Confinement in quasi-one-dimensional quantum wires

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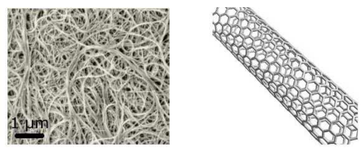
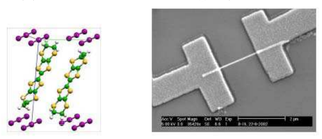
Experimental realization of 1D systems

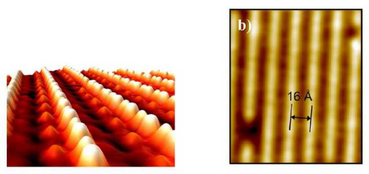


single-walled carbon nanotubes

http://www.ipt.arc.nasa.gov/cabonnano.html



Bechgaard salts and semiconductor wires



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

Confinement models of wire

Hamiltonian for simulating spin-polarized (ferromagnetic) N-electrons

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} + \sum_{i<j}\tilde{V}(x_{ij}) + \frac{N}{2}V_{\mathrm{Mad}}$$

Ewald sum $\tilde{V}(x_{ij})$, Madelung energy $V_{\mathrm{Mad}} = \lim_{x\to 0}\left[\tilde{V}(x) - V(0)\right]$
Hartree atomic units (a.u.), $\hbar = |e| = m_e = \epsilon = 1$ a.u.

1. model

soften Coulomb potential $V(x) = 1/\sqrt{x^2+b^2}$ where b transverse width parameter of the cylindrical wire

$$V(q) = 2K_0(bq) = -2\left[\ln\left(\frac{bq}{2}\right)+\gamma\right] - \frac{b^2q^2}{2}\left[\ln\left(\frac{bq}{2}\right)+\gamma-1\right] + O\left(b^3\right)$$

2. model

harmonically regularized Coulomb potential $V_\perp(r_\perp) = r_\perp^2/8b^4$, integrating transverse degrees of freedom: $\frac{\sqrt{\pi}}{2b}e^{\frac{x^2}{4b^2}}\mathrm{erfc}\left(\frac{|x|}{2b}\right)$ and

$$V(q) = E_1(b^2q^2) = -2\left[\ln(bq)+\frac{\gamma}{2}\right] - b^2q^2\left[2\ln(bq)+\gamma-1\right] + O\left(b^3\right)$$

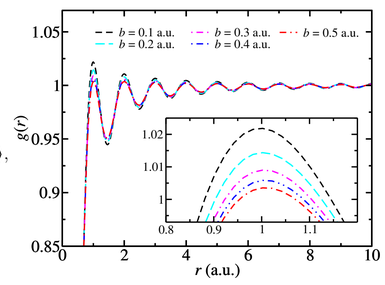
Quantum Monte Carlo simulation

casino code R. J. Needs et al., J. Phys. Condens. Mat. 22 (2010) 023201
details: V. Ashokan et al., Phys. Rev. B 98 (2018) 125139
harmonic wire for N = 99 at $r_s = 0.5$

parallel-spin pair-correlation function

$$g_{\uparrow\uparrow}(x) = \frac{1}{\rho_\uparrow^2}\left\langle\sum_{i>j}^{N_\uparrow}\delta(|x_{i,\uparrow}-x_{j,\uparrow}|-x)\right\rangle,$$

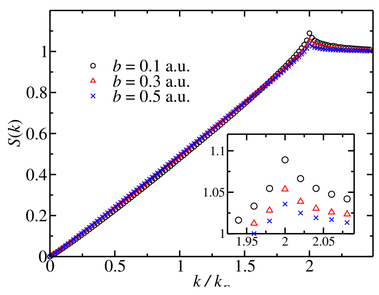
with spin σ, electron density ρ_σ



static structure factor

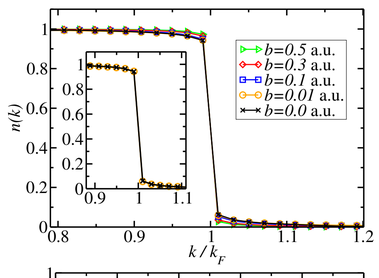
$$S(k) = \frac{1}{N}\langle\rho(-k)\rho(k)\rangle$$

where $\rho(k) = \sum_i e^{ikr_i}$



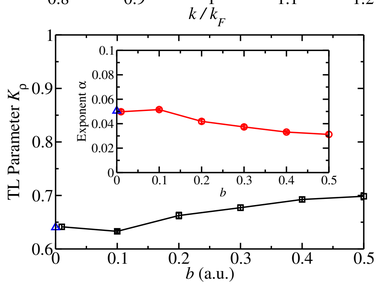
momentum distribution

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



Tomonaga-Luttinger parameter

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



Density response function

parameter λ indicates the order of expansion

$$\chi(q,\omega) = \chi_0(q,\omega) + \lambda\, v(q)\chi_0^2(q,\omega) + \lambda\,\chi_1^{se}(q,\omega) + \lambda\,\chi_1^{ex}(q,\omega)$$

non-interacting polarizability

$$\chi_0(q,\omega) = \frac{g_s m}{2\pi q}\ln\left[\frac{\omega^2-(\frac{q^2}{2m}-\frac{qk_F}{m})^2}{\omega^2-(\frac{q^2}{2m}+\frac{qk_F}{m})^2}\right],$$

self-energy contribution

$$\chi_1^{se}(q,\omega) = 2g_s\sum_{k,p}n_k n_p[v(k-p)-v(k-p+q)]\frac{\Omega_{k,q}^2+\omega^2}{(\Omega_{k,q}^2-\omega^2)^2}$$

exchange contribution

$$\chi_1^{ex}(q,\omega) = -2g_s\sum_{k,p}\left\{v(k-p)[n_{k-\frac{q}{2}}n_{p-\frac{q}{2}}-n_{k-\frac{q}{2}}n_{p+\frac{q}{2}}] \times\frac{(\Omega_{k-\frac{q}{2},q}\,\Omega_{p-\frac{q}{2},q}+\omega^2)}{(\Omega_{k-\frac{q}{2},q}^2-\omega^2)(\Omega_{p-\frac{q}{2},q}^2-\omega^2)}\right\}$$

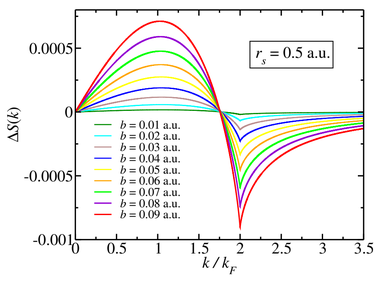
with $\Omega_{k,q} = \omega_k - \omega_{k+q}$, $\Omega_{p,q} = \omega_p - \omega_{p+q}$, spin degeneracy g_s, Fermi-Dirac distribution function n_k

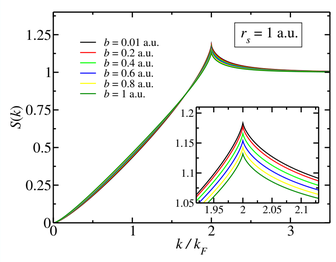
Analytical results

static structure factor

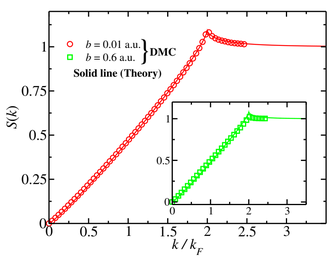
$$S(q) = -\frac{1}{\pi\, n}\int_0^\infty d\omega\,\mathrm{Im}\,\chi(q,\omega) = S_0(q) + S_1^d(q) + S_1^{se}(q) + S_1^{ex}(q)$$

$$\Delta S(k) = S_1^{Hr.}(x,b) - S_1^{Hr.}(x)$$
$r_s = 0.5$





harmonic wire as a function of k/k_F at $r_s = 1$

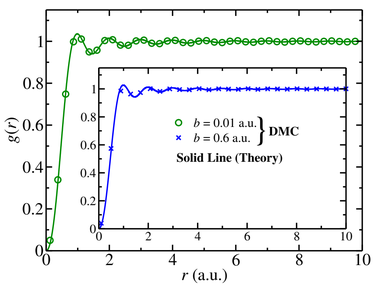


comparison with DMC for $N = 99$ at $r_s = 0.5$

pair-correlation function

$$g(r) = 1 - \frac{1}{2\pi n}\int_{-\infty}^{\infty}dq\, e^{iqr}[1-S(q)]$$

theoretical result compared with DMC for $N = 99$ at $r_s = 0.5$ for harmonic wire, main plot for $b = 0.01$ and inset for $b = 0.6$



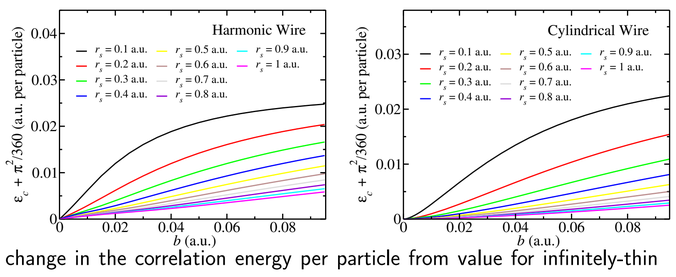
Correlation energy

fluctuation-dissipation theorem

$$E_g = E_0 + \frac{n}{2}\sum_{q\neq 0}V(q)\left(-\frac{1}{n\pi}\int_0^1 d\lambda\int_0^\infty\chi(q,\iota\omega;\lambda)\,d\omega - 1\right) = E_0 + E_x + E_c$$

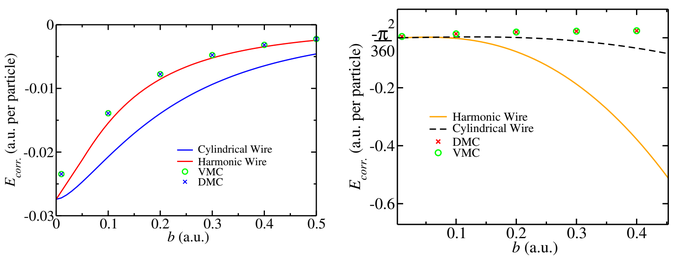
with kinetic energy $E_0 = \pi^2/24r_s^2$, analytical expression for wire-width-dependent correlation energy up to $O\left(b^2\right)$ Grindhar et al., Phys. Rev. B 105 (2022) 115140

$$\epsilon_c(b,r_s) = -\frac{\pi^2}{360} - \frac{b^2}{216{g_s}^2{r_s}^2}\left[6\left(3+\pi^2\right)\ln\left(\frac{\pi b}{g_s r_s}\right) + 72\zeta(3) + \begin{cases}3\gamma\left(3+\pi^2\right) - 2\pi^2 - 42\right] & \text{harmonic wire}\\ 6\gamma\left(3+\pi^2\right) - 5\pi^2 - 51 - \pi^2\ln(64) - 18\ln(2))\right] & \text{cylindrical wire}\end{cases}$$



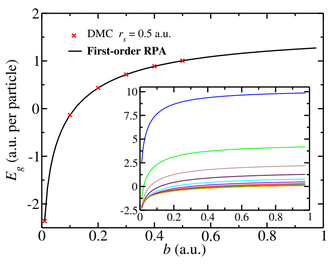
change in the correlation energy per particle from value for infinitely-thin wire for harmonic (left) and cylindrical wire (right)

Comparision with QMC

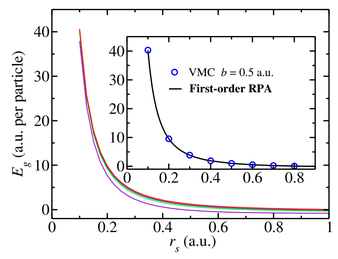


Ground-state energy

$$E_g = E_0 + E_x + E_c$$



main plot for $r_s = 0.5$ compared with DMC simulation an inset for $r_s = 0.2$ - 1 in steps of 0.1 (top to bottom)



as function of density parameter r_s, main plot for $b = 0.1, 0.3, 0.5, 0.7, 0.9$ (bottom to top), inset for $b = 0.5$ compared with VMC

- as the wire width is reduced the ground state energy decreases
- becomes negative beyond some b signifying existence of a more stable and bounded system

Summary

- ground-state properties of ferromagnetic quasi-quantum wire using quantum Monte Carlo (QMC) method for various thicknesses and densities
- correlation energy, pair-correlation function, static structure factor, and momentum density are calculated for various wire widths at high-density
- the peak in static-structure factor at $k = 2k_F$ grows sub-linearly as the wire width decreases
- thermodynamic limit of Tomonager-Luttinger parameter for several wire widths at high densities, varies about 10% for wire widths $b = 0.01$ to $b = 0.5$
- first-order RPA with exchange and self-energy contributions leads to analytical expressions for the structure factor and correlation energy
- high-density analytical results in agreement with quantum Monte Carlo simulation
- exact correlation energy varies as b^2 for $b << r_s$ from its value of an infinitely-thin wire, significantly depends on two wire models used

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

1. Eur. Phys. J. B 91 (2018) 29, *Dependence of structure factor and correlation energy on the width of electron wires*, Vinod Ashokan, Renu Bala, Klaus Morawetz, and Karem N. Pathak
2. Phys. Rev. B 97 (2018) 155147, *Conditions where RPA becomes exact in the high-density limit*, Klaus Morawetz, Vinod Ashokan, Renu Bala, and Karem N. Pathak
3. Phys. Rev. B 101 (2020) 075130, *Exact ground-state properties of the one-dimensional electron gas at high density* ,Vinod Ashokan, Renu Bala, Klaus Morawetz, and K. N. Pathak
4. Phys. Rev. B 104 (2021) 035149, *Ground-state properties of electron-electron biwire systems*, R. O. Sharma, N. D. Drummond, V. Ashokan, K. N. Pathak, K. Morawetz
5. Phys. Rev. B 105 (2022) 115140, *Electron correlation and confinement effects in quasi-one-dimensional quantum wires at high density*, A. Girdhar, V. Ashokan, N. D. Drummond, K. Morawetz, K. N. Pathak