Electron-electron biwire systems

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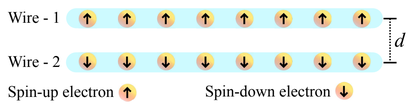
Model

electron density n in each wire, coupling parameter $r_s = 1/(2na_\mathrm{B})$, Bohr radius $a_\mathrm{B} = \epsilon/(e^2 m_e)$, Hartree atomic units ($\hbar = |e| = m_e = \epsilon = 1$)

electron-electron biwire: identical except spin



Hamiltonian

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{N}\left(\frac{\partial^2}{\partial \mathbf{x}_{i,1}^2}+\frac{\partial^2}{\partial \mathbf{x}_{i,2}^2}\right)+\sum_{i<j}\{V(x_{ij,1})+V(x_{ij,2})\}+\sum_{i,j}\frac{1}{\sqrt{|\mathbf{x}_{i,1}-\mathbf{x}_{j,2}|^2+d^2}}+NV_\mathrm{Mad}$$

where $x_{ij,m} = |x_{i,m} - x_{j,m}|$ distance between electron i located at $x_{i,m}$ and electron j located at $x_{j,m}$ in wire m, Ewald interaction $V(x_{ij,m})$ and Madelung energy V_Mad

Method

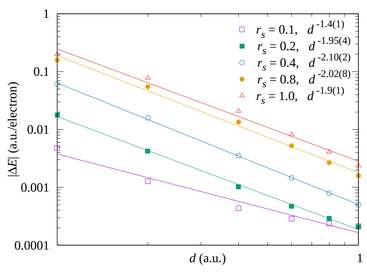
- variational Monte Carlo for Slater-Jastrow trial wave function
$$\Psi_T = D[\phi^\uparrow(x(\mathbf{R}))]D[\phi^\downarrow(x(\mathbf{R}))]e^{J(\mathbf{R})},$$
with orbital spin-up electron $\phi^\uparrow$, Slater determinant D
- backflow transformation: oordinates of electrons in Slater determinants are replaced by "quasi-particle coordinates" related to actual electron positions by backflow functions consisting of polynomial expansions in electron in-wire separation up to 8th order
- CASINO's Jastrow factors N. D. Drummond, M. D. Towler, and R. J. Needs, Phys. Rev. B 70, 235119 (2004)
- non-reweighted variance minimization N. D. Drummond and R. J. Needs, Phys. Rev. B 72, 085124 (2005) to optimize free parameters of trial wave function, 5×10^6 statistically independent steps and 1024 configurations
- comparison of variational MC and diffusive MC yields better than 99.9% agreement in ground state energy but less computationally costly

Correlational energy

interaction energy per electron $\Delta E = E_\mathrm{g}^2 - E_\mathrm{g}^1$ as difference between biwure and single wire

best fit $\Delta E = \dfrac{\exp(c)}{d^a}$

r_s	a	c
0.1	1.4(1)	-8.7(2)
0.2	1.95(4)	-8.59(5)
0.4	2.10(2)	-7.59(3)
0.8	2.02(8)	-6.3(1)
1.0	1.9(1)	-5.9(1)
2.0	1.5(1)	-4.4(2)
5.0	0.73(7)	-2.92(9)
10.0	0.45(3)	-2.71(4)
15.0	0.36(2)	-2.80(3)
20.0	0.32(2)	-2.92(2)



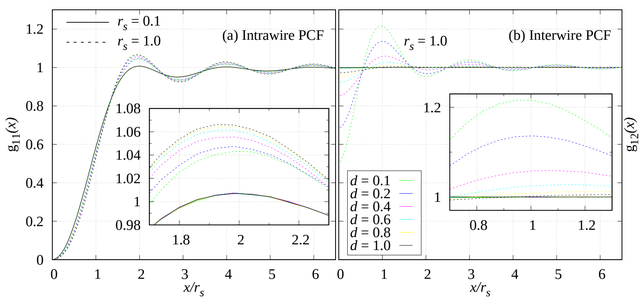
symbols calculated data and solid lines fitting, works for $1 < r_s < 20$ too

- interaction energy $\Delta E(d)$ and correlation energy of single wire $E_c(d) = E_c^1 + \Delta E(d)$, therefore, dependence of correlation energy on wire separation d is similar to $\Delta E(d)$

Pair-correlation function

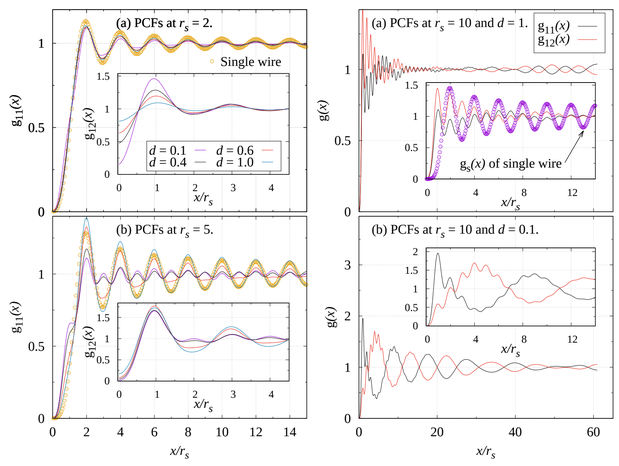
intra-wire (parallel-spin) $m = 1$, inter-wire (anti-parallel-spin) $m = 2$

$$g_{1m}(x) = \frac{1}{Ln_1n_m}\left\langle \sum_i \sum_j \delta(x_{i,1} - x_{j,m} - x)\right\rangle$$



- oscillations in g_{12} increases, in g_{11} decreases, as d decreases
- correlations between electrons of different wires are build on and intra-wire correlations are suppressed as two wires approach
- first peak in g_{11} and g_{12} near $r = 2r_s$ and $r = r_s$, both g_{11} and g_{12} oscillates with a period $2r_s$
- as d reduces, first peak of g_{12} rises and shifts towards origin while for g_{11} it shrinks and shifts away from origin
- $g_{12}(r)$ at $r = 0$ shifts towards zero as d reduces, because with decreasing d, electrons in different wires repel each other and $g_{12}(0)$ becomes smaller

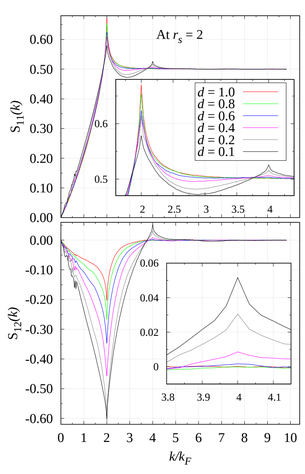
Low-density pair-correlation function



Symbols represents data for single wire

- for $r_s = 5$ a small peak develops in g_{11} at $r = r_s$ when inter-wire distance is reduced to 0.6 a.u. rising with reduction in d
- at distance $d = 0.4$ a.u. g_{11} oscillates with period of r_s rather than with $r = 2r_s$
- similar to g_{11}, also g_{12} oscillates at period $r = r_s$ for $d \leq 0.4$ a.u.
- at $r_s = 5$ for close proximity of two wires, we interpret change in period as tendency towards formation of Wigner crystal phase
- at $r_s = 10$ oscillations in both inter- and intra-wire PCFs are enhanced further, inter-wire correlations are comparatively stronger than intra-wire correlations as range of d is significantly smaller than r_s
- two kinds of osculations, period of r_s enveloped by second kind of oscillation due to interplay between intra- and inter-wire correlations

Static structure factor



$$S(k) = 1 + \frac{2N}{L}\int [g(x) - 1]e^{-ikx}dx$$

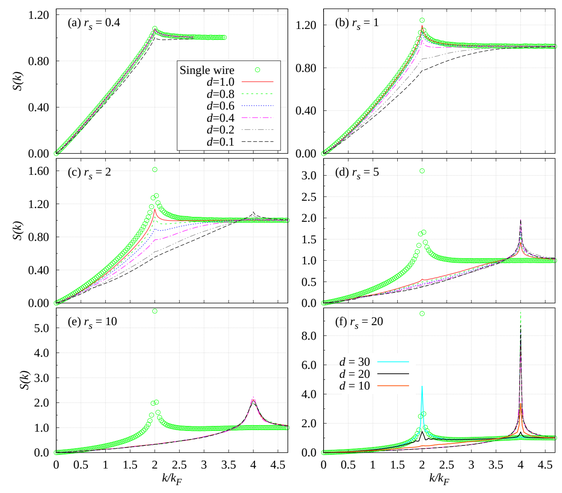
with

$$g(x) = \sum_a \sum_b \frac{n_a n_b}{n^2} g_{ab}$$

- inter-wire SSF $S_{12}(k)$ negative for small k and has strong peak at $2k_F$
- $S_{12}(k)$ gets positive before $4k_F$ and a second peak builds up at $4k_F$ for $d = 0.4$ whose height increases as d reduced further

Sum over spin pairs

$$S(k) = S_{11}(k) + S_{12}(k) + S_{21}(k) + S_{22}(k)$$



open circles: isolated single wire

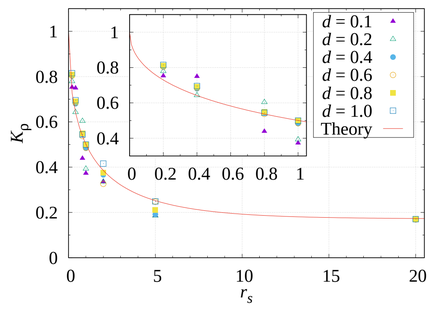
- for high densities small peak at $2k_F$ whose height decreases as d becomes smaller (a), (b)
- lower density, correlation effects become more important (c), for $r_s = 2$ a second peak appears at $4k_F$ when d is reduced to 0.2 a.u., no such peak in single isolated wire
- increasing r_s, the $4k_F$ peak rises while no $2k_F$ peak d $1...0.1$
- at $r_s = 20$ the peak at $2k_F$ reappears (f)
- peak at $4k_F$ signals ordered structure, Wigner crystallization at much lower densities as compared to the single wire

Momentum distribution

fitting $n(k)$ within the range $|k - k_F| < \epsilon k_F$

$$n(k) = \frac{1}{2\pi}\left\langle \int \frac{\Psi_T(r)}{\Psi_T(x_1)} e^{ik(x_1 - r)}dr \right\rangle = n(k_F) + A[\mathrm{sign}(k - k_F)]|k - k_F|^\alpha$$

Luttinger parameter $K_\rho = 1 + 2\alpha - 2\sqrt{\alpha + \alpha^2}$



$K_\rho > 1$ attractive, $0 < K_\rho < 1$ repulsive

solid line: isolated single wire $\alpha = \tanh\left(\dfrac{r_s}{8}\right)$ which passes closely to larger d data

Summary

- parallel infinitely-thin electron-electron quantum biwire system studied by variational Monte Carlo method
- interaction energy falls off as d^{-2} for high densities where d is comparable to r_s, for low densities $d \ll r_s$ smaller exponent
- pair correlation function shows oscillatory behavior with two frequencies
- as wires approach, inter-wire correlations increase while intra-wire correlations decrease
- static structure factor shows a peak at $2k_F$ at higher densities, a second peak starts to appear at $4k_F$ when $r_s = 2$ and $d = 0.2$ a.u., which is not found for $d > 0.2$
- for lower densities, first peak completely disappears and the height of the second peak keeps increasing with r_s and d
- electron-electron biwire system goes into a quasi-Wigner crystalline state at densities higher compared to the case of a single wire
- momentum distribution reveals a Tomonaga-Luttinger (TL) liquid behavior with power law nature near k_F even in presence of an extra interwire interaction

books and paper: http://www.k-morawetz.de

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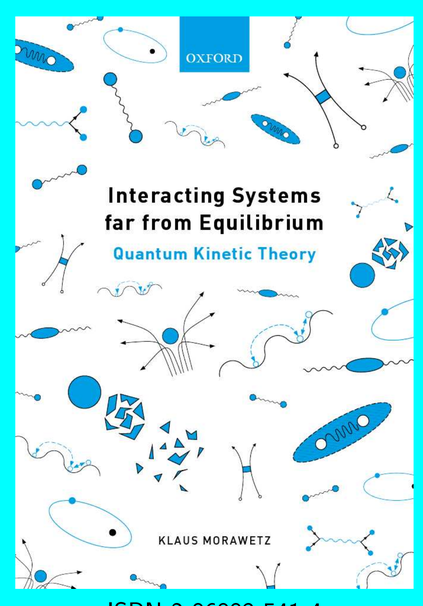

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