QMC and the 1d electron gas

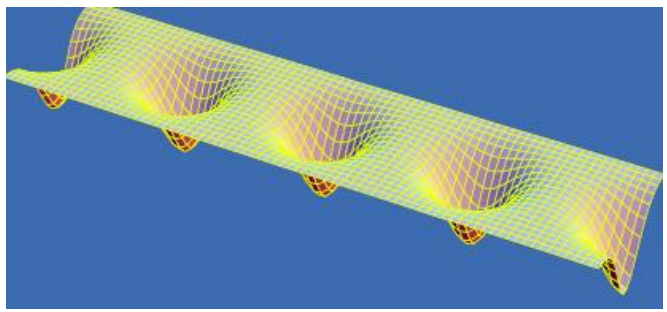
Robert Lee

ESDG talk

21st October 2009

Contents

- Main features of the 1d HEG model
- Experimental application/relevance
- Quantum Monte Carlo calculations
- Conclusions



https://www.jyu.fi/fysiikka/en/research/material/clusters/wires.html

The ideal 1d model

The model is simply 1d electrons on a uniform positive background

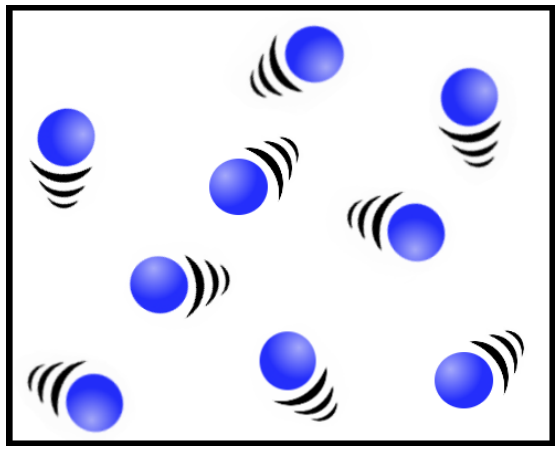
Many previous studies used regularized interactions

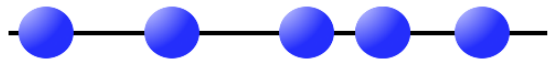
Here we consider the Coulomb interaction, diverging as $1/r$ at coalescence points

$$\hat{\mathcal{H}} = -\frac{1}{2}\sum_{i=1}^{n}\nabla_i^2 + \sum_{i<j}\frac{1}{|x_i - x_j|} + C \ ,$$

where C includes background terms.

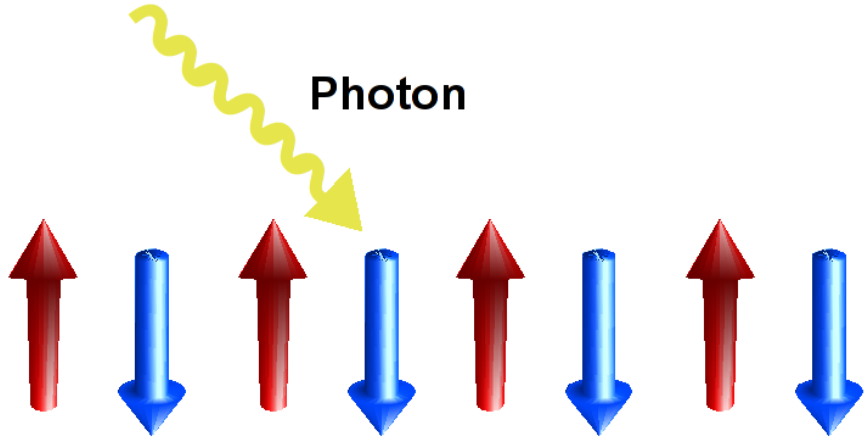
In 1d, particles cannot avoid each other

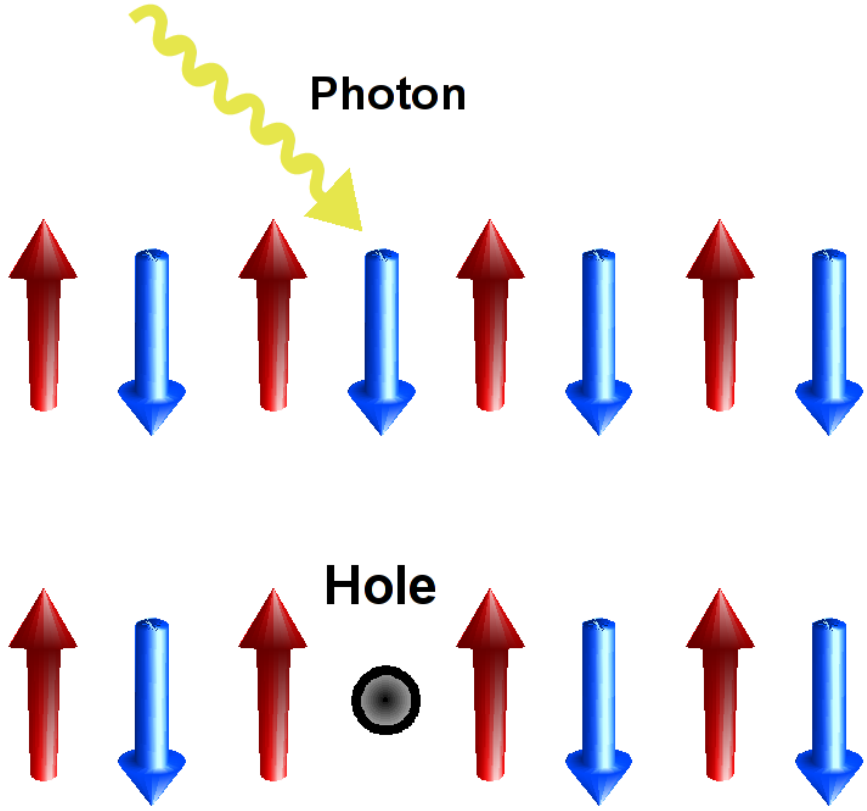


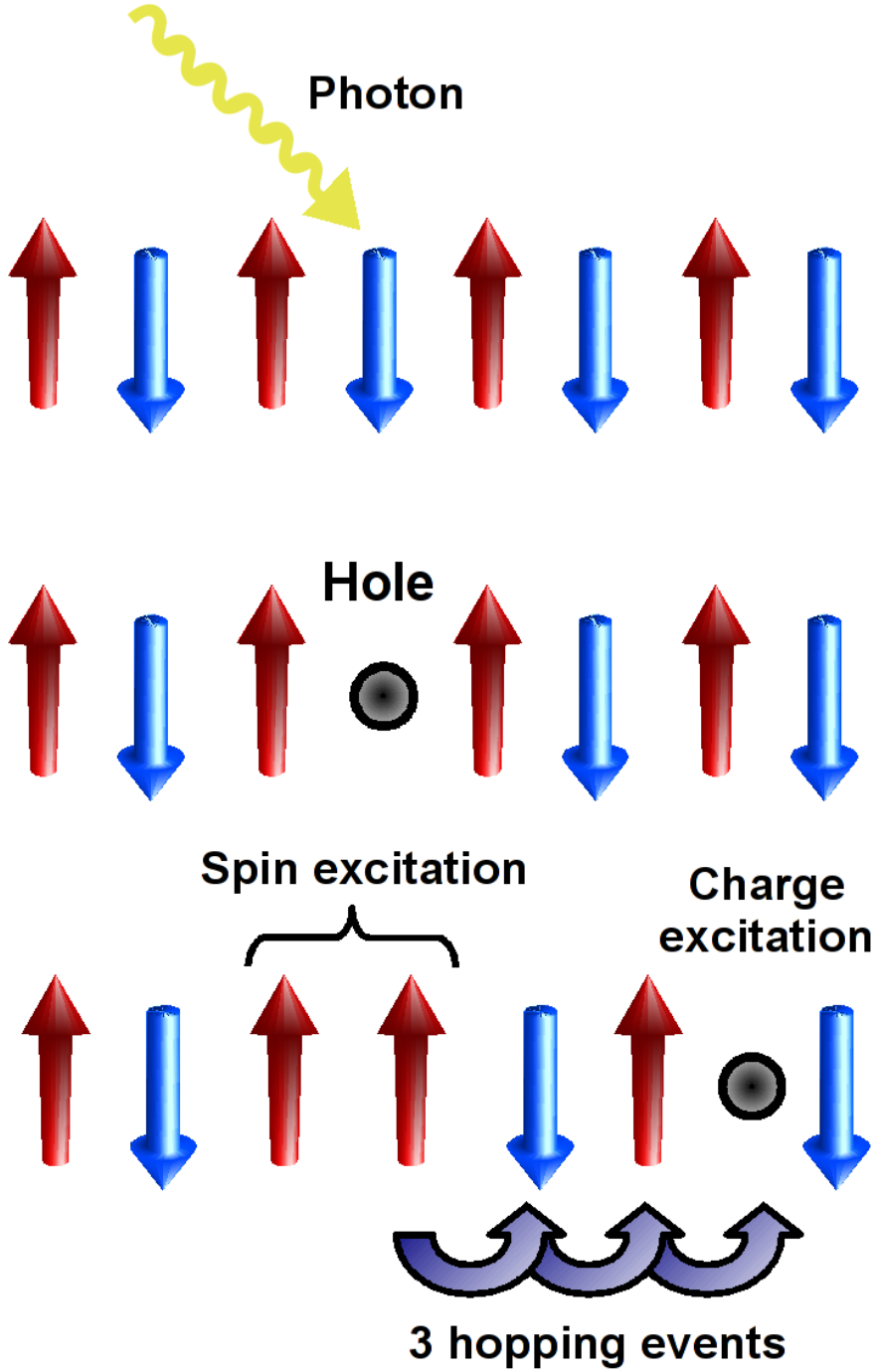


The interesting physics comes from the reduced dimensionality and the strong correlation that is a consequence of the dimensionality.

Experimentalists look for power law behaviour in various quantities and spin-charge separation as a signature of 1d behaviour...


Photon


Photon
Hole


Photon
Hole
Spin excitation
Charge
excitation
3 hopping events

Strong correlation

Non-Fermi liquid behaviour is characterized by

$$\lim_{N\to\infty} Z = 0 \,,$$

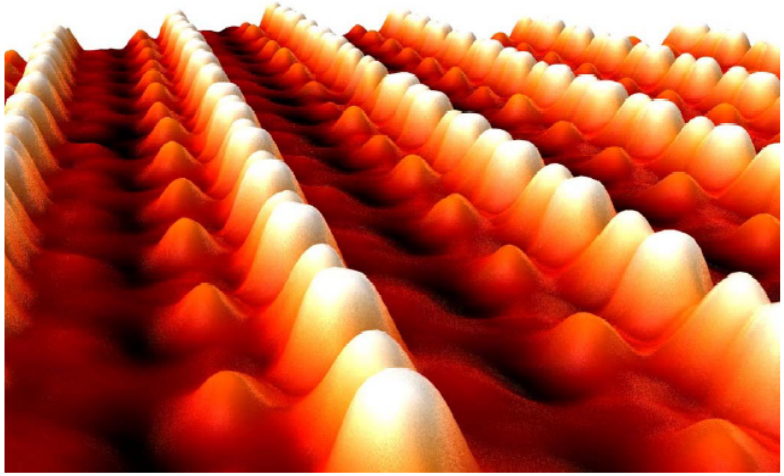
where

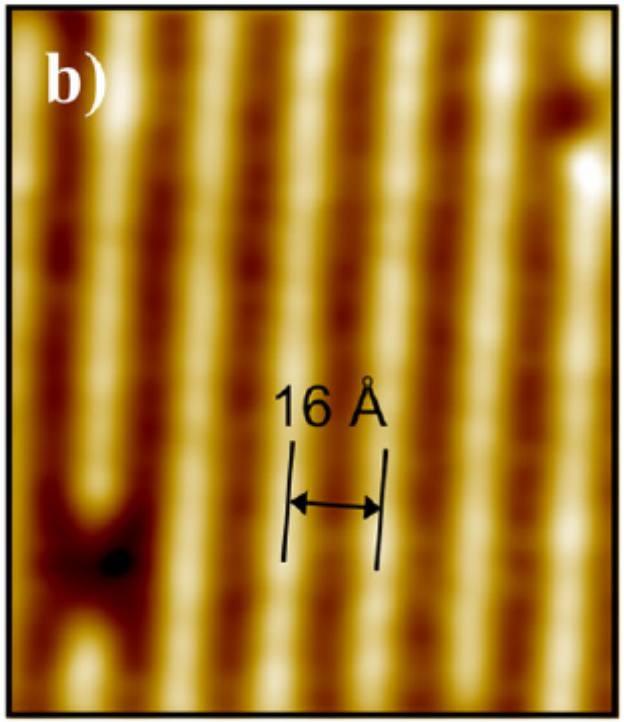
$$Z_{\sigma,k_F} = \left| \langle 0, N+1 \mid \hat{a}^{\dagger}_{\sigma,\mathbf{k}} \mid 0, N \rangle \right|^2_{|\mathbf{k}|=k_F}$$

is the renormalization constant.

You may recognize Z as the size of the step at k_F in the momentum distribution - this is a result of Z also being the weight under the quasiparticle peak in the spectral function.

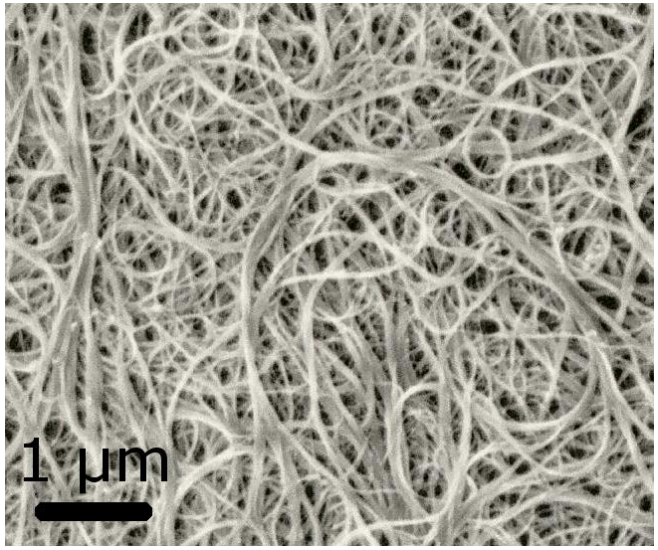
Nanowires of atoms

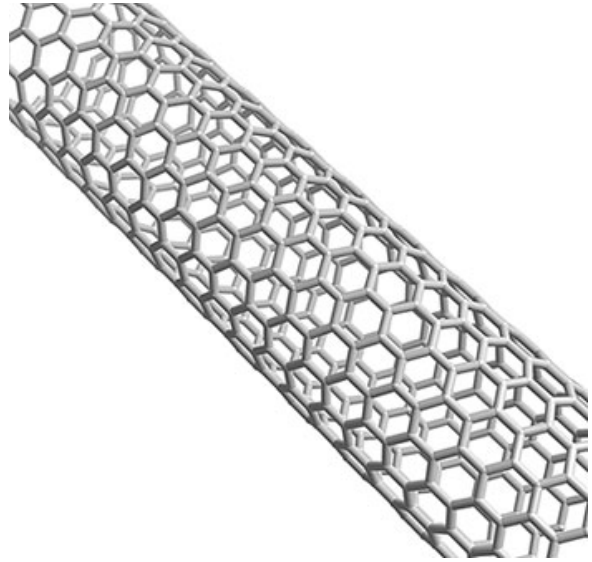




(left) Pt atoms on Ge., Oncel *et al.* PRL **95**, 116801 (2005)
(right) Au atoms on Ge., Schäfer *et al.* PRL **101**, 236802 (2008)

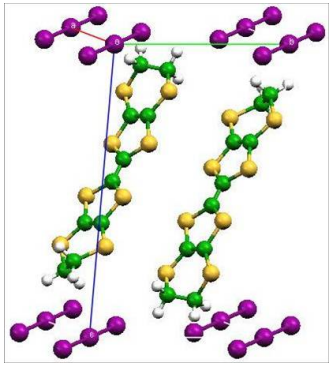
Carbon nanotubes

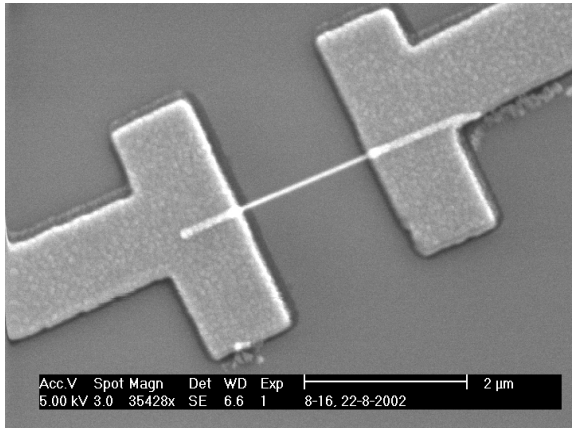




Single-walled CNTs in particular seem to exhibit behaviour characteristic of electrons in 1d.

(images: http://www.ipt.arc.nasa.gov/carbonnano.html)





(left) charge-transfer salts (e.g. $(\text{BEDT-TTF})_2\text{X}$)
(right) semiconductor devices

Atoms in anisotropic traps, transition metal oxides, quantum Hall edge states, etc.

QMC calculations on the ideal 1d electron liquid

- The g.s. nodes are known - no fermion sign problem
- The geometry makes twist averaging simple
- We can get very good wavefunctions - expectation values hardly differ at all between VMC and DMC

The wavefunction

$$\psi(\mathbf{R}) = \exp\left[J(\mathbf{R})\right] \begin{vmatrix} \phi_1(x_1') & \phi_2(x_1') & \dots & \phi_n(x_1') \\ \phi_1(x_2') & \phi_2(x_2') & \dots & \phi_n(x_2') \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(x_n') & \phi_2(x_n') & \dots & \phi_n(x_n') \end{vmatrix}$$

where $\phi_n(x) = \exp(ik_n x)$ and x' is related to x by a backflow transformation. The Jastrow factor is

$$J(\mathbf{R}) = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left[\sum_{A=1}^{N_p} a_A \cos\left(\frac{2\pi A}{L} x_{ij}\right) + (x_{ij} - L_u)^C \Theta(L_u - x_{ij}) \sum_{r=0}^{N_u} \alpha_r x_{ij}^r \right]$$

where $x_{ij} = |x_i - x_j|$.

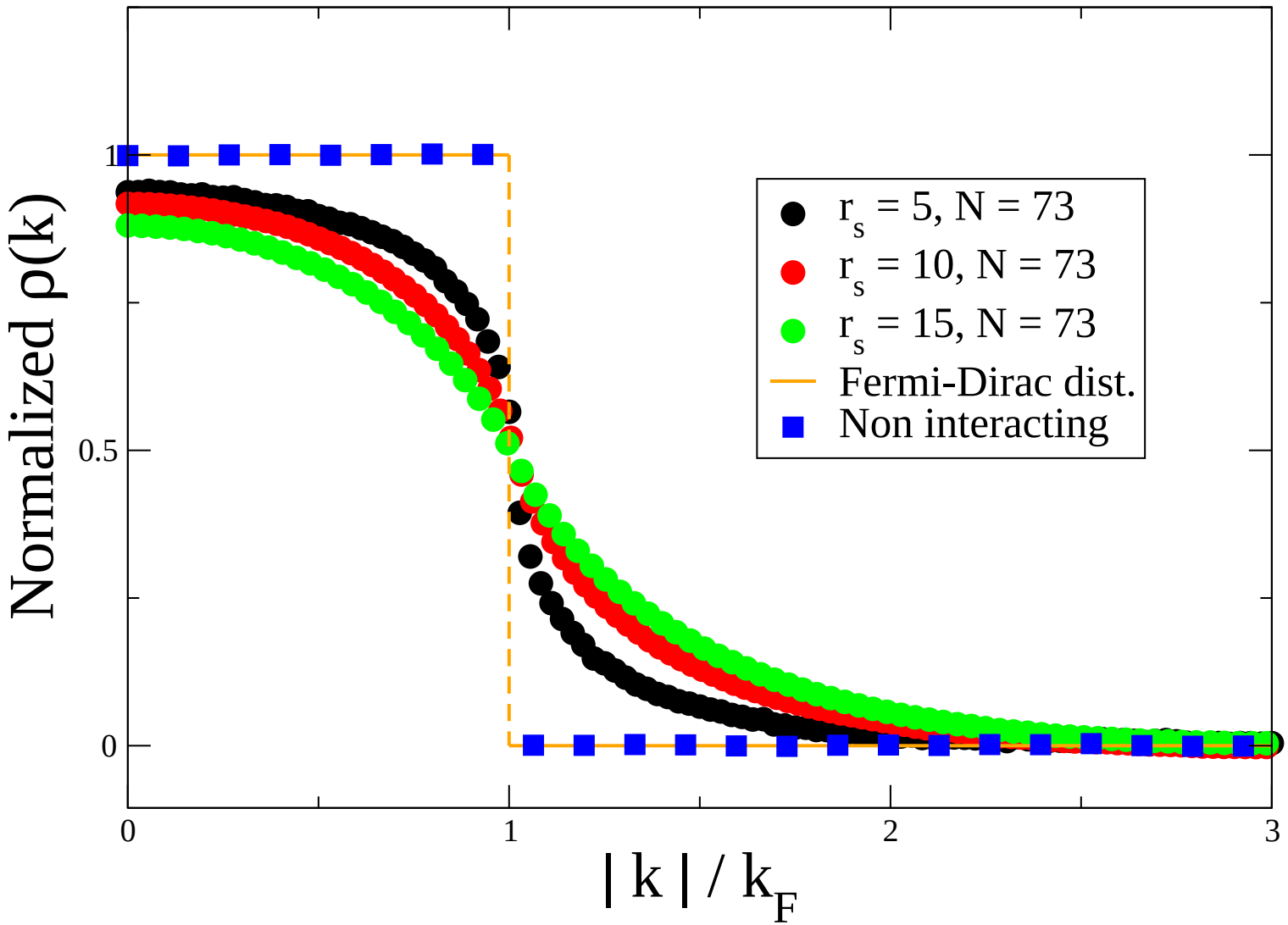
Wavefunction quality

Method	% $E_{\text{correlation}}$
DMC	100
VMC-SJ3BF	100.000(6)
VMC-SJ3	99.999(6)
VMC-SJ2BF	99.99996(6)
VMC-SJ2	99.9752(6)
HF	0

(this is for $r_s = 15$ au, $N = 15$ - the numbers above are typical)

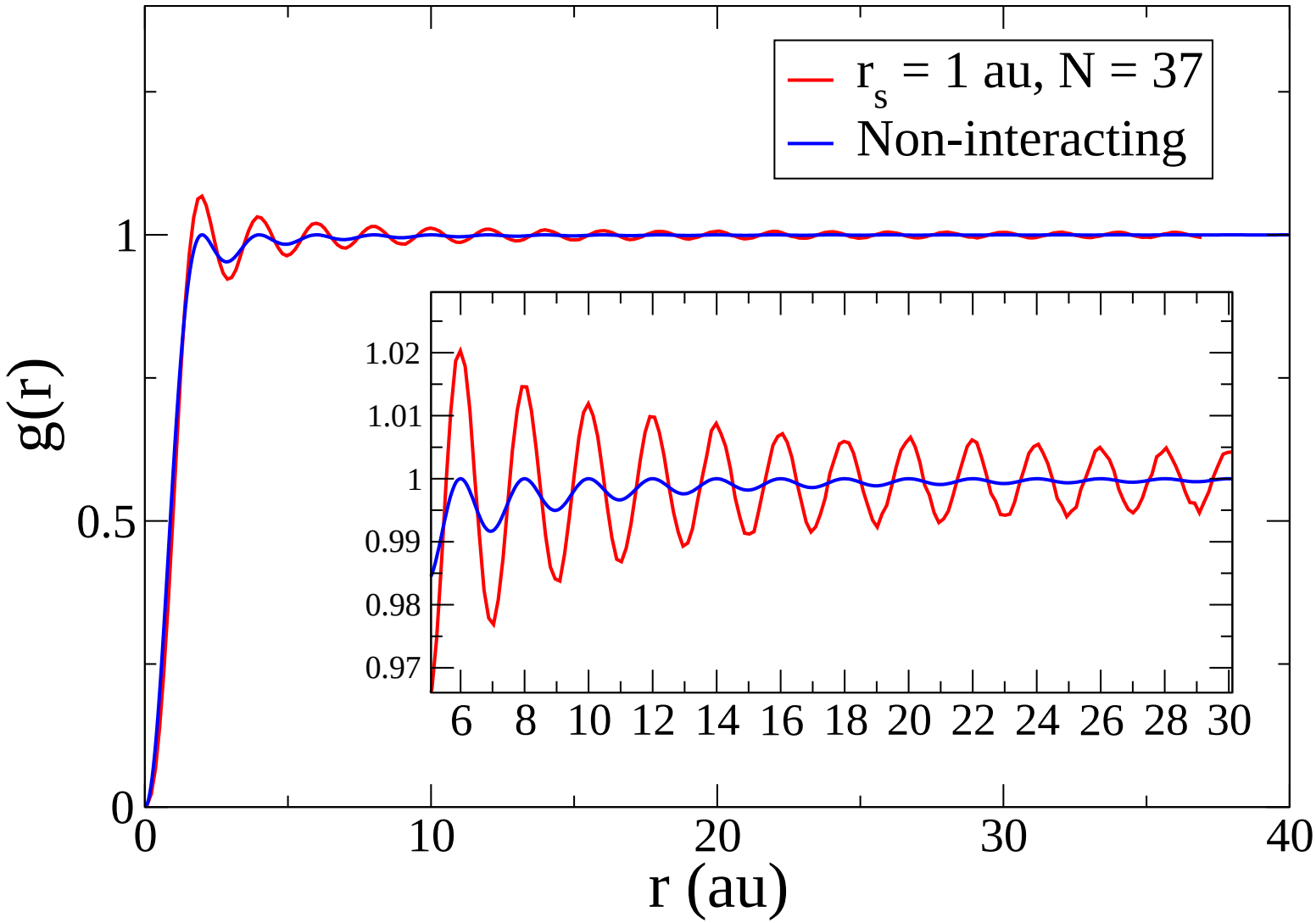
Momentum density

$$\rho(k) = \left\langle \frac{1}{2\pi} \int \frac{\Psi(r, x_2, x_3, \ldots, x_N)}{\Psi(x_1, x_2, x_3, \ldots, x_N)} \exp[ik(x_1 - r)]\, dr \right\rangle_{x_1,\ldots,x_n}$$



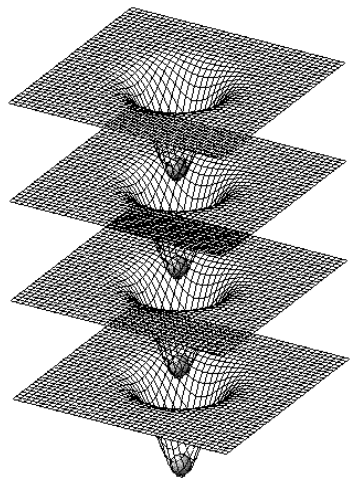
Pair correlation function

$$g(|x_1 - x_2|) = \frac{n(x_1, x_2)}{n(x_1)n(x_2)}, \qquad g_{\mathrm{non-int}}(x) = 1 - \left| \frac{\sin(k_F x)}{k_F x} \right|^2$$



Harmonic wire

A more sophisticated model has a wire of finite width - the confinement comes from a harmonic potential



If the confinement is strong enough, we can factorise the wavefunction

$$\Psi(\mathbf{R}) = \phi(x)\,\theta(r_\perp)$$

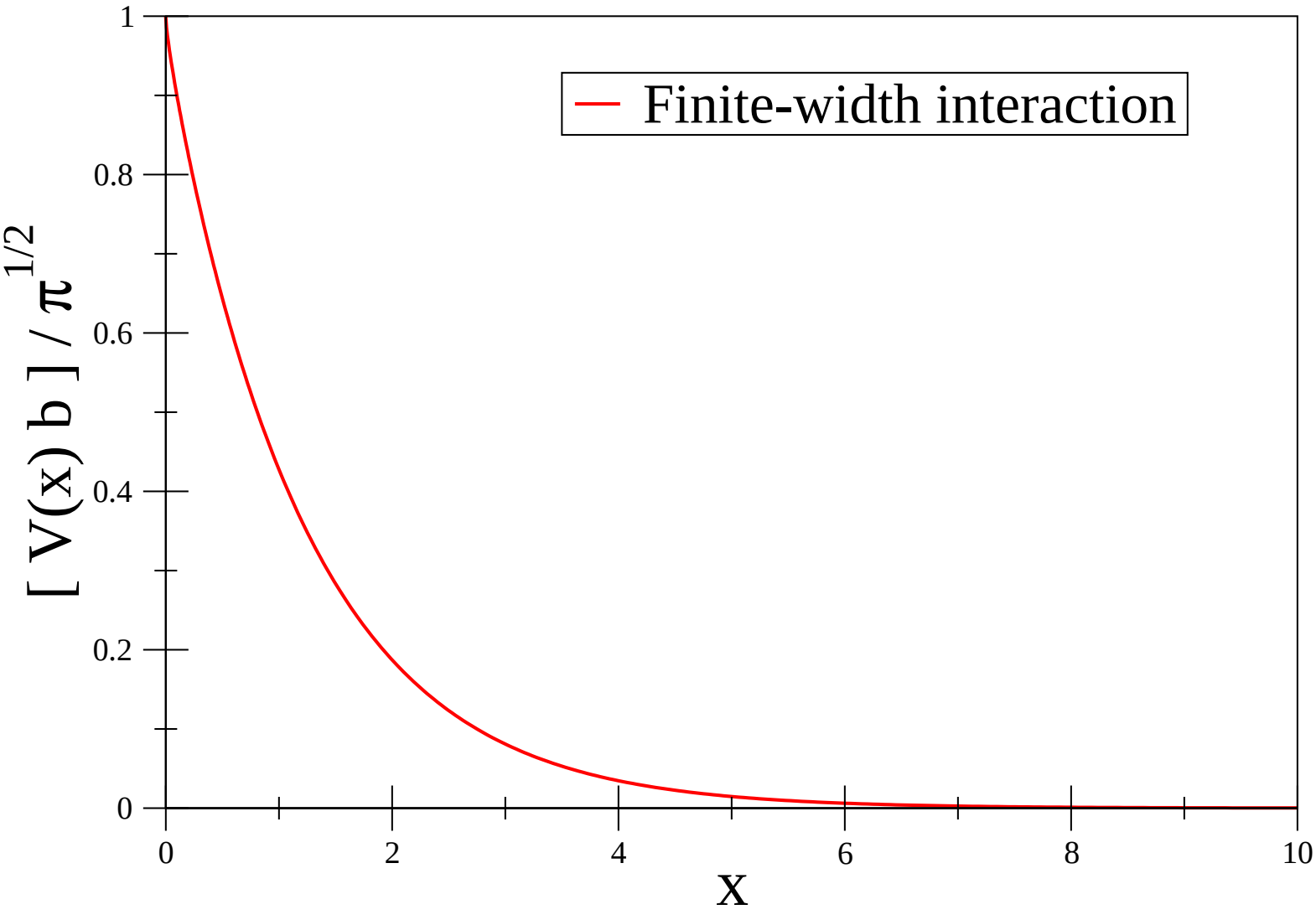
...and we know that $\theta(r_\perp)$ is a Gaussian

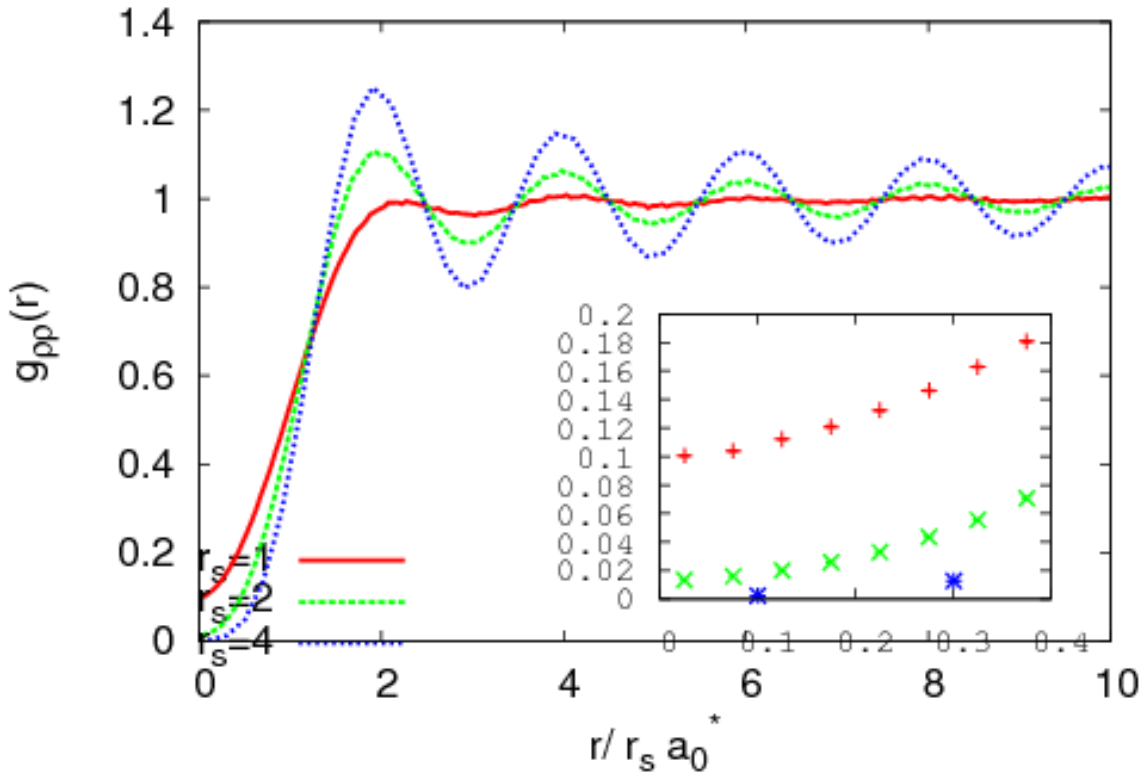
We can work out the interaction as a function of x by integrating over the transverse part of Ψ,

$$V(x) = \int \frac{|\theta(\mathbf{r}'_\perp)|^2 |\theta(\mathbf{r}_\perp)|^2}{\left[x^2 + (\mathbf{r}'_\perp - \mathbf{r}_\perp)^2\right]^{1/2}} \, d\mathbf{r}'_\perp \, d\mathbf{r}_\perp \, ,$$

putting in a Gaussian form for $\theta(\mathbf{r})$ yields

$$V(x) = \frac{\sqrt{\pi}}{b} \exp\left(\frac{x^2}{4b^2}\right) \operatorname{erfc}\left(\frac{|x^2|}{2b}\right) \, .$$


Finite-width interaction
[V(x) b] / π^1/2
X
0
0.2
0.4
0.6
0.8
1
0
2
4
6
8
10



Data kindly provided by Michele Casula

Summary

- Calculating the energy, PCF, SF and MD of the 1d HEG for both infinitely-thin and harmonic wire models
- Doing some fitting to the observables to compare with experimental literature
- Reliable calculations of the momentum density have not been seen before...

Acknowledgements

Neil Drummond

Richard Needs

EPSRC

Cambridge High Performance Computing Service

Step in the momentum distribution

The spectral function $A(\boldsymbol{\alpha}, \omega)$ is the probability density for increasing **or** decreasing the energy by an amount between $\hbar\omega$ and $\hbar(\omega + d\omega)$ upon adding **or** removing a single particle in the state $|\, \psi_{\boldsymbol{\alpha}}\rangle$

$\boldsymbol{\alpha}$ can describe spin, momentum, etc.

Forget spin for the moment and look at momentum states. The $T = 0$ momentum density is given by

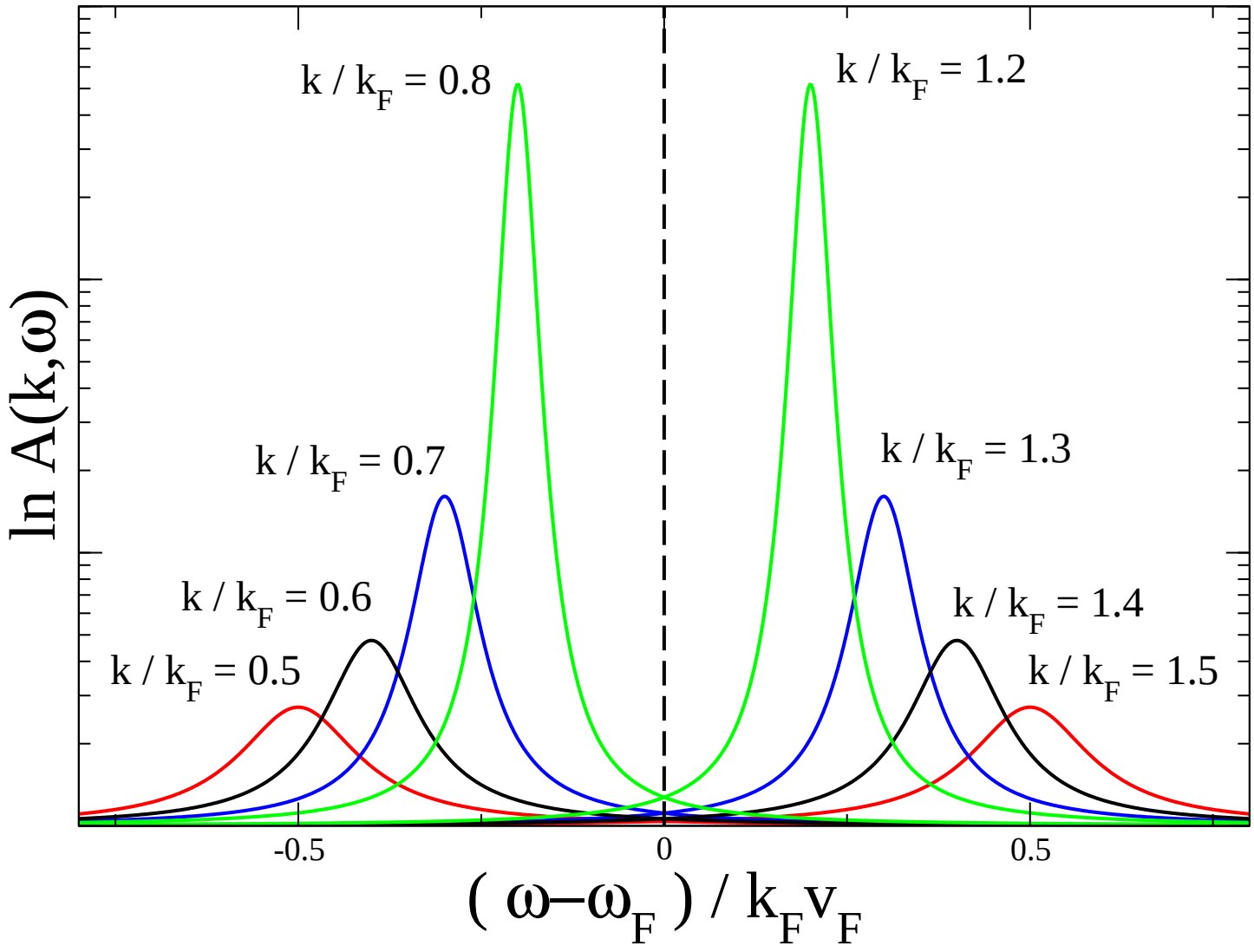
$$n_{\mathbf{k}} = \int_{-\infty}^{\mu/\hbar} A(\mathbf{k}, \omega) d\omega$$

In 2 and 3d, $A(\boldsymbol{\alpha}, \omega)$ has a (Lorentzian) quasiparticle peak, the width of which vanishes in the limit $k \longrightarrow k_F$ as $|k - k_F|^2$.

When $k > k_F$, the quasiparticle peak is at a frequency $\omega > \mu/\hbar$ and so does not fall within the limits of the integral, whereas for $k < k_F$ its contribution is its weight, Z.

Since it is a δ-function at the Fermi surface, the passing of the quasiparticle peak through $\omega = \mu/\hbar$ at $k = k_F$ results in the value of $n_{\mathbf{k}}$ having a discontinuity.

In 1d, there are no quasiparticles and the system is strongly-correlated ($Z = 0$), so there is no step in $n_{\mathbf{k}}$.


k / k_F = 0.8
k / k_F = 1.2
k / k_F = 0.7
k / k_F = 1.3
k / k_F = 0.6
k / k_F = 1.4
k / k_F = 0.5
k / k_F = 1.5
ln A(k,ω)
-0.5
0
0.5
(ω–ω_F) / k_F v_F