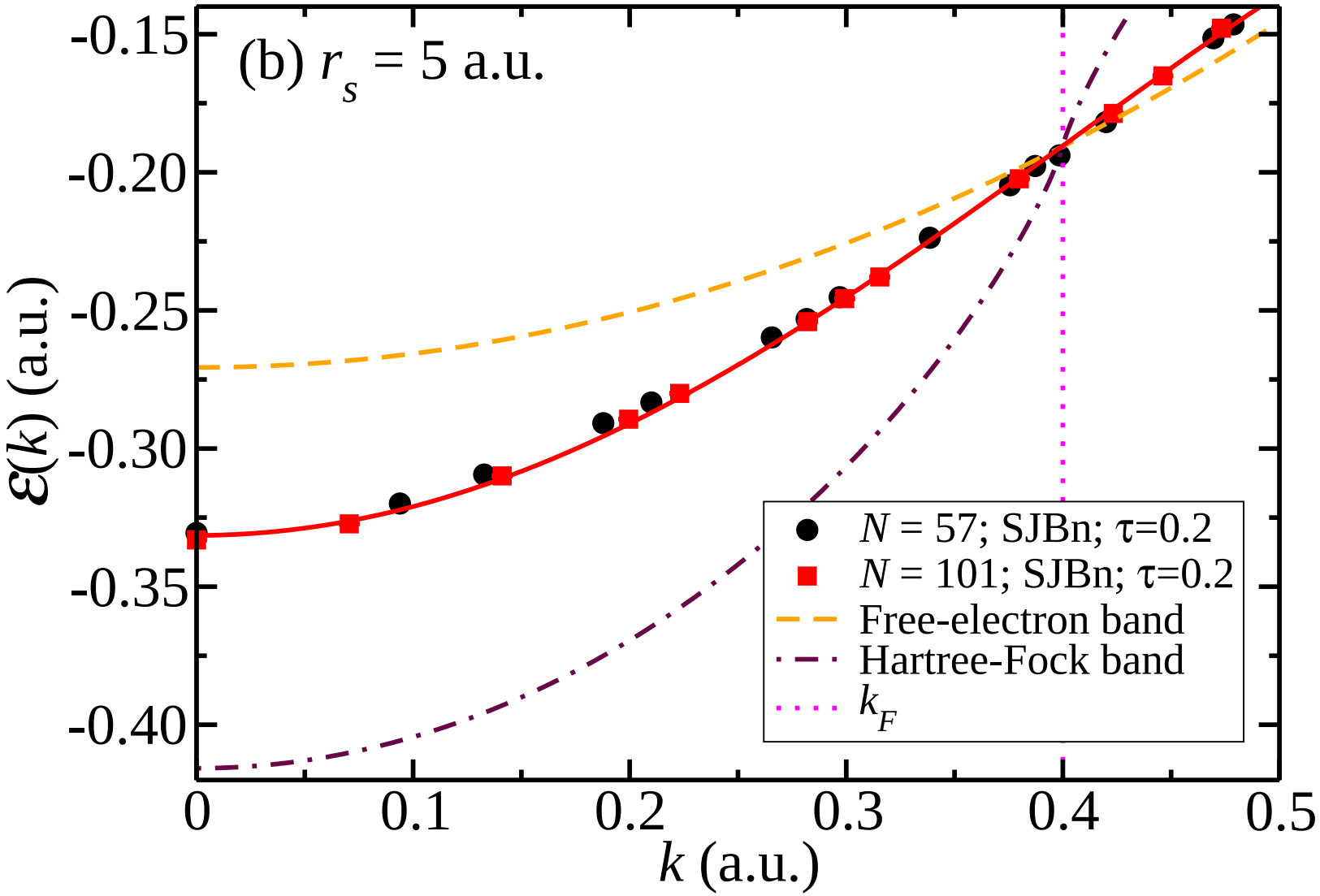
Paramagnetic Electronic Energy Band: $r_s = 10$ a.u.



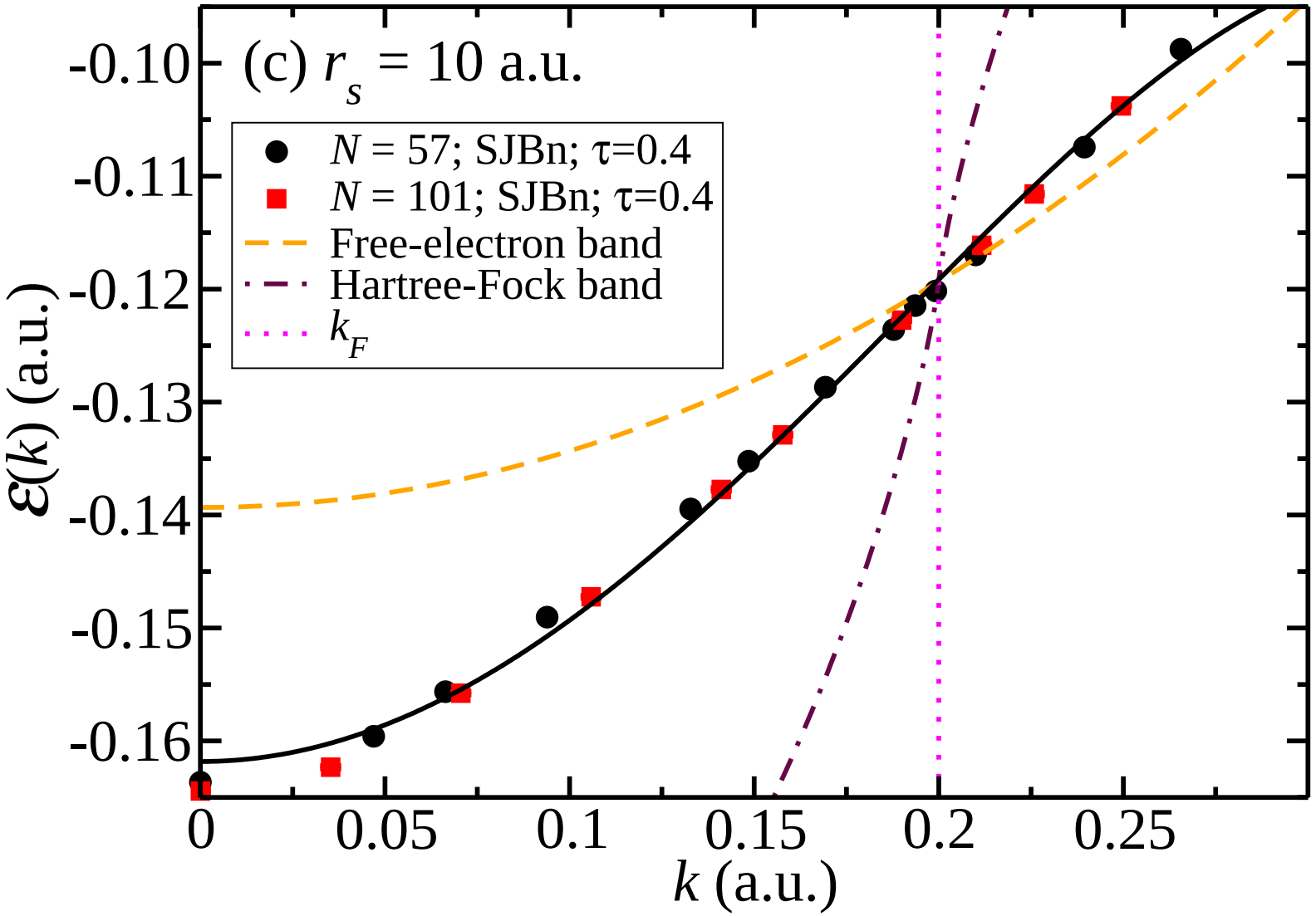
Ferromagnetic Electronic Energy Band: $r_s = 1$ a.u.



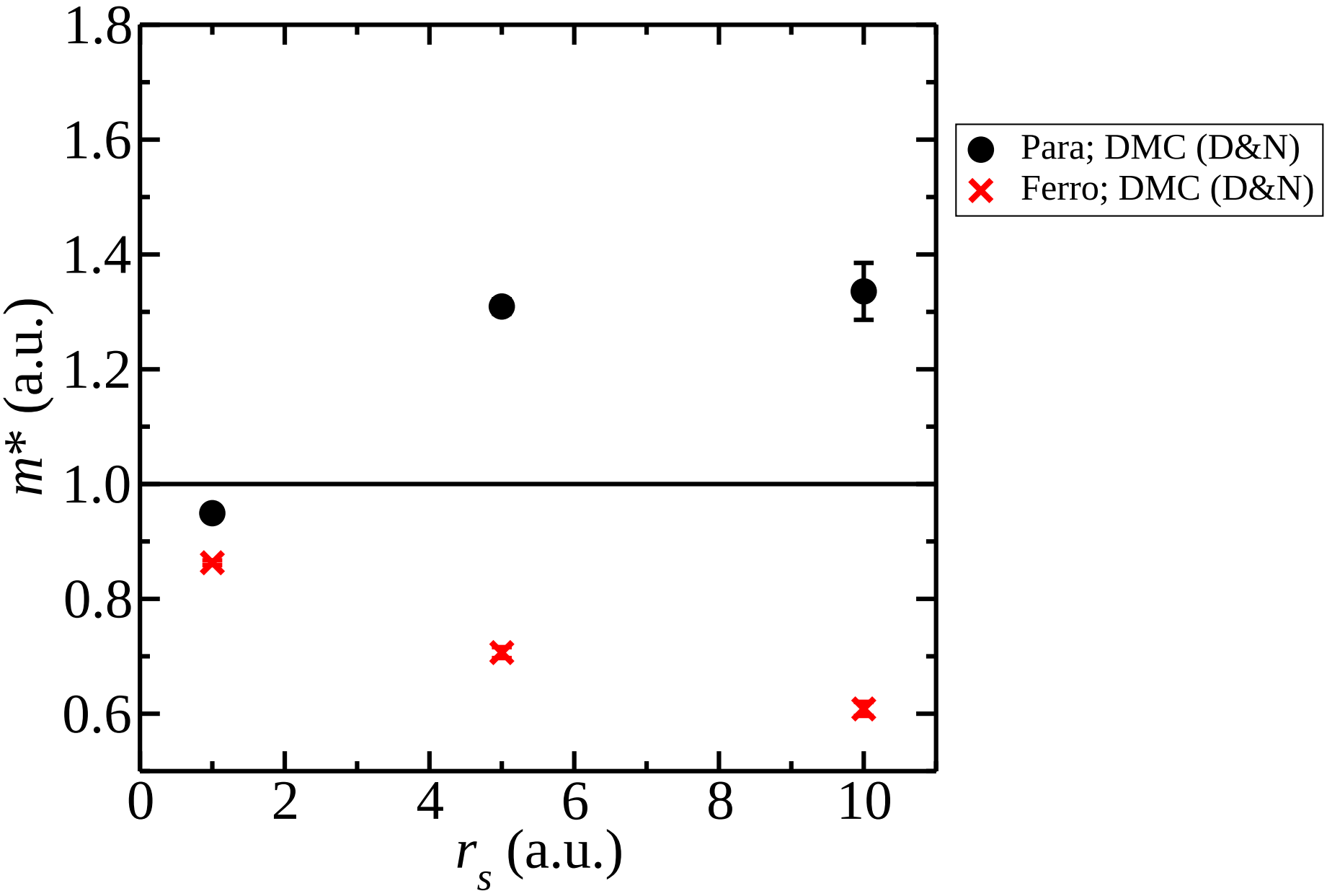
Ferromagnetic Electronic Energy Band: $r_s = 5$ a.u.



Ferromagnetic Electronic Energy Band: $r_s = 10$ a.u.



Quasiparticle Effective Masses (I)



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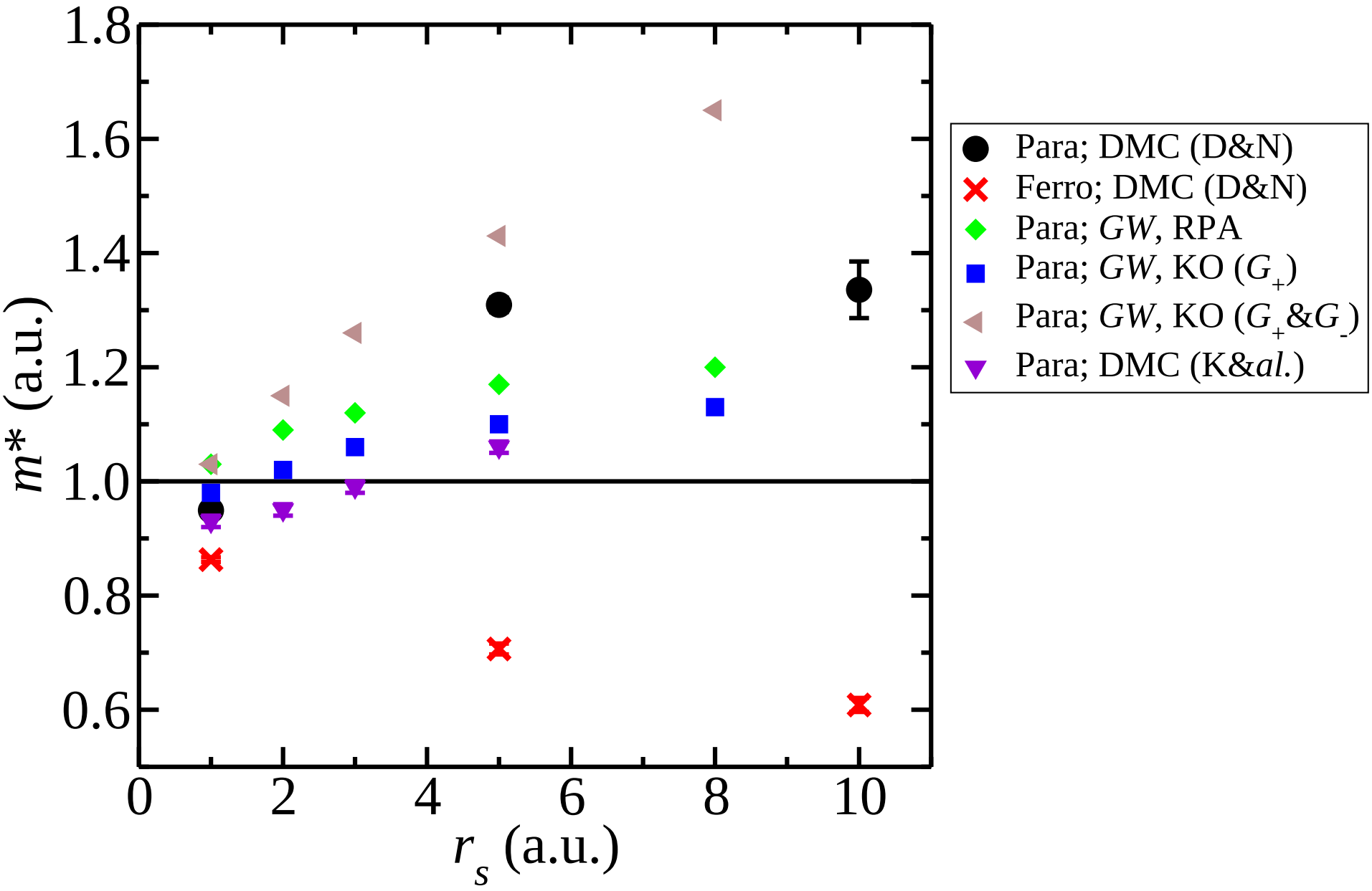

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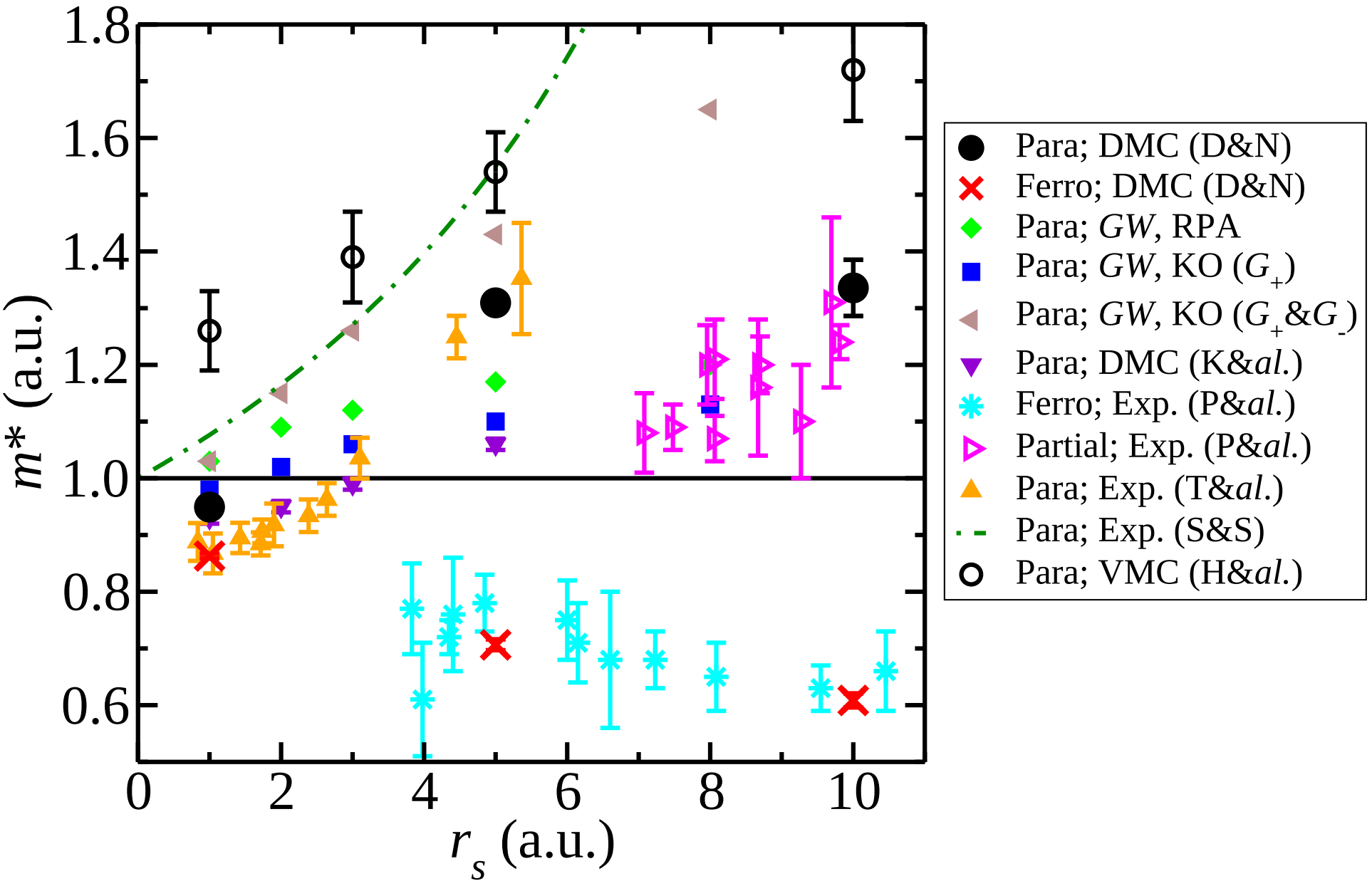


Quasiparticle Effective Masses (II)

Paramagnetic HEG

- At $r_s = 1$ a.u. the EM is slightly less than the bare electron mass, but at $r_s = 5$ a.u. the EM is significantly enhanced.
- EM does not continue to grow rapidly when the density is reduced beyond $r_s \simeq 5$ a.u.
- DMC EMs are in quantitative agreement with experimental results of Tan *et al.*

Ferromagnetic HEG

- The EM *decreases* when the density is lowered. Our results therefore support the qualitative conclusions of Padmanabhan *et al.*
- DMC EMs are in quantitative agreement with exp. results of Padmanabhan *et al.*

Conflict

Very recently, Holzmann *et al.*[7] have carried out a VMC study of the 2D HEG EM. Their EMs differ significantly from our DMC results.

They considered only additions of electrons immediately outside the Fermi surface.

They found substantial finite-size effects in the EM, which they corrected using an approximate analytical expression, derived by considering the finite-size behaviour of the discontinuity in the momentum density at the Fermi surface.

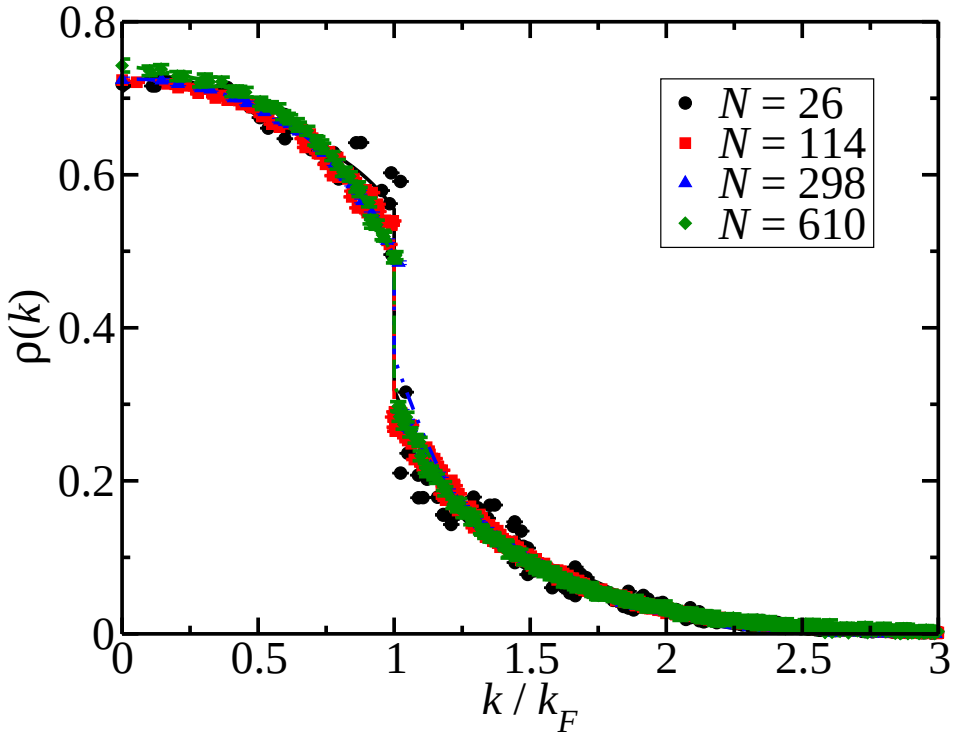
Our EMs do not suffer from these finite-size effects; if anything, our EMs show the opposite trend with system size.

There is a much larger error in Holzmann *et al.*'s VMC results due to the finite fraction of correlation energy retrieved than there is in our DMC results.

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

Momentum Density

Holzmann *et al.* derived an expression for the finite-size error in the momentum density. Error is significant at the Fermi edge, but not elsewhere.

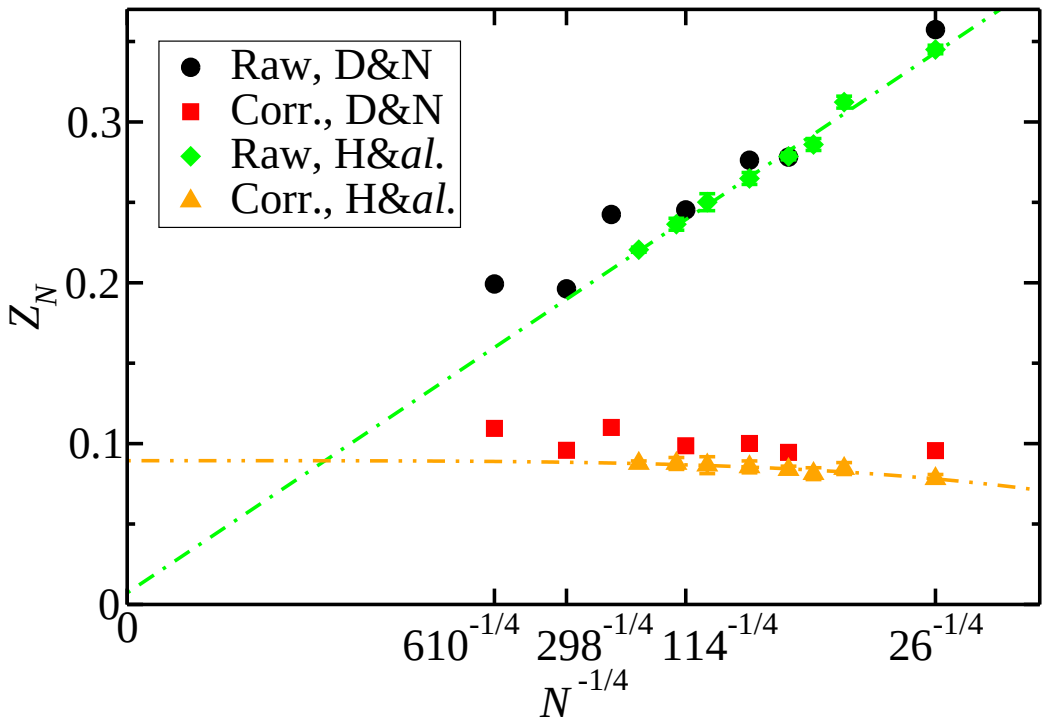


VMC momentum density of paramagnetic HEG at $r_s = 10$ *a.u.*

Renormalisation factor: discontinuity Z at Fermi edge.

Finite-size correction to Z_N: $\Delta Z_N = -Z_N[\pi r_s^2/(4N)]^{1/4} \sim N^{-1/4}$.

Renormalisation Factor



VMC renormalisation factor of paramagnetic HEGs at $r_s = 10$ *a.u.*

Finite-size effects predicted by Holzmann *et al.* are indeed present in Z.

Adding an electron introduces a spike of size Z_N in the momentum density. So finite-size correction to band evaluated by addition of an electron just outside k_F is $\Delta Z_N k_F^2/2$.

Should find significant finite-size effects in the energy band close to the Fermi surface. Finite-size effects are less significant away from the Fermi surface.

Possible Reason For Disagreement?

Possible reason for the disagreement with Holzmann *et al.*: we used a fit to the entire occupied (and part of the unoccupied) band to compute the EM. Therefore, pathological behaviour at the Fermi surface has little effect on the fitted band.

Apparent objection: *Fermi liquid theory is only concerned with excitations close to the Fermi surface. It is therefore inappropriate to calculate the EM by examining excitations over a wider range of k. These are not quasiparticle excitations.*

Response: *We have calculated the electronic energy band (describing electronic additions and subtractions), not the quasiparticle band. The electronic band is an interesting and useful quantity in its own right. Our data are well described by a quartic function over the range of k for which we have data. The pathological behaviour of the QMC band at k_F due to (i) retrieving a finite fraction of the correlation energy and (ii) finite-size effects has a negligible effect on the fitted band. According to Fermi liquid theory, the quasiparticle band coincides with the electronic band at the Fermi surface and, furthermore, the band is smooth at k_F. We may therefore take the derivative of our fitted electronic band at k_F to obtain the EM.*

Holzmann *et al.* added electrons close to the Fermi surface and corrected for finite-size errors, but don't seem to have considered the legacy of HF theory in the QMC band.

Conclusions

- Our data confirm that the EM of the paramagnetic HEG increases when the density is lowered, while that of the ferromagnetic HEG decreases.

- Our ferromagnetic and paramagnetic EMs are in agreement with the experimental results of Padmanabhan *et al.* and Tan *et al.*, respectively.

- However, our results disagree with those of another QMC study. We believe this is because the other QMC study only looked at excitations close to the Fermi surface.

Future work:

- Use the approach taken by Kwon *et al.* to calculate the Fermi liquid parameters.

- Padmanabhan *et al.* used a magnetic field to polarise the HEG. The field was mostly in-plane (which has no effect on an ideal 2D HEG other than to spin-polarise it), but a small perpendicular component may have affected their results. *Study 2D HEG in the presence of a magnetic field.*

Acknowledgements

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