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Electronic properties of junctions of quantum wires

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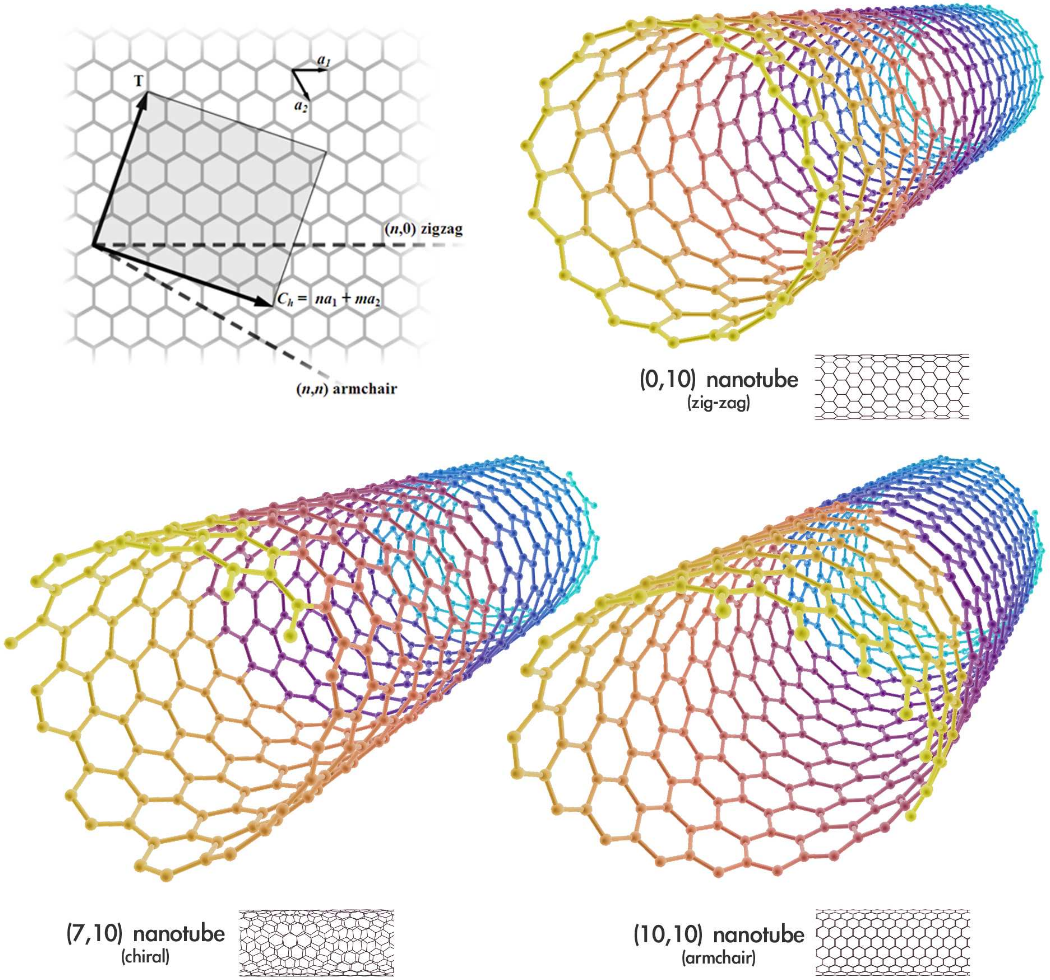
Based on *V.C, E. Ragoucy, Nucl. Phys. B828 (2010), 515 and arXiv:0907.5359* and preliminary work with M. Minthev

INTRODUCTION

Motivation: theoretical description of circuits of carbon nanotubes



Amazing realizations:

- transistors

- simple electronic circuits

This talk in a nutshell

Why can we hope to get such a description?

3 facts

- Low energy properties of interacting electrons in single wall carbon nanotubes have been shown[1] to be captured by an integrable one-dimensional effective model: the Tomonaga-Luttinger model.

- This model has been solved on a star graph[2]. Crucial ingredient: scattering properties at the central vertex.

- Scattering properties on any finite connected graph with external edges can be effectively described by a star graph[3].

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[1] R. Egger and A. Gogolin, Phys. Rev. Lett. 79 (1997) 5082; C. Kane, L. Balents, M. Fisher, Phys. Rev. Lett. 79 (1997) 5086

[2] B. Bellazzini, M. Mintchev, P. Sorba, J.Phys.A40:2485-2508,2007

[3] V. Caudrelier, E. Ragoucy, Nucl.Phys.B828:515-535,2010

Conclusion : to model an arbitrary circuit of nanotubes, put the model on a graph: edges=nanotubes and vertices=connections.

Plan

1. The ingredients

- Solution of the Tomonaga-Luttinger model via bosonization
- Solution on a star graph: role of Reflection-Transmission algebras and scattering matrix
- Effective description of an arbitrary graph as a star graph

2. The recipe: example of a ring in a magnetic field

- Total scattering matrix
- Conductance

3. Conclusions

1.1 Solution of the Tomonaga-Luttinger model via bosonization

- Model on the line for two fermionic fields ψ_1, ψ_2 with Lagrangian density

$$\mathcal{L} = i\psi_1^\dagger(\partial_t+\partial_x)\psi_1+i\psi_2^\dagger(\partial_t-\partial_x)\psi_2-g_+(\psi_1^\dagger\psi_1+\psi_2^\dagger\psi_2)^2-g_-(\psi_1^\dagger\psi_1-\psi_2^\dagger\psi_2)^2 .$$

- Solvable by expressing the fermionic fields in terms of bosonic free massless fields φ, $\widetilde{\varphi}$ satisfying

$$(\partial_t^2 - \partial_x^2)\varphi = 0 \quad , \quad \partial_t\widetilde{\varphi} = -\partial_x\varphi \quad , \quad \partial_x\widetilde{\varphi} = -\partial_t\varphi$$

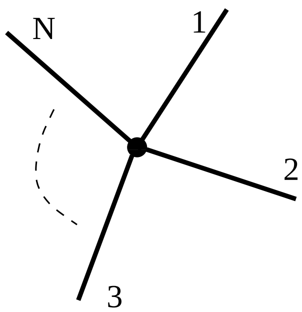
- The fields φ, $\widetilde{\varphi}$ are expressed in the usual way in terms of creation/annihilation operators

$$[a(k_1)\,,\,a(k_2)] = 0 = [a^\dagger(k_1)\,a^\dagger(k_2)] \quad , \quad [a(k_1)\,,\,a^\dagger(k_2)] = 2\pi\,\delta(k_1-k_2)$$

- The correlation functions of the quantum fermionic theory can then be computed using a representation of this algebra.

1.2 Solution on a star graph

- Put the previous model on a star graph with N external edges and one central vertex: fermionic fields $\psi_1(x, t, j)$, $\psi_2(x, t, j)$, $j = 1, ..., N$, $x > 0$.



- On top of interactions on the external edges, presence of interactions at the vertex encoded in boundary conditions on the fields at $x = 0$.

- Same principle of solution as before: N pairs of free bosonic massless fields $\varphi(x, t, j)$, $\widetilde{\varphi}(x, t, j)$, $j = 1, ..., N$, $x > 0$ but with boundary conditions at $x = 0$ now.

- Set of boundary conditions ensuring unitarity is known[4].

- Associated scattering matrix describing transition and reflexion probabilities between edges satisfies important properties

$$S^\dagger(k)S(k) = \mathbb{1} \quad , \quad S(k)S(-k) = \mathbb{1} \, .$$

- Key to solve the problem: change the oscillator algebra into a Reflection-Transmission algebra [5]

$$[a_j(p), a_k(q)] = 0 = [a_j^\dagger(p), a_k^\dagger(q)] \, ,$$

$$[a_j(p), a_k^\dagger(q)] = 2\pi\delta_{jk}\delta(p-q) + 2\pi S_{jk}(p)\delta(p+q)\mathbf{1} \, ,$$

$$a_j(p) = \sum_{k=1}^{n} S_{jk}(p) a_k(-p) \quad , \quad a_j^\dagger(p) = \sum_{k=1}^{n} a_k^\dagger(-p) S_{kj}(-p) \qquad (1)$$

[4] V. Kostrykin, R. Schrader, J. Phys. A: Math. Gen. Vol.32 (1999) 595-630

[5] M. Mintchev, E. Ragoucy, P. Sorba, J. Phys. A36 (2003),10407.

Application: computation of the conductance

- Method: couple the field to a classical electric field A_μ and compute the response of the vacuum expectation value of the current $J(x,t,j) = (\psi_1^\dagger \psi_1 - \psi_2^\dagger \psi_2)(x,t,j)$.

- Response theory yields

$$\langle J(x,t,j) \rangle_{A_\mu} = \langle J(x,t,j) \rangle + i \int_{-\infty}^{t} \langle [H_{int}(\tau), J(x,t,j)] \rangle d\tau$$

$$H_{int}(\tau) = \sum_{j=1}^{n} \int_0^\infty dx \left[\frac{1}{\alpha\pi} J\, A_x - \frac{1}{2\pi} A^\mu A_\mu \right] (x, \tau, j)$$

- All calculations can be reduced to using the RT algebra relations to get an exact result.

The result[6]:

$$\langle J(x,t,j)\rangle_{A_\mu} = G_{line}\sum_{k=1}^{n}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\hat{A}_x(\omega,k)e^{-i\omega t}$$

$$\times\left[\delta_{kj} - S_{kj}(\omega) - \sum_{\eta\in Res}\frac{\eta}{\eta+i\omega}Res(S_{kj},\eta)e^{(t-t_0)(\eta+i\omega)}\right]$$

- The conductance $G_{kj}(\omega, t-t_0)$ is the term in brackets (in units of G_{line}, the conductance of an infinite line).

- Main message: behaviour of physical quantities completely determined by $S(p)$ and its analytic structure (as expected).
$\longrightarrow$ One needs an efficient method to compute $S(p)$.

[6] assuming a constant electric field $E(t,j) = \partial_t A_x(t,j)$ in the Weyl gauge $A_t = 0$ and switched on at $t = t_0$.

1.3 Total scattering matrix of an arbitrary graph

- Several existing results in the literature[7] but all with drawbacks for our purposes: no explicit formula or impractical recursive methods.

Goal: knowing all the local scattering matrices, obtain the total scattering matrix simply and explicitly.

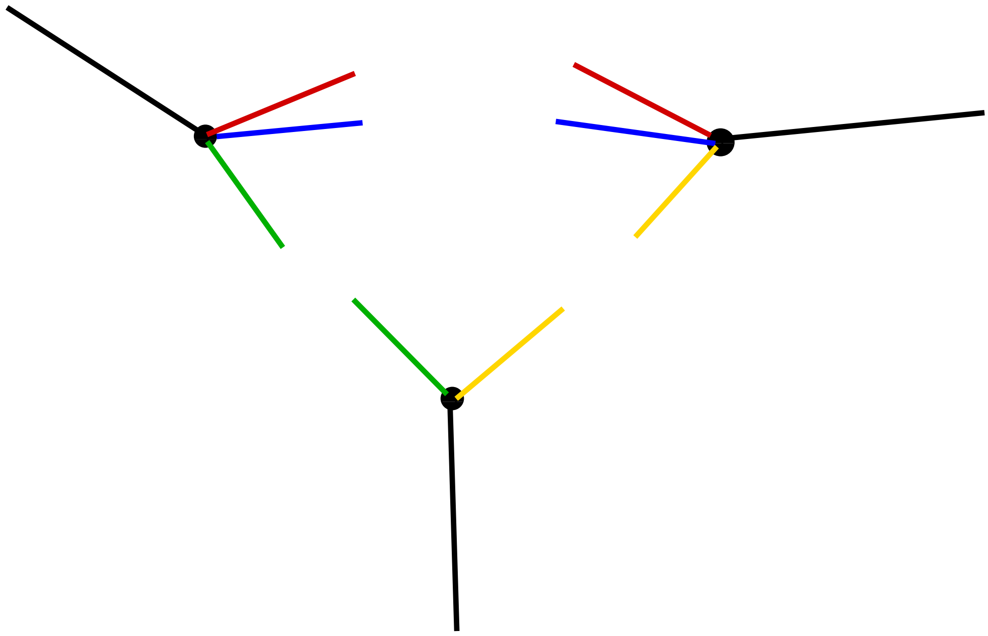
- Our method is based on a simple gluing procedure and uses only linear algebra!

Idea: Lego-type approach

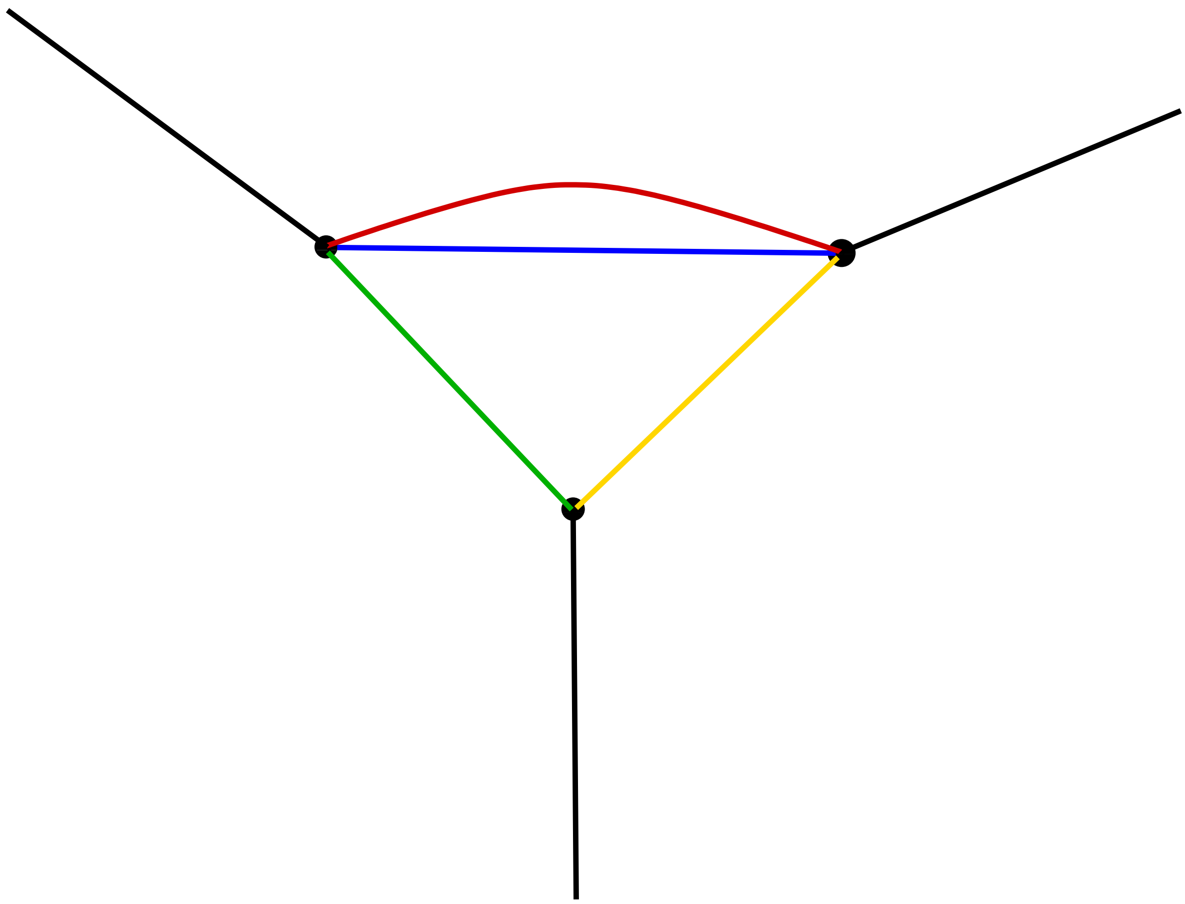
arbitrary graph = collection of star graphs glued together

See figures

[7] V. Kostrykin, R. Schrader, J. Phys. A32 (1999) 595 ; Sh. Khachatryan, R. Schrader, A. Sedrakyan, J. Phys. A42 (2009) 304019 ; E. Ragoucy J. Phys. A42 (2009) 295205

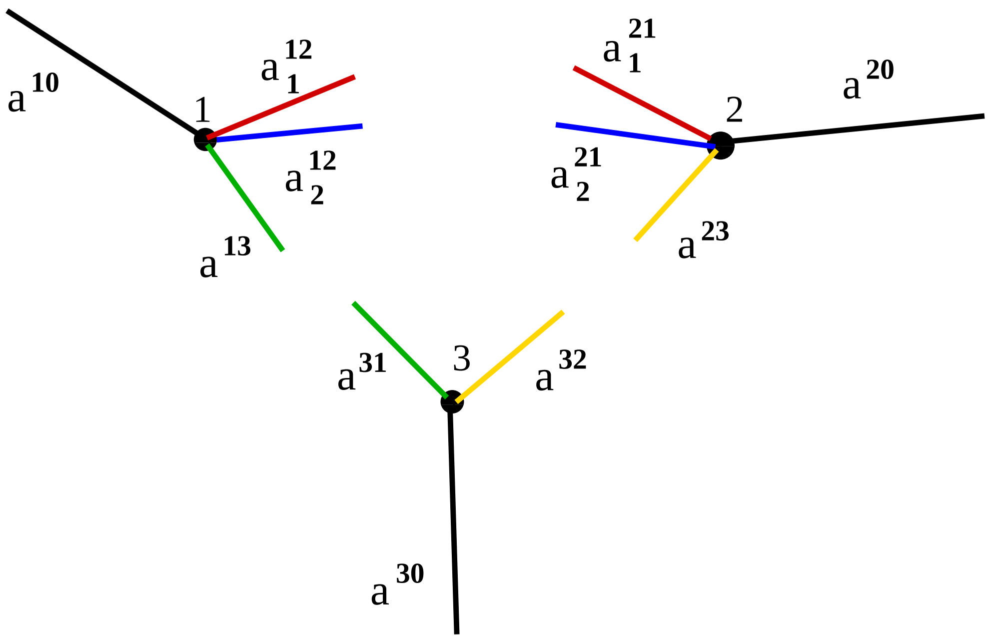


(a) Star graphs before gluing

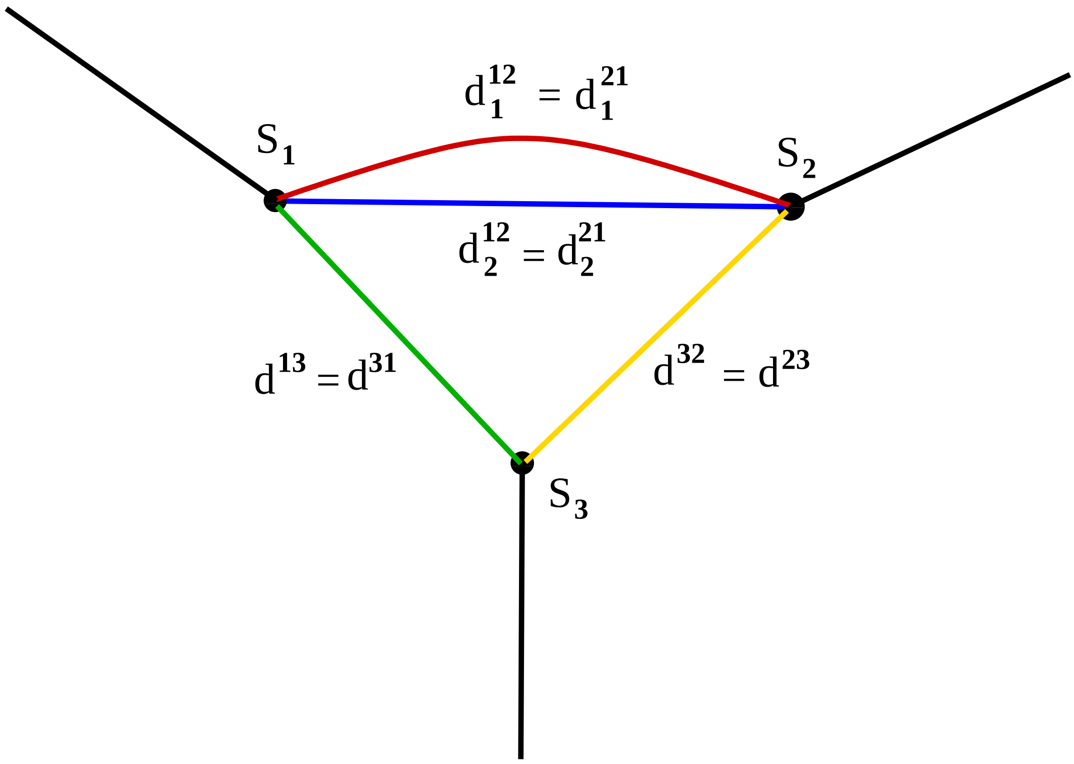


(b) The resulting graph after gluing

Figure 1: Three star graphs to be glued together



(a) Labelling of the star graphs



(b) Local and topological information

Figure 2: Labelling and physical information

Some general notations

- Modes on the edges $a_j^{\alpha\beta}(p)$ (p: momentum)

  - $\alpha = 1, 2, \dots, N$ denotes the vertex to which the edge is attached;
  - $\beta = 0, 1, 2, \dots, N$ denotes the vertex linked to α by the edge under consideration, with the convention that external edges corresponds to $\beta = 0$;
  - $j = 1, \dots, N_{\alpha\beta}$ numbers the different edges between α and β, $N_{\alpha\beta}$ being their total number. We set $N_{\alpha\beta} = 0$ if α is not connected to β. $N_{\alpha\beta} = N_{\beta\alpha}$.
  - $d_j^{\alpha\beta} = d_j^{\beta\alpha}$ is the length of edge (α, β, j).

Two fundamental set of relations:

- Local scattering at vertex α:

$$a_j^{\alpha\beta}(p) = \sum_{\gamma=0}^{N} \sum_{k=1}^{N_{\alpha\gamma}} s_{\alpha;jk}^{\beta\gamma}(p)\, a_k^{\alpha\gamma}(-p)$$

where $s_{\alpha;jk}^{\beta\gamma}(p)$ are the components of the local scattering matrix $S_\alpha(p)$ which satisfies $S_\alpha(p)S_\alpha(-p) = \mathbb{1}$.

- Propagation on edge $(\alpha\beta j)$:

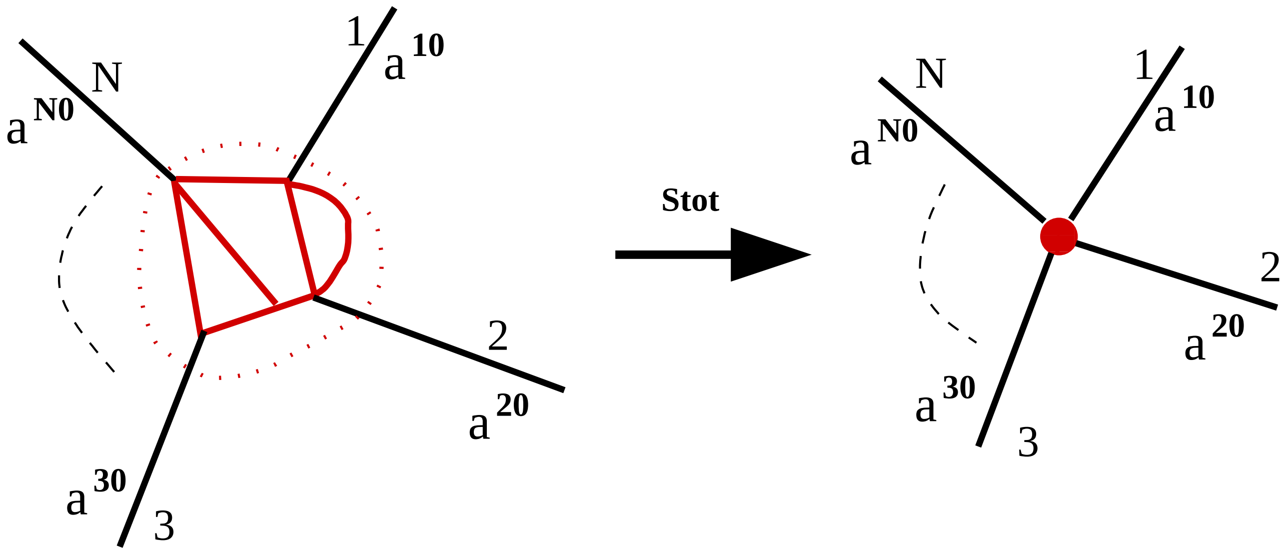
$$a_j^{\alpha\beta}(p) = \exp(-i\, d_j^{\alpha\beta}\, p)\, a_j^{\beta\alpha}(-p)\,.$$

Question: what is the equivalent star graph with total scattering matrix Stot?

Answer: we seek the scattering relations directly between the external modes $i.e.$ relations of the form

$$a_j^{\alpha 0}(p) = \sum_{\gamma=1}^{N} \sum_{k=1}^{N_{\gamma 0}} S_{tot;jk}^{\alpha\gamma}(p)\, a_k^{\gamma 0}(-p) \qquad \forall j = 1, \ldots, N_{\alpha 0}\ ;\ \forall \alpha = 1, \ldots, N\ ,$$

where $S_{tot;jk}^{\alpha\gamma}(p)$ are the components of the total scattering matrix for the graph, $S_{tot}(p)$.



Derivation of the result: put modes in vectors and use linear algebra.

- All external modes in vector $A(p)$, internal modes in $B(p)$.
- Collect external elements of the local S's in $S_{11}(p)$.
- Collect internal elements in $S_{22}(p)$.
- Collect the elements linking external to internal modes in $S_{21}(p)$
- Collect the elements linking internal to external in $S_{12}(p)$.

- Finally, let $E(p)$ be the connectivity matrix encoding the propagation: it has one $e^{-ipd_j^{\alpha\beta}}$ term in each row and column and connects the elements of $B(p)$

- The set of scattering and propagation relations becomes

$$
\begin{aligned}
A(p) &= S_{11}(p)\, A(-p) + S_{12}(p)\, B(-p) \\
B(p) &= S_{21}(p)\, A(-p) + S_{22}(p)\, B(-p) \\
B(p) &= E(p) B(-p)
\end{aligned}
$$

Assuming that $E(p) - S^{(22)}(p)$ is invertible this yields the desired relations

$$
A(p) = S_{tot}(p) A(-p)\,,
$$

with

$$
S_{tot}(p) = S_{11}(p) + S_{12}(p)\, \left[E(p) - S_{22}(p)\right]^{-1} S_{21}(p)\,.
$$

- The internal modes can be deduced from the external ones through

$$
B(p) = \left[E(-p) - S_{22}(-p)\right]^{-1} S_{21}(-p)\, A(p)
$$

2.1 Ring a magnetic field

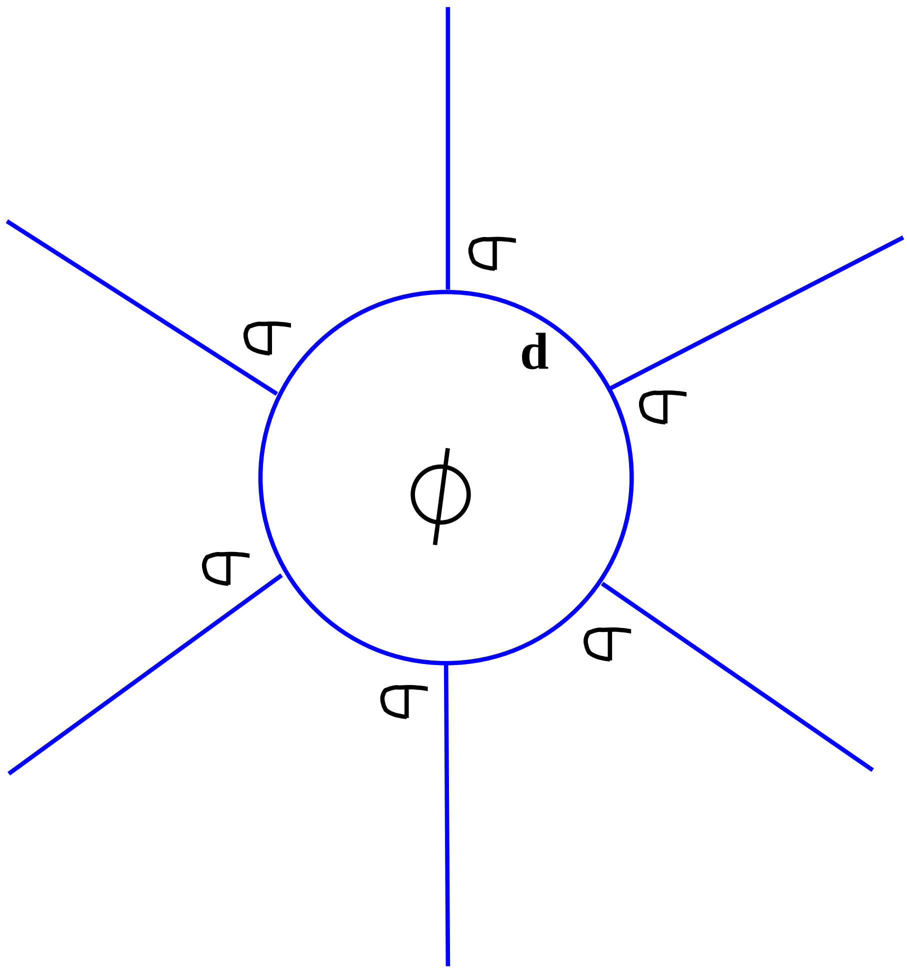


Figure 3: Example of a regular ring with 6 external edges, identical local scattering matrices σ and length d between edges pierced by a flux ϕ.

- For N external edges, $S_{tot}(p,\phi)$ is a $N \times N$ circulant matrix. Can be diagonalised and using our method we find

$$S_{tot}(p,\phi) = W \begin{pmatrix} \lambda_1(p,\frac{\phi}{N}) & & \\ & \ddots & \\ & & \lambda_N(p,\frac{\phi}{N}) \end{pmatrix} W^{-1}$$

With

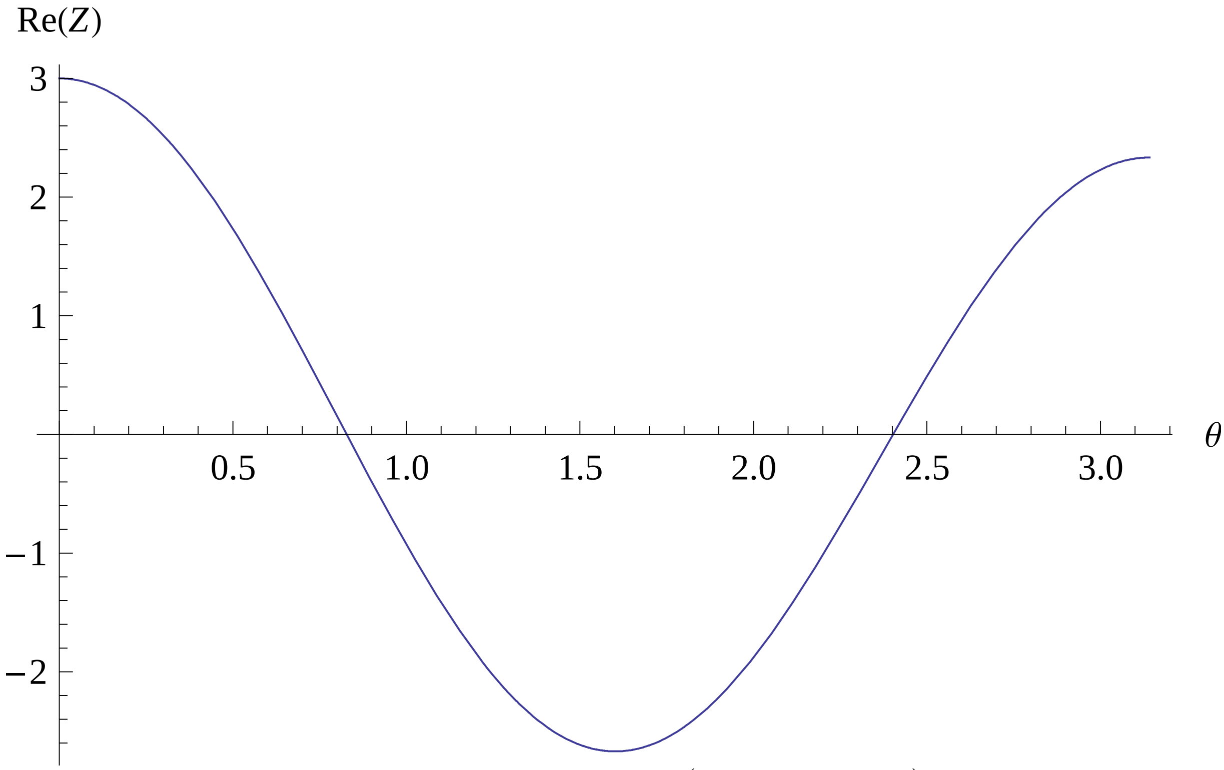
$$W = \begin{pmatrix} 1 & 1 & \dots & 1 \\ 1 & \omega & \dots & \omega^{N-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{N-1} & \dots & (\omega^{N-1})^{N-1} \end{pmatrix} \quad , \quad \omega = e^{\frac{2i\pi}{N}} ,$$

and

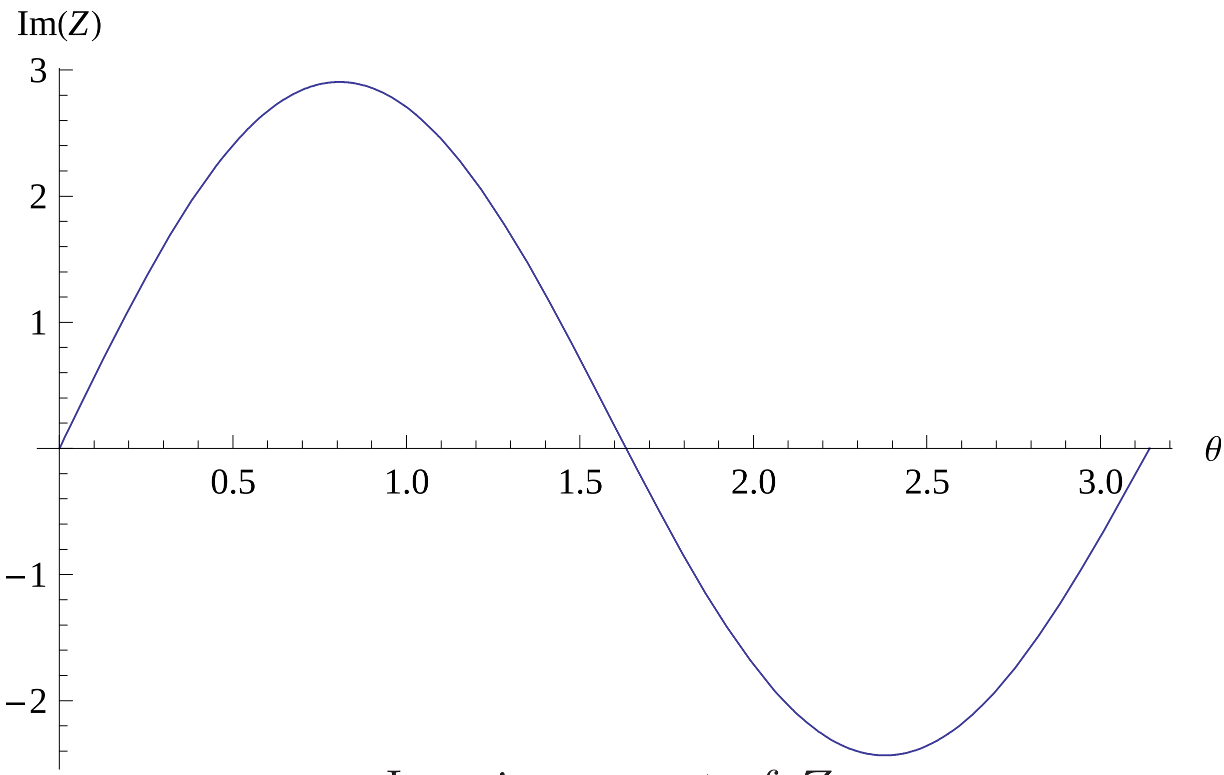
$$\lambda_j(p,\theta) = \frac{e^{2ipd}\det\sigma + e^{ipd}\left[(\sigma_{11}\sigma_{23} - \sigma_{13}\sigma_{21})e^{i\theta}\omega^{j-1} + (\sigma_{11}\sigma_{32} - \sigma_{31}\sigma_{12})e^{-i\theta}\omega^{1-j}\right] - \sigma_{11}}{e^{2ipd}(\sigma_{22}\sigma_{33} - \sigma_{23}\sigma_{32}) + e^{ipd}(\sigma_{23}e^{i\theta}\omega^{j-1} + \sigma_{32}e^{-i\theta}\omega^{1-j}) - 1},$$

- Thanks to this explicit expression, the conductance tensor can be computed exactly. In general, one gets complex entries: resistance and inductance/capacitance effects.

- Next page: impedance Z_{12} between the edges 1 and 2 in the limit $d = 0$ with the flux θ held finite (result for $N = 3$, σ a given constant matrix).



(a) Real part of Z_{12} (resistance).



(b) Imaginary part of Z_{12}

Figure 4: Impedance Z_{12} (between edges 1 and 2) as a function of the flux θ.

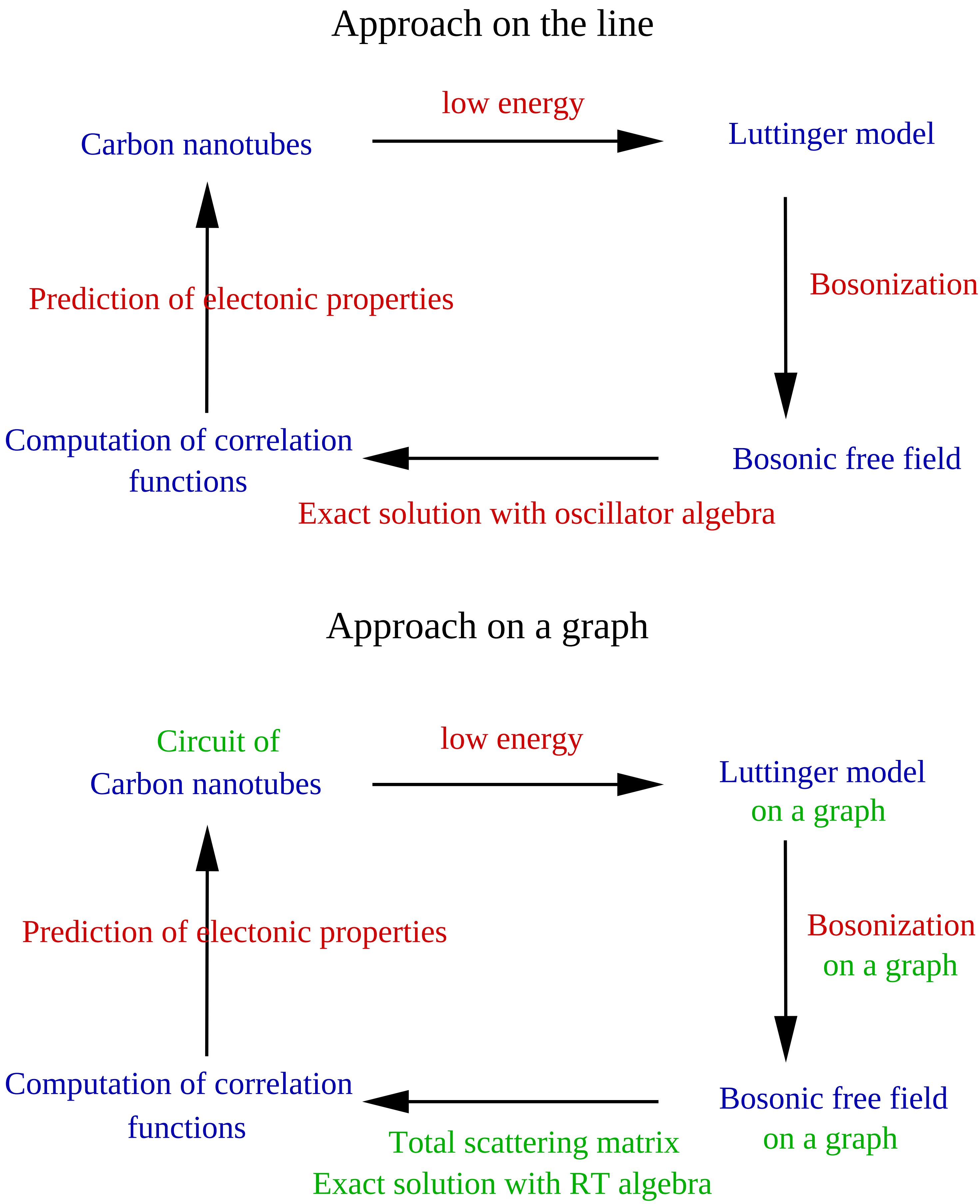


Figure 5: Summary

3 Conclusions

- Complete solution of the Tomonaga-Luttinger model on an arbitrary graph $\longrightarrow$ study of electronic properties of circuits of quantum wires (carbon nanotubes).

- Application: preliminary results for the conductance on a ring in a magnetic field. Comparison with previous works in condensed matter physics [8] employing different, perturbative methods in progress.

- Question of conductance for simple graphs already addressed in the context of integrable QFT [9]. Use of TBA and form factor to get finite temperature conductance of free fermions on a 1D array of impurities.

Prospectives

- Brings us closer to the understanding of integrable QFT on graphs.

- Case of finite temperature can be tackled along the same lines: only difference is to take a Gibbs representation of the RT algebra instead of Fock representation.

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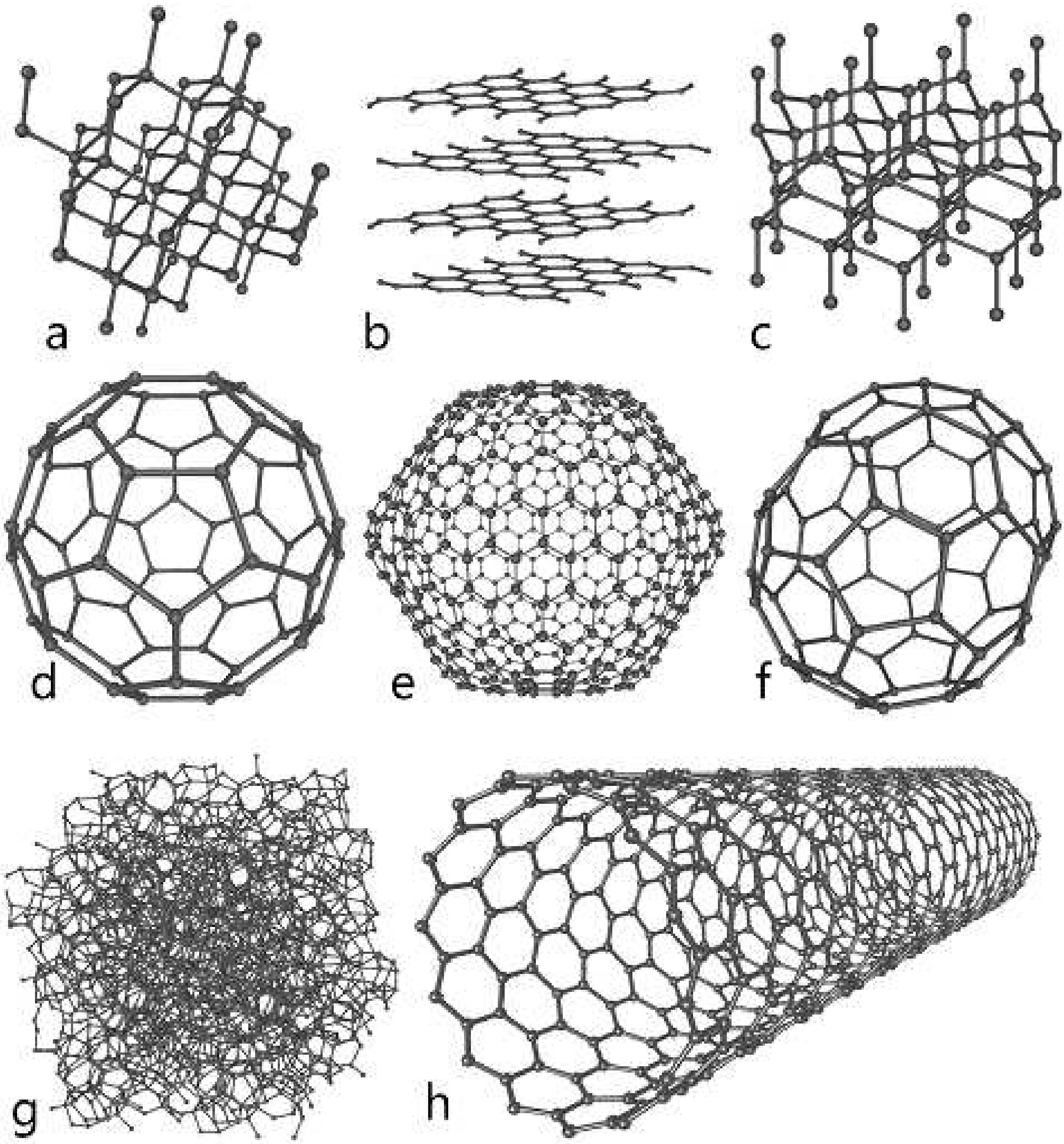
[8] M. Oshikawa, C. Chamon, I Affleck, J.Stat.Mech. 0602 (2006) P008.

[9] O. Castro-Alvaredo, A. Fring, Nucl.Phys. B649 (2003) 449-490.

THANK YOU!



Sources of inspiration: a) Diamond, b) Graphite, c) Lonsdaleite, d) C60 (Buckminsterfullerene or buckyball), e) C540, f) C70, g) Amorphous carbon, and h) single-walled carbon nanotube or buckytube.