QMC and the 1d electron liquid

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- How we expect it to behave
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The ideal 1d model

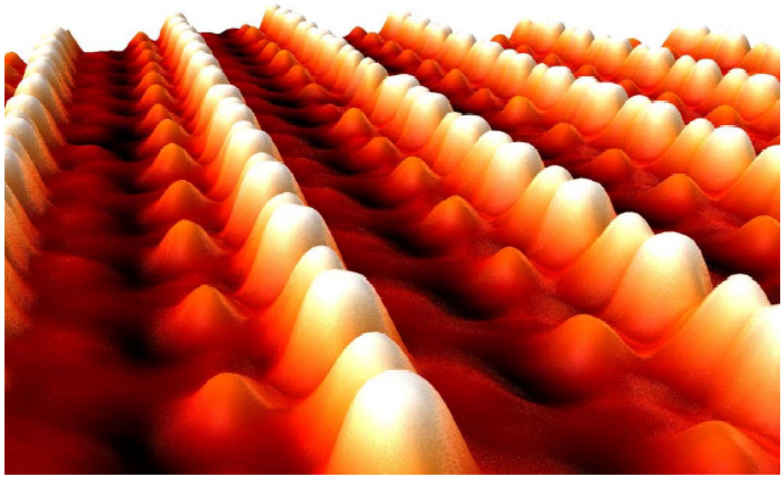
The model is simply 1d electrons on a uniform positive background

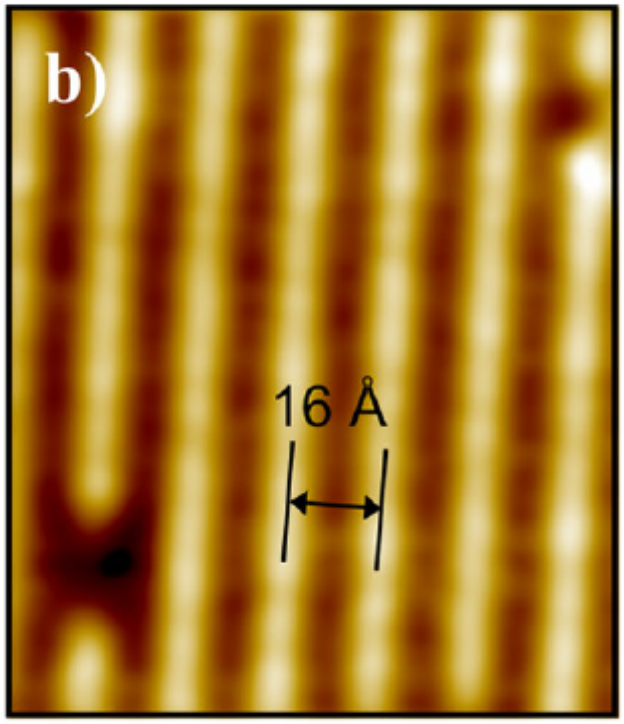
Many previous studies used regularized interactions so that the electrons may coalesce (and get past each other)

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

Where might this model be relevant?

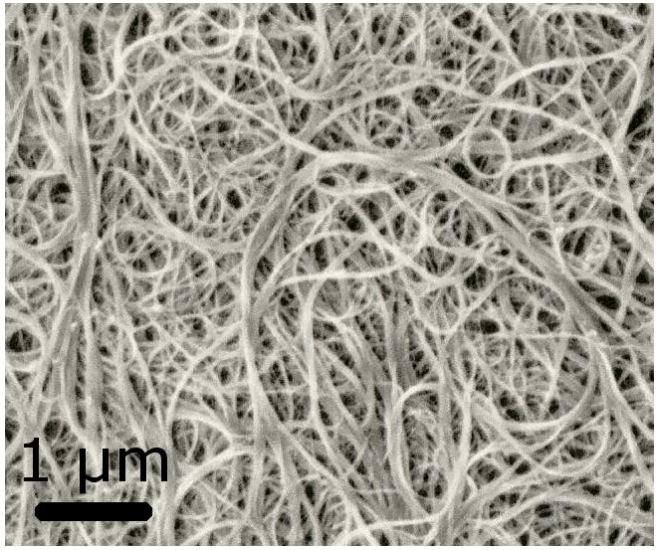
Nanowires of atoms

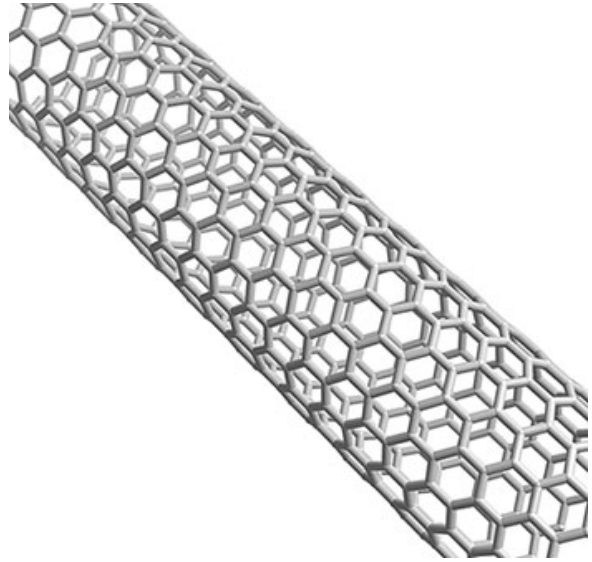




(left) Pt atoms on Ge. From Oncel *et al.* PRL **95**, 116801 (2005)
(right) Au atoms on Ge. From Schäfer *et al.* PRL **101**, 236802 (2008)

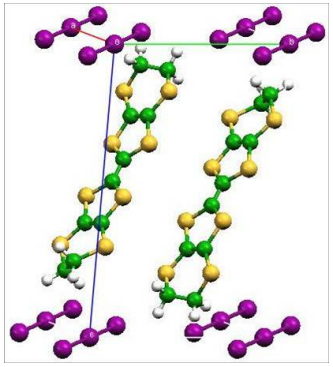
Carbon nanotubes

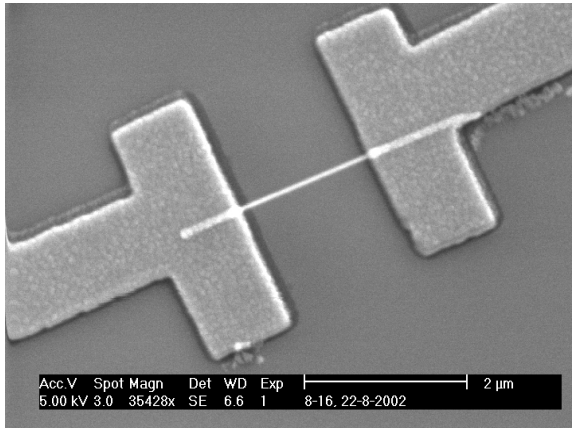




Single-walled CNTs in particular seem to exhibit behaviour characteristic of electrons in 1d.

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

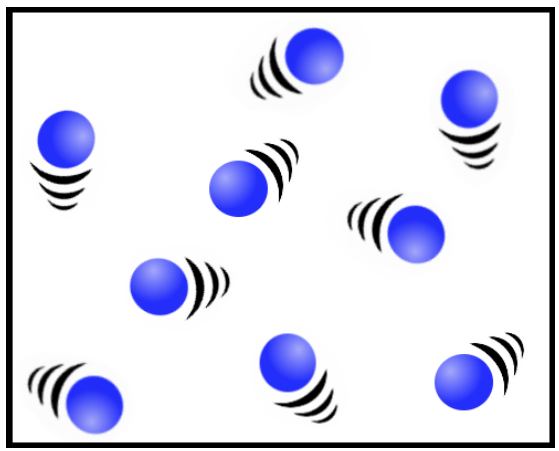


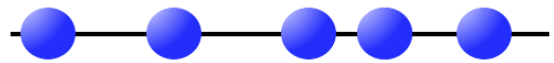


(left) charge-transfer salts (e.g. $(\text{BEDT-TTF})_2\text{X}$)
(right) semiconductor devices

Atoms (both fermions and bosons) in anisotropic traps, quantum Hall edge states, etc.

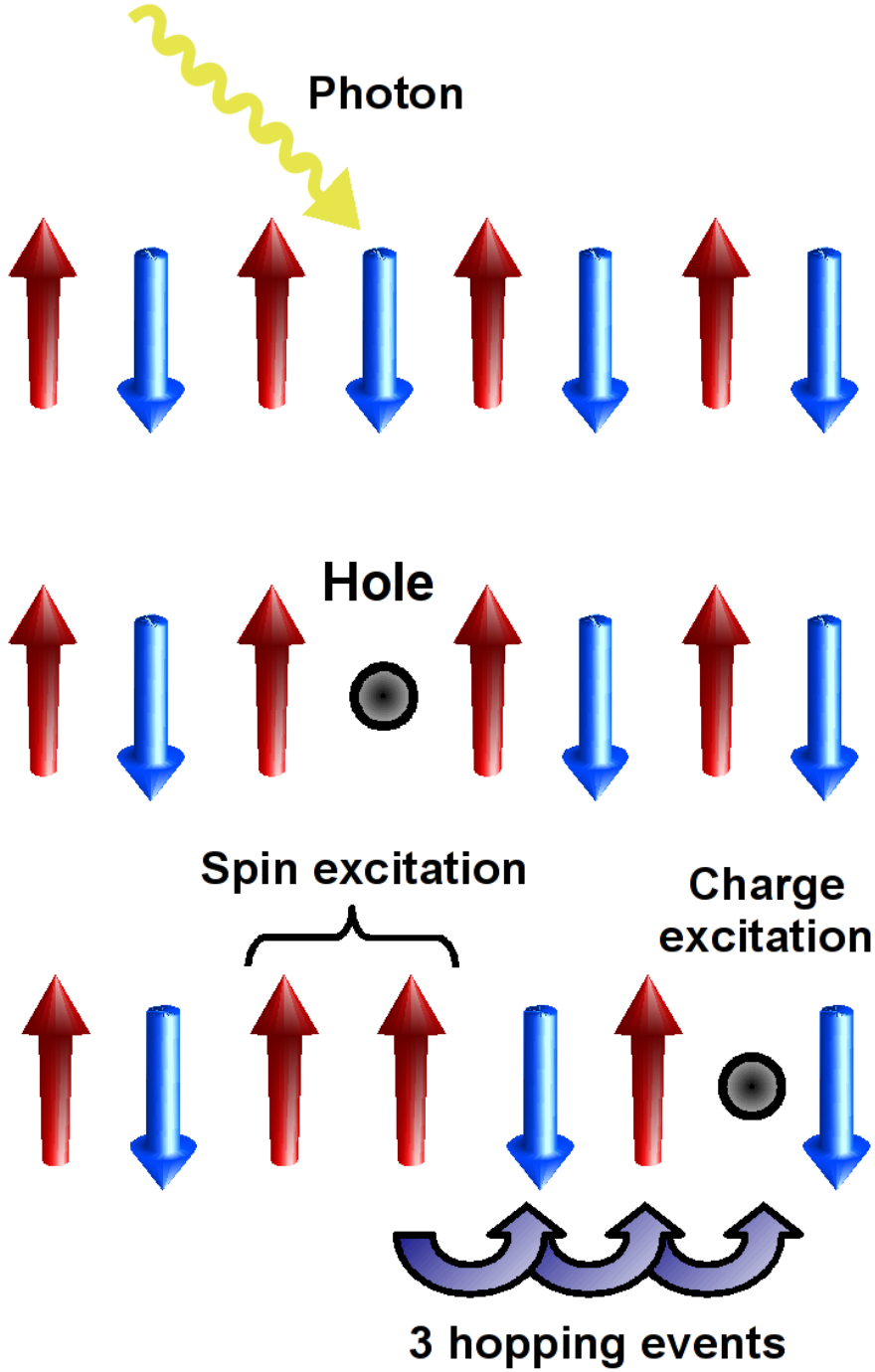
In 1d, particles cannot avoid each other





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
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 being the weight under the quasiparticle peak in the spectral function.

QMC calculations on the ideal 1d electron liquid

- The g.s. nodes are known - no fermion sign problem
- Twist averaging is simple - the grand canonical ensemble is the same as the canonical ensemble
- 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 $x_{ij} = |x_i - x_j|$.

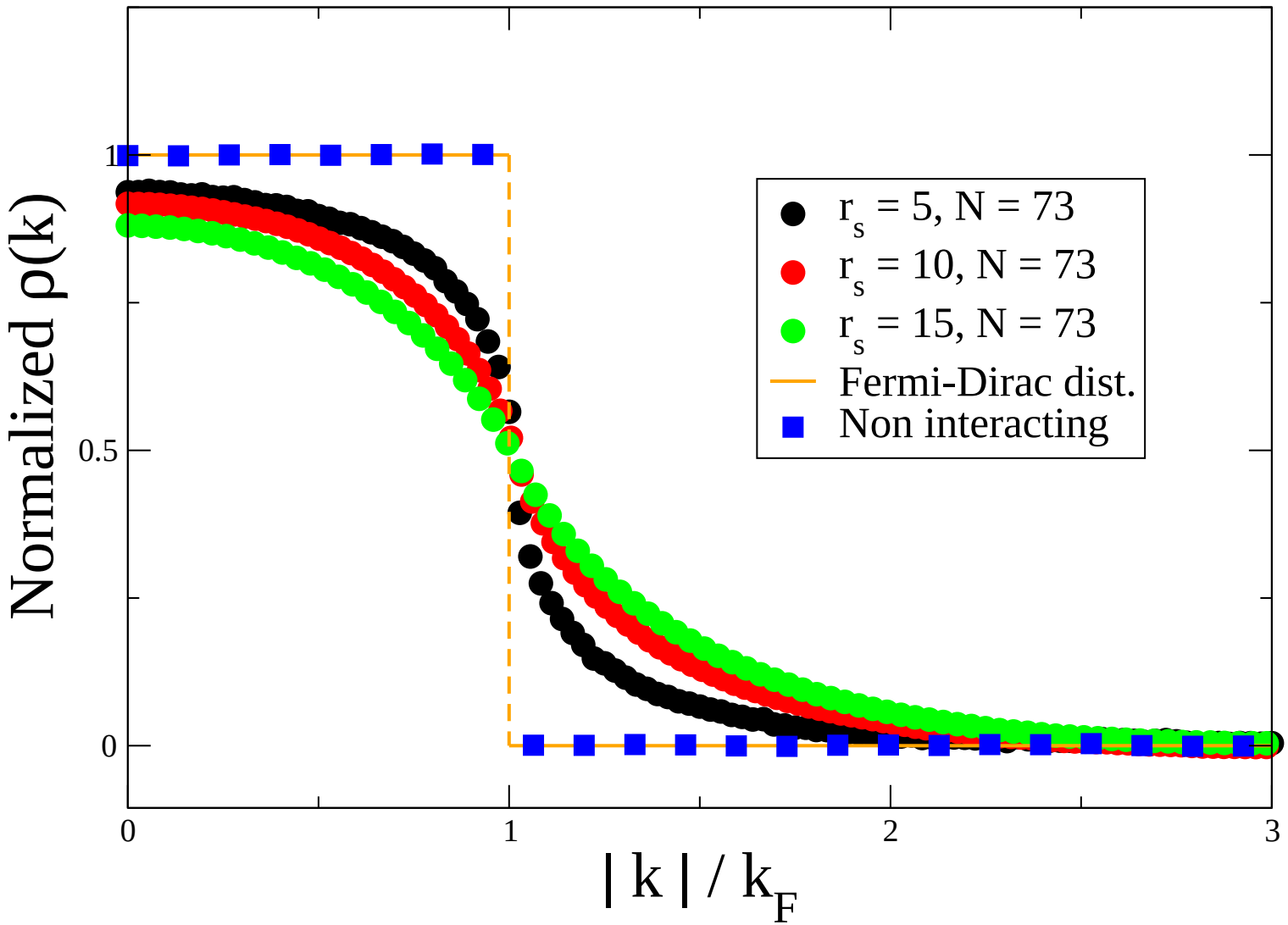
Wavefunction quality

Method	% E_{corr} retrieved
DMC	100
VMC-SJBF	99.99996(6)
VMC-SJ	99.9752(6)
HF	0

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

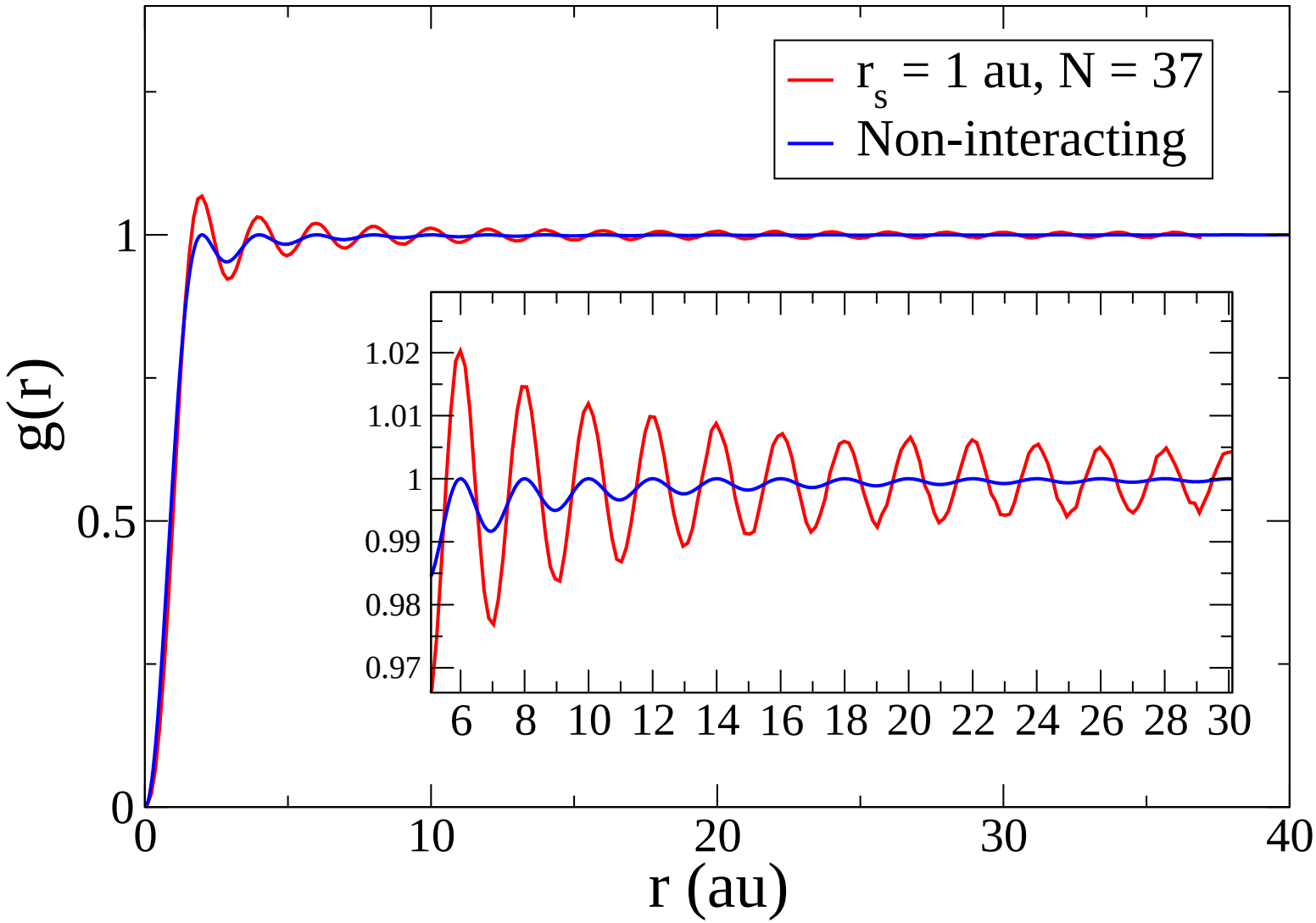
Momentum density

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



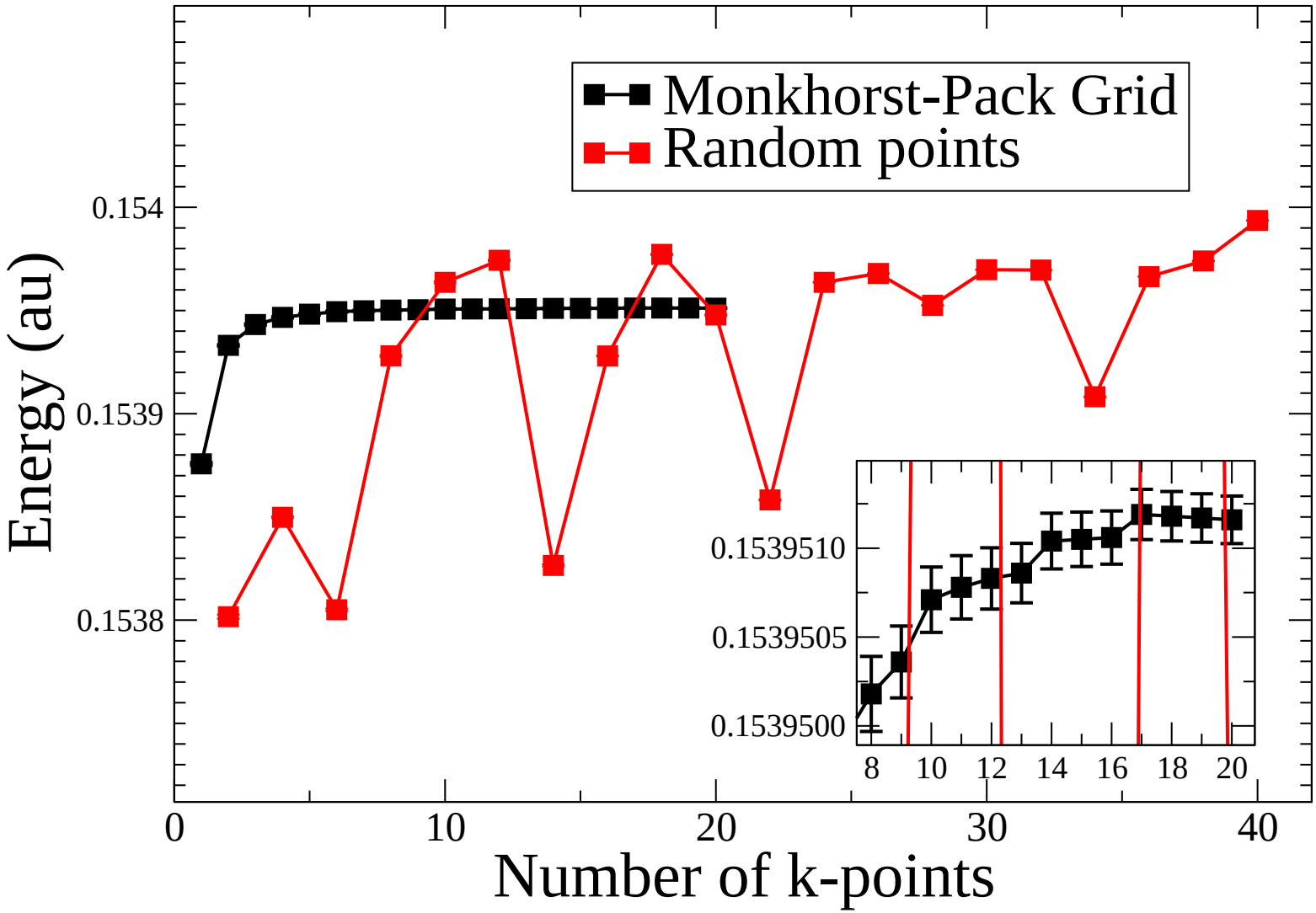
Pair correlation function

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



The nth point in MP grid of size $N/2$ (symmetry) was chosen by

$$k_n = \frac{2n - N - 1}{2N} G$$



Luttinger model parameters

GS correlation functions may be found exactly (for the model, at least) by bosonization, but the parameters may not.

For example, the momentum density behaves as

$$n(k) - n(k_F) \propto \mathrm{sgn}\{k - k_F\}|k - k_F|^{\alpha}$$

when $|k - k_F|$ is small. The oscillations in the PCF also decay characteristically $\propto \exp(-c\sqrt{\ln x})$

α may be written in terms of the Luttinger liquid parameter K_ρ,

$$\alpha = \frac{1}{4}\left(K_\rho + \frac{1}{K_\rho} + 2\right)$$

Many people have calculated these quantities for real systems...

R. Egger (Eur. Phys. J. B **3**, 281 (1998)) calculated (approximately) the parameter for a single-wall carbon nanotube

$$K_\rho = \left(1 + \frac{8e^2}{\pi\kappa\hbar v}\left[\ln\left(\frac{L}{2\pi R}\right) + 0.51\right]\right)^{-1/2},$$

which gives $K_\rho = 0.18$ for experimentally-determined parameters and a tube of length 3μm.

Others have found $K_\rho = 0.2$ for SWNTs and $0.20 < K_\rho < 0.23$ for the Bechgaard salts.

Getting K_ρ from our data is the next thing to do...

Summary

- Finding (density dependent) values of K_ρ so that experimentalists can say how close they are to ideal
- Observing LL-like behaviour and confirming the region of validity of the Luttinger model
- Producing exact results for the idealized system

Acknowledgements

Neil Drummond

Richard Needs

Mike Towler

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 $\mid \psi_{\boldsymbol{\alpha}} \rangle$

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

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

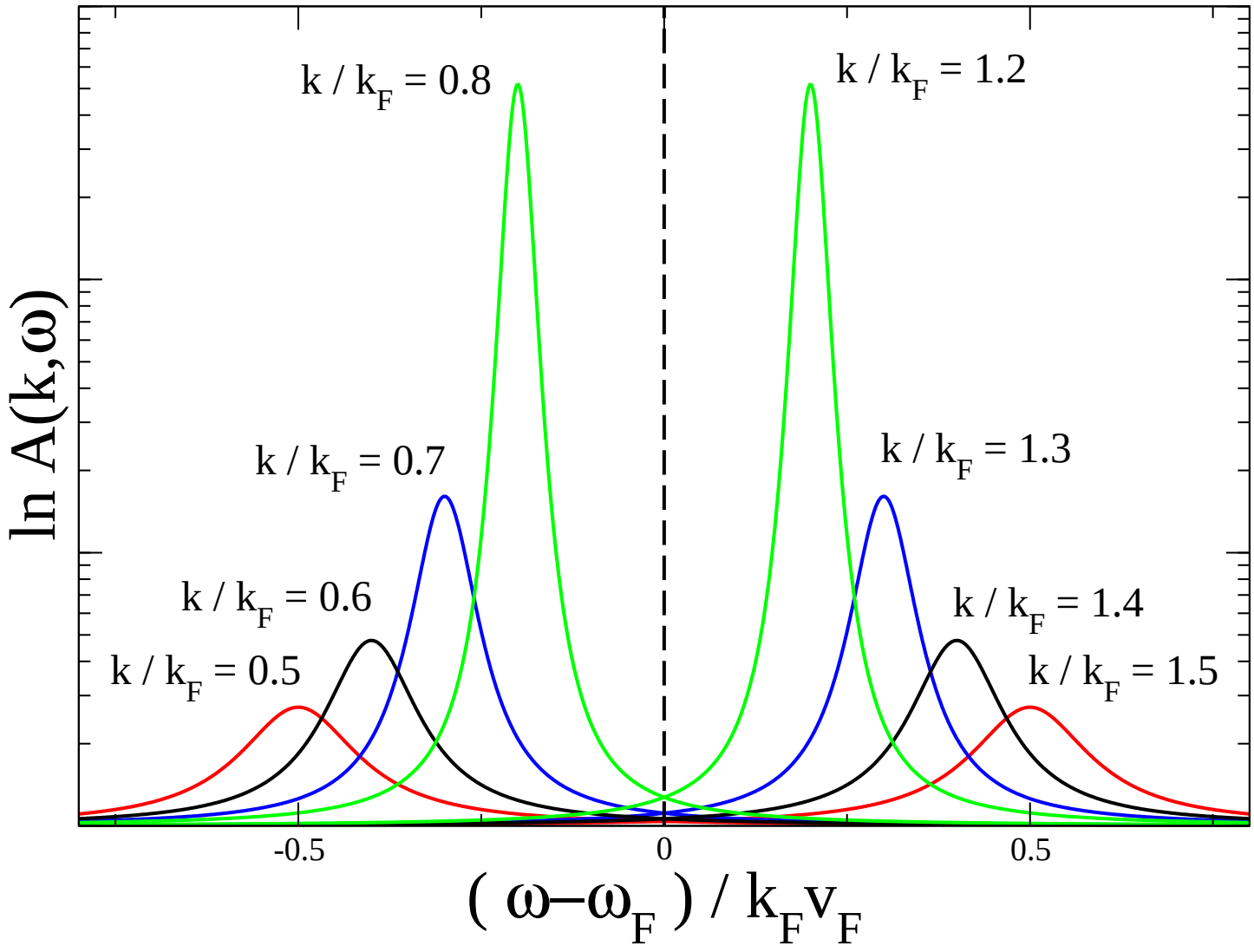
$$n_{\mathbf{k}} = \int_{-\infty}^{\mu/\hbar} A(\mathbf{k}, \omega) d\omega$$

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