Kazimierz Dolny, 26 June 2007

Application of a continuous unitary transformation in the quantum statistics

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Outline

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- **Unitary transformation**

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- **Mathematical justification of CUT**
- **Applications**

1. Unitary transformations (UT)

Application to the eigenproblems

$$\hat{H}\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle$$

$$\downarrow$$

$$\hat{S}\hat{H}\hat{S}^{-1}\,\hat{S}\,|\Psi_n\rangle = E_n\,\hat{S}\,|\Psi_n\rangle$$

$$\downarrow$$

$$\hat{\tilde{H}}\,\left|\tilde{\Psi}_n\right\rangle = E_n\,\left|\tilde{\Psi}_n\right\rangle$$

where

$$\hat{\tilde{H}} \equiv \hat{S}\hat{H}\hat{S}^{-1}$$

$$\left|\tilde{\Psi}_n\right\rangle \equiv \hat{S}\,|\Psi\rangle$$

Unitary transformations preserve the eigenvalues.

1. Unitary transformations (UT)

Example 1

Exact diagonalization of the bilinear structures

$$\hat{H} = \varepsilon \left(\hat{c}^{\dagger}_{\uparrow} \hat{c}_{\uparrow} + \hat{c}^{\dagger}_{\downarrow} \hat{c}_{\downarrow} \right) + \Delta \, \hat{c}^{\dagger}_{\uparrow} \hat{c}^{\dagger}_{\downarrow} + \Delta^{*} \, \hat{c}_{\downarrow} \hat{c}_{\uparrow}$$

via the **Bogoliubov transformation (1947)**

$$\begin{pmatrix} \hat{\tilde{c}}_{\uparrow} \\ \hat{\tilde{c}}^{\dagger}_{\downarrow} \end{pmatrix} = \begin{bmatrix} u & v \\ -v & u \end{bmatrix} \begin{pmatrix} \hat{c}_{\uparrow} \\ \hat{c}^{\dagger}_{\downarrow} \end{pmatrix}$$

This is often used for studying:

– fermion systems with the **BCS**-like structure,

– boson systems in presence of the **BE condensate**.

1. Unitary transformations (UT)

Example 2

Exact solution of the lattice vibrations coupled to a single level state

$$\hat{H} = \varepsilon\, \hat{c}^\dagger \hat{c} + \hbar\omega\, \hat{a}^\dagger \hat{a} + V_{el-ph}\, \hat{c}^\dagger \hat{c} \left(\hat{a}^\dagger + \hat{a}\right)$$

via the **Lang-Firsov transformation (1962)**

$$\hat{S} = \frac{V_{el-ph}}{\hbar\omega}\; \hat{c}^\dagger \hat{c}\left(\hat{a}^\dagger - \hat{a}\right)$$

This result is often used as a starting point for studying the influence of lattice vibrations on mobile electrons in conductors and superconductors.

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and we thus have to resort to some other methods.

2. UT in a perturbative scheme

Suppose, that we want to solve the eigenvalue problem of

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Applying the transformation $\hat{S} = e^{\hat{A}}$ we have

$$\begin{aligned}
\hat{\tilde{H}} &= e^{\hat{A}}\hat{H}e^{-\hat{A}} \\
&= \left(1 + \hat{A} + \frac{\hat{A}^2}{2} + \ldots\right)\hat{H}\left(1 - \hat{A} + \frac{\hat{A}^2}{2} - \ldots\right) \\
&= \hat{H} + \left[\hat{A}, \hat{H}\right] + \frac{1}{2}\left[\hat{A}, \left[\hat{A}, \hat{H}\right]\right] + \ldots
\end{aligned}$$

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$$\hat{\tilde{H}} = \hat{H}_0 + \frac{1}{2}\left[\hat{A}, \lambda \hat{V}\right] + O(\lambda^3)$$

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This is a routine procedure for the perturbative studies.

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The derivative

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\frac{d\hat{H}(l)}{dl} &= \frac{d\hat{S}(l)}{dl}\hat{H}\hat{S}^{\dagger}(l) + \hat{S}(l)\hat{H}\frac{d\hat{S}^{\dagger}(l)}{dl} \\
&= \frac{d\hat{S}(l)}{dl}\hat{S}^{\dagger}(l)\hat{H}(l) + \hat{H}(l)\hat{S}(l)\frac{d\hat{S}^{\dagger}(l)}{dl}
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Using the unitary transform. identity $\hat{S}(l)\hat{S}^{\dagger}(l) = \mathbf{1}$, so that $\frac{d\hat{S}(l)}{dl}\hat{S}^{\dagger}(l) + \hat{S}(l)\frac{d\hat{S}^{\dagger}(l)}{dl} = \mathbf{0}$ we obtain **the flow equation**

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$$\frac{d\hat{H}(l)}{dl} = [\hat{\eta}(l), \hat{H}(l)]$$

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$$\frac{d\hat{H}(l)}{dl} = [\hat{\eta}(l), \hat{H}(l)]$$

where

$$\hat{\eta}(l) = \frac{d\hat{S}(l)}{dl}\hat{S}^{\dagger}(l) = -\hat{\eta}^{\dagger}(l).$$

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For operators

$$\hat{H} = \hat{H}_{diag} + \hat{H}_{off}$$

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Other possible ways for constructing the generating operator $\hat{\eta}$ have been discussed by various authors. For a detailed information see for instance:

S. Kehrein, Springer Tracts in Modern Physics **217**, (2006);

F. Wegner, J. Phys. A: Math. Gen. **39**, 8221 (2006).

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CUT schemes invented so far in physics:

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Similar ideas have been also earlier independently developed by mathematicians in the field of **control theory**. They are known under the names:

- *"double bracket flow"*

  R.W. Brockett, Lin. Alg. and its Appl. **146**, *79 (1991).*

- *"isospectral flow"*

  M.T. Chu and K.R. Driessel, J. Num. Anal. **27**, *1050 (1990).*

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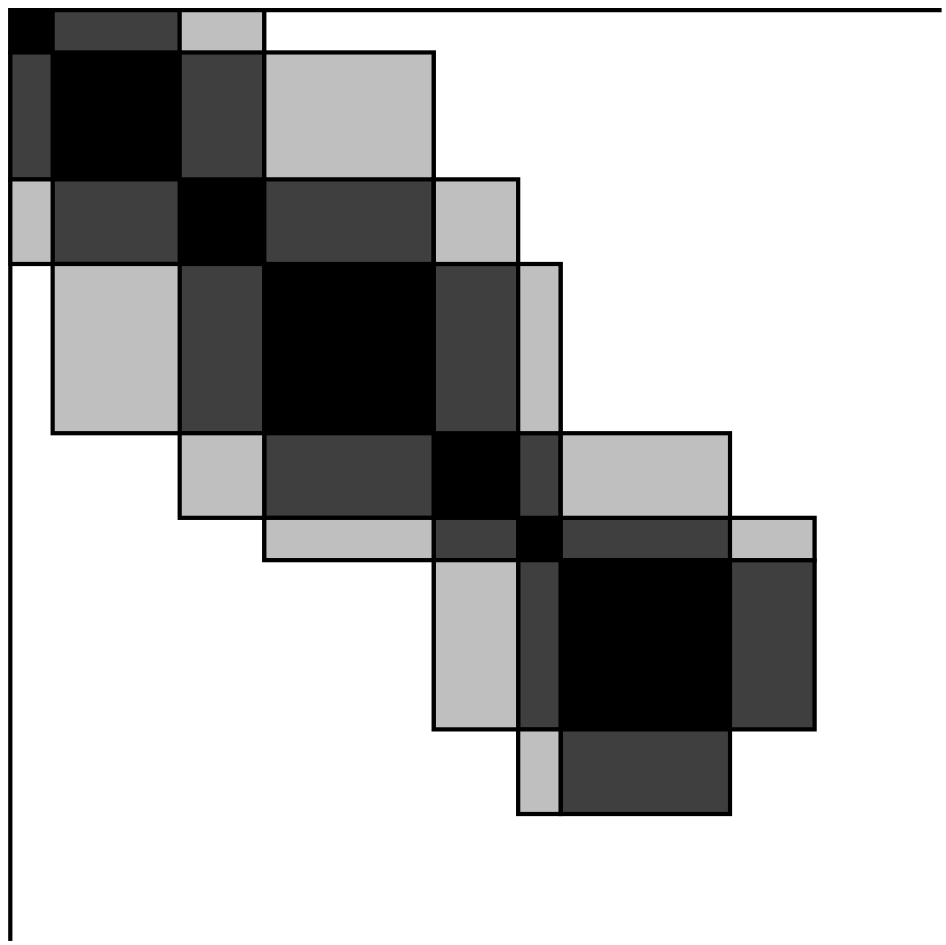

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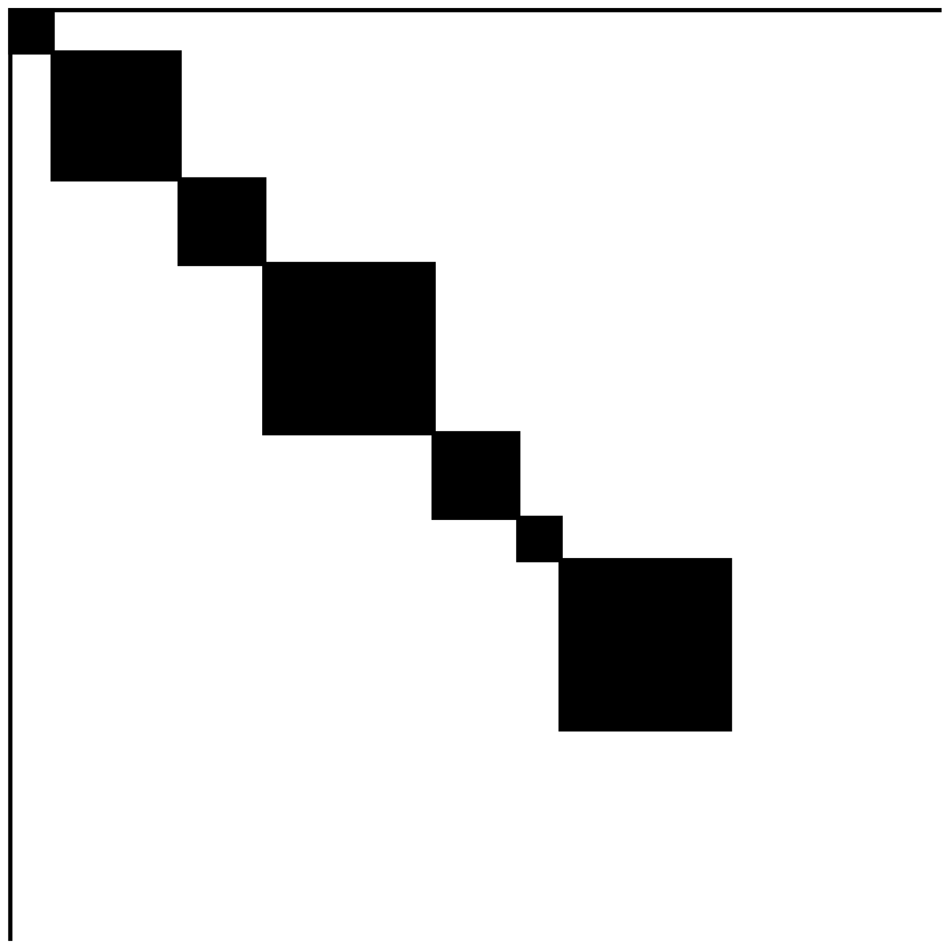

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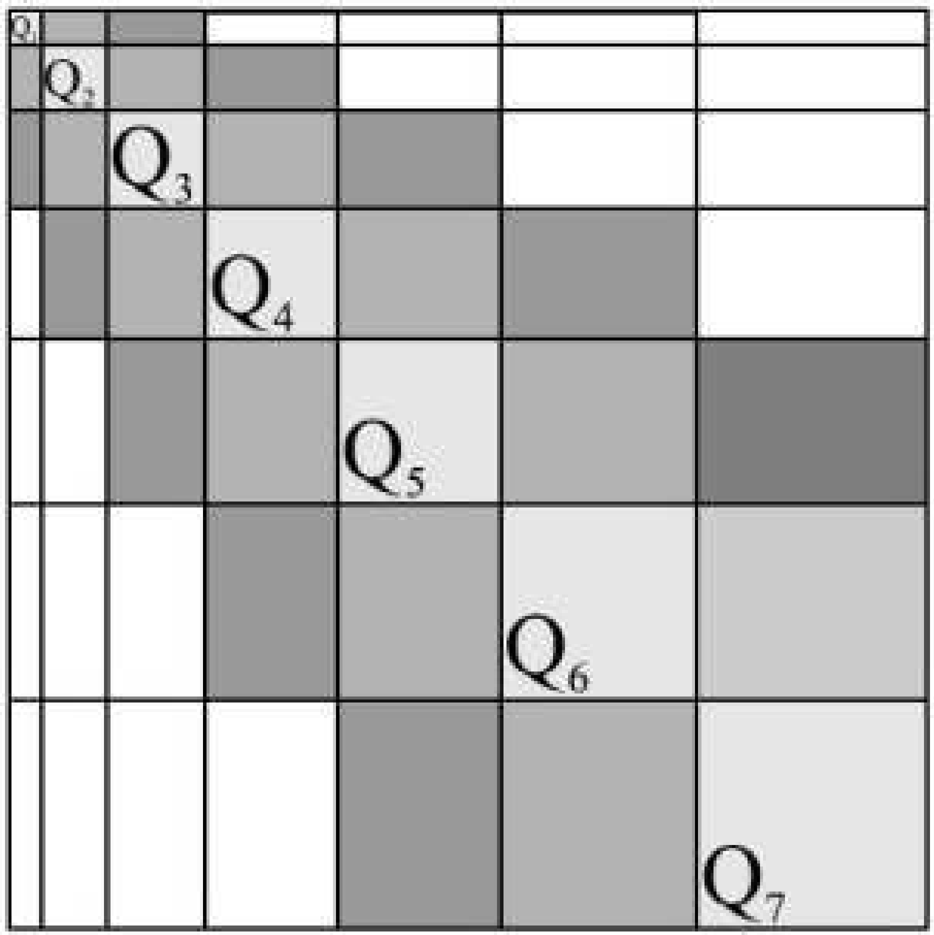

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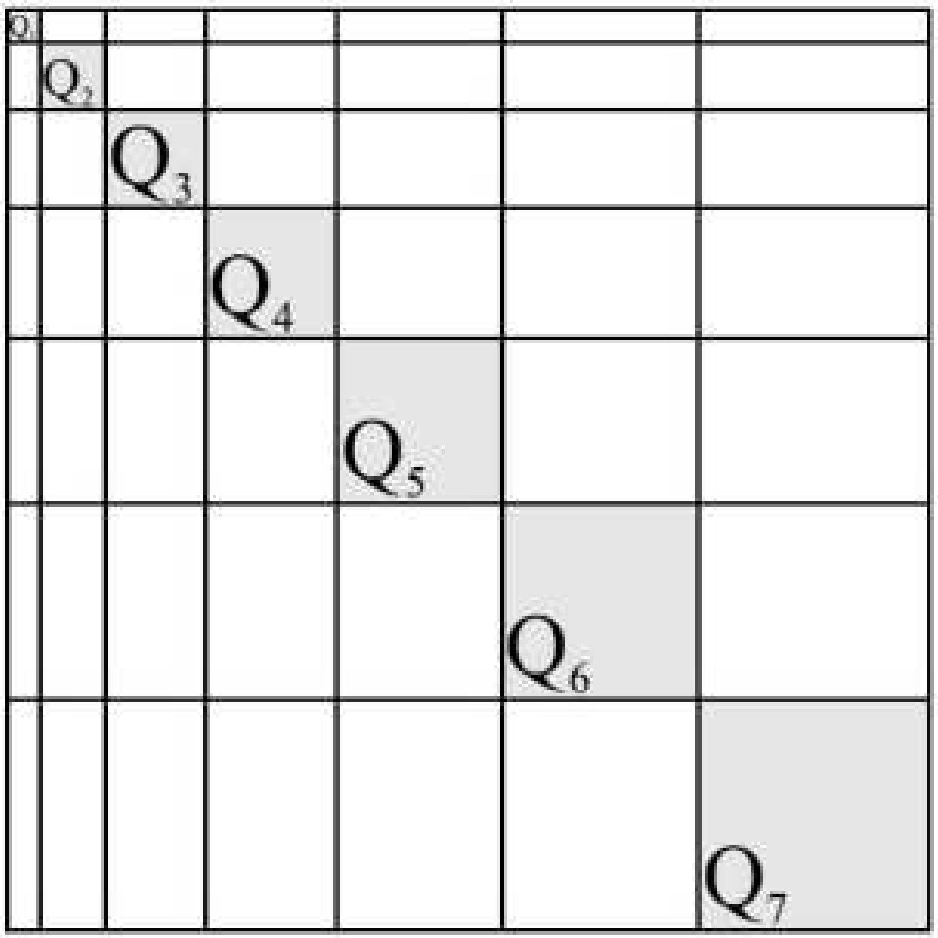

4. Mathematical justification of CUT

We can express the operators $\hat{H}$ and $\hat{\eta}$ in a certain basis of the orthonormal states $|\mathbf{k}\rangle$ so, that

$$
\begin{aligned}
< k|\hat{H}|q > &\equiv h_{k,q} \\
< k|\hat{\eta}|q > &= h_{kk}h_{kq} - h_{kq}h_{qq} = (h_{k,k} - h_{q,q})h_{k,q}
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From the flow equation we obtain

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\frac{dh_{k,q}}{dl} = \sum_p \left(h_{kk} + h_{q,q} - 2h_{p,p}\right) h_{k,p}h_{p,q}
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and in particular, for the diagonal elements

$$\frac{dh_{k,k}}{dl} = 2\sum_p (h_{k,k} - h_{p,p})\, h_{k,p}^2 \qquad (1)$$

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Since the trace $Tr(\hat{H}^n)$ is invariant under unitary transf.

$$0 = \frac{d\, Tr(\hat{H}^2)}{dl} = \frac{d}{dl} \sum_{k,q} h_{k,q} h_{q,k} \qquad (2)$$

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we can write that

$$\begin{aligned} \frac{d}{dl}\sum_{k,q\neq k} h_{k,q}h_{q,k} &= -\frac{d}{dl}\sum_{k} h_{k,k}^2 \\ &= -2\sum_{k} h_{k,k}\frac{dh_{k,k}}{dl} \end{aligned}$$

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Applying (2) to the flow equation (1) we arrive at

$$\begin{aligned}
\frac{d}{dl} \sum_{k,q \neq k} |h_{k,q}|^2 &= -4 \sum_{k} h_{kk} \sum_{q} (h_{kk} - h_{qq}) h_{kq}^2 \\
&= -2 \sum_{k,q} (2h_{kk}^2 - 2h_{kk}h_{qq}) h_{kq}^2 \\
&= -2 \sum_{k,q} (h_{kk}^2 + h_{qq}^2 - 2h_{kk}h_{qq}) h_{kq}^2 \\
&= -2 \sum_{k,q} \left(h_{k,k} - h_{q,q}\right)^2 h_{k,q}^2 \\
&= -2 \sum_{k,q} \eta_{k,q}^2 \quad \leq \quad 0 \qquad \text{!!!}
\end{aligned}$$

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Using a continuous unitary transf. a lá Wegner,

the off-diagonal terms are monotonously reduced

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Because of $\sum_{k,q \neq k} h_{k,q}^2 \geq 0$, the derivative with respect to l is bounded from below therefore

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$$\lim_{l \to \infty} \frac{d}{dl} \sum_{k,q \neq k} h_{k,q}^2 = 0.$$

From relation $\frac{d}{dl} \sum_{k,q\neq k} |h_{k,q}|^2 = -2 \sum_{k,q} \eta_{k,q}^2$ one finally obtains

$\lim_{l\to\infty} \eta_{k,q} = 0$ and $\lim_{l\to\infty} h_{k,q\neq k} = 0$

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S.R. White, J. Chem. Phys. **117**, *7472 (2002).*

This procedure has been further applied by the same author to *ab initio* calculations in the quantum chemistry.

5. Correlation functions

In the quantum statistical physics one often needs to determine various correlation functions

$$\langle \hat{A}\ \hat{B} \rangle$$

with the Boltzmann averaging

$$\langle \ldots \rangle = \text{Tr}\left\{ e^{-\beta \hat{H}} \ldots \right\} / \text{Tr}\left\{ e^{-\beta \hat{H}} \right\}.$$

where $\beta = (k_B T)^{-1}$.

This can be done making use of the invariance

$$\begin{aligned} \text{Tr}\left\{ e^{-\beta \hat{H}} \hat{O} \right\} &= \text{Tr}\left\{ e^{\hat{S}(l)} e^{-\beta \hat{H}} \hat{O} e^{-\hat{S}(l)} \right\} \\ &= \text{Tr}\left\{ e^{\hat{S}(l)} e^{-\beta \hat{H}} e^{-\hat{S}(l)} e^{\hat{S}(l)} \hat{O} e^{-\hat{S}(l)} \right\} \\ &= \text{Tr}\left\{ e^{-\beta \hat{H}(l)} \hat{O}(l) \right\} \end{aligned}$$

where

$$\hat{H}(l) = e^{\hat{S}(l)} \hat{H} e^{-\hat{S}(l)} \qquad \hat{O}(l) = e^{\hat{S}(l)} \hat{O} e^{-\hat{S}(l)}$$

5. Correlation functions

SOME REMARKS:

- ⋆ The easiest way for calculating $< ... >$ is the limit $l \longrightarrow \infty$ when $\hat{H}(\infty)$ becomes (block-)diagonal.

- ⋆ All operators must be however transformed

$$\hat{O} \longrightarrow ... \longrightarrow \hat{O}(l) \longrightarrow ... \longrightarrow \hat{O}(\infty)$$

- ⋆ according to **the flow equation**:

$$\frac{\partial \hat{O}(l)}{\partial l} = \left[\hat{\eta}(l), \hat{O}(l)\right]$$

6. Applications

6.1. BCS problem: an exercise

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$$\hat{H} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} \left(\Delta_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} + \Delta^{*}_{\mathbf{k}} \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} \right)$$

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This (reduced BCS) Hamiltonian can be solved exactly using e.g. the Bogoliubov transformation

$$\begin{aligned} \hat{c}_{\mathbf{k}\uparrow} &= u_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow} + v_{\mathbf{k}} \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \\ \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} &= -v_{\mathbf{k}} \hat{c}_{\mathbf{k}\uparrow} + u_{\mathbf{k}} \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \end{aligned}$$

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N.N. Bogoliubov, Sov. Phys. JETP **7**, *41 (1948)*

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$$\partial_l \hat{H} = \left[\hat{\eta}, \hat{H}\right]$$

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we obtain a set of the flow equations

$$\begin{aligned} \partial_l \, \xi_{\mathbf{k}}(l) &= 4\xi_{\mathbf{k}}(l) \, |\Delta_{\mathbf{k}}(l)|^2 \\ \partial_l \, \Delta_{\mathbf{k}}(l) &= -4|\xi_{\mathbf{k}}(l)|^2 \, \Delta^*_{\mathbf{k}}(l) \end{aligned}$$

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which yield the following identity

$$|\Delta_{\mathrm{k}}(l)| = |\Delta_{\mathrm{k}}| e^{-4\int_0^l dl' [\xi_{\mathrm{k}}(l')]^2}.$$

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$$\partial_l \hat{H} = \left[\hat{\eta}, \hat{H}\right]$$

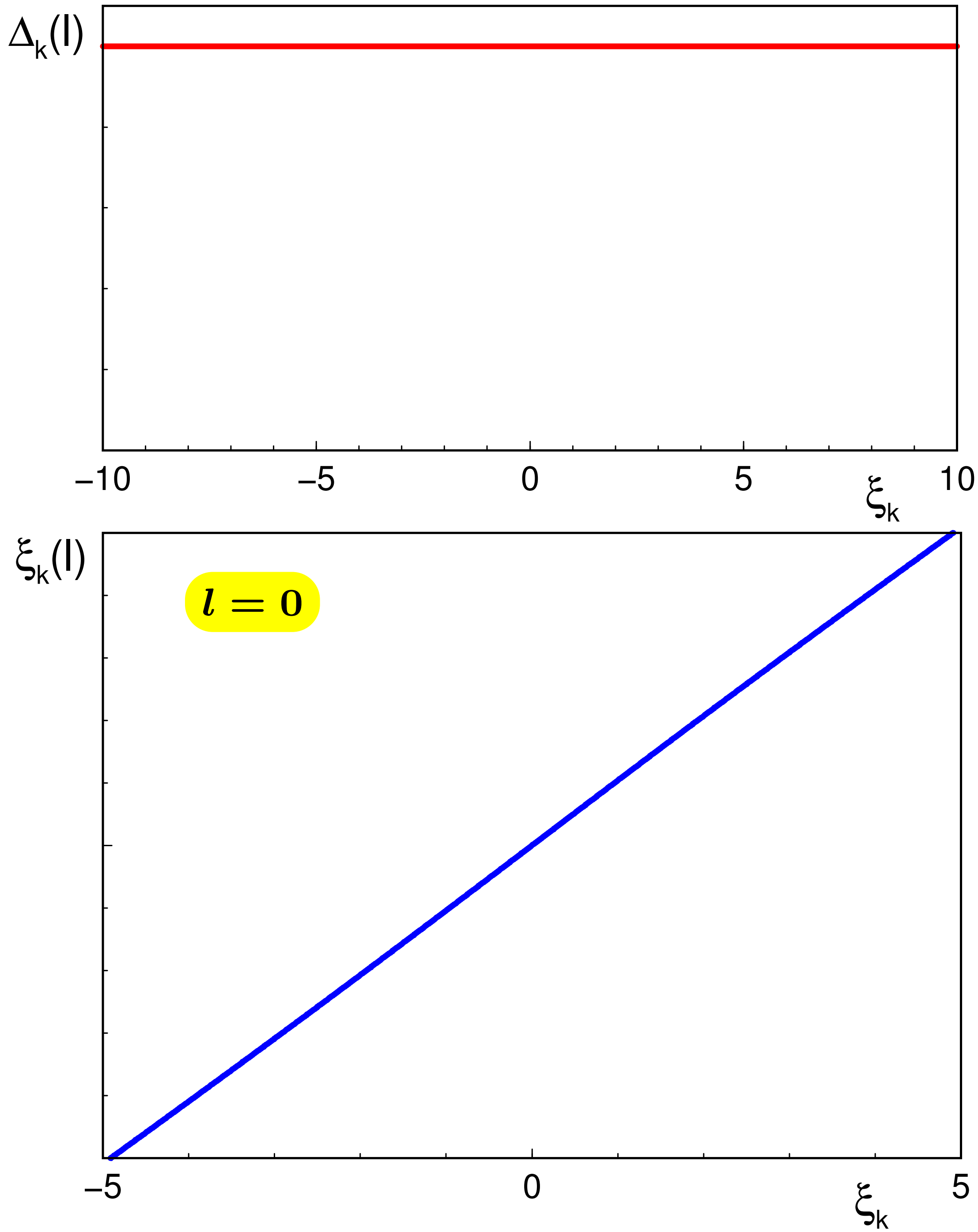
we obtain a set of the flow equations

$$\begin{aligned} \partial_l\ \xi_{\mathbf{k}}(l) &= 4\xi_{\mathbf{k}}(l)\ |\Delta_{\mathbf{k}}(l)|^2 \\ \partial_l\ \Delta_{\mathbf{k}}(l) &= -4|\xi_{\mathbf{k}}(l)|^2\ \Delta_{\mathbf{k}}^*(l) \end{aligned}$$

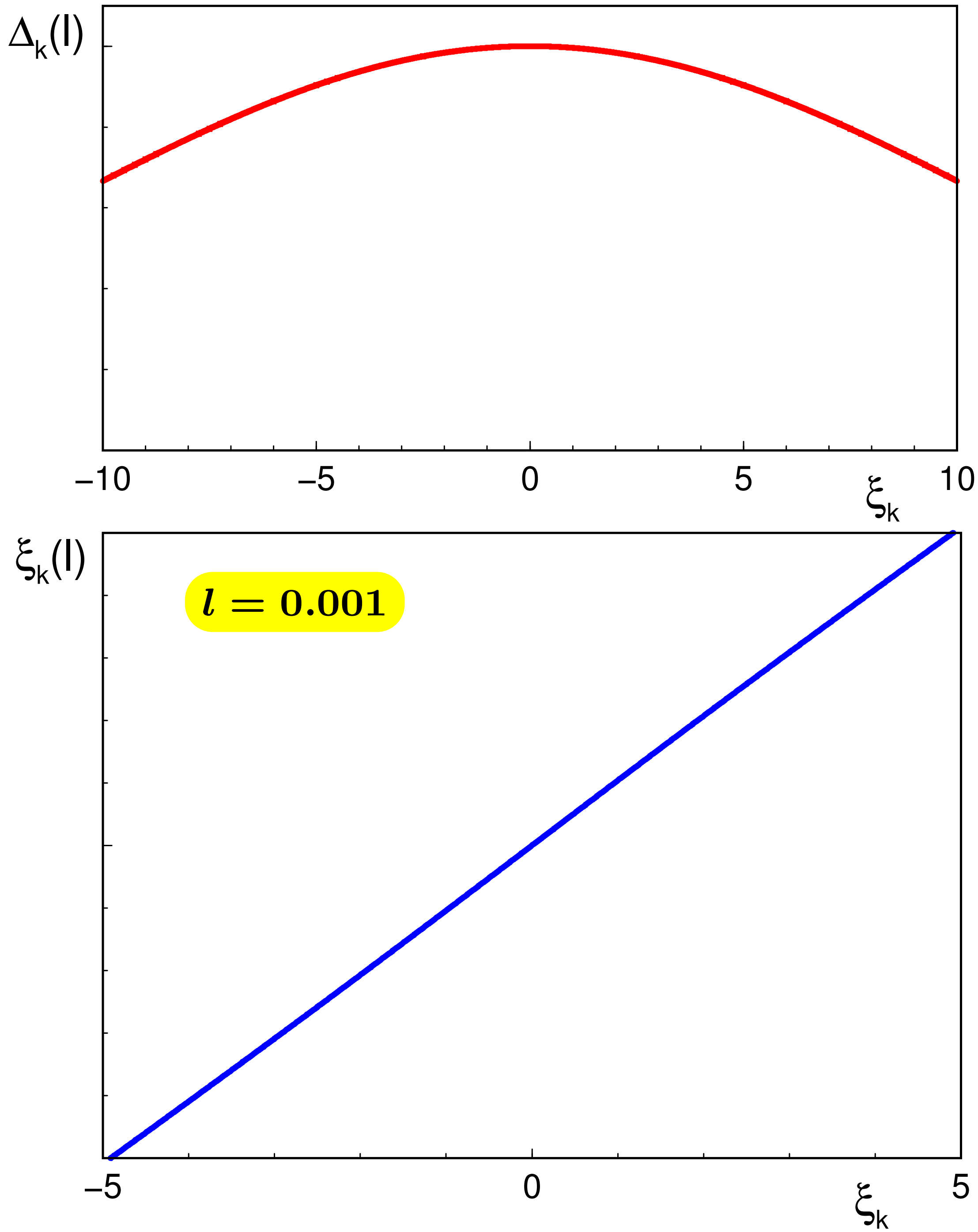
which yield the following identity

$$|\Delta_{\mathbf{k}}(l)| = |\Delta_{\mathbf{k}}| e^{-4\int_0^l dl' [\xi_{\mathbf{k}}(l')]^2}.$$

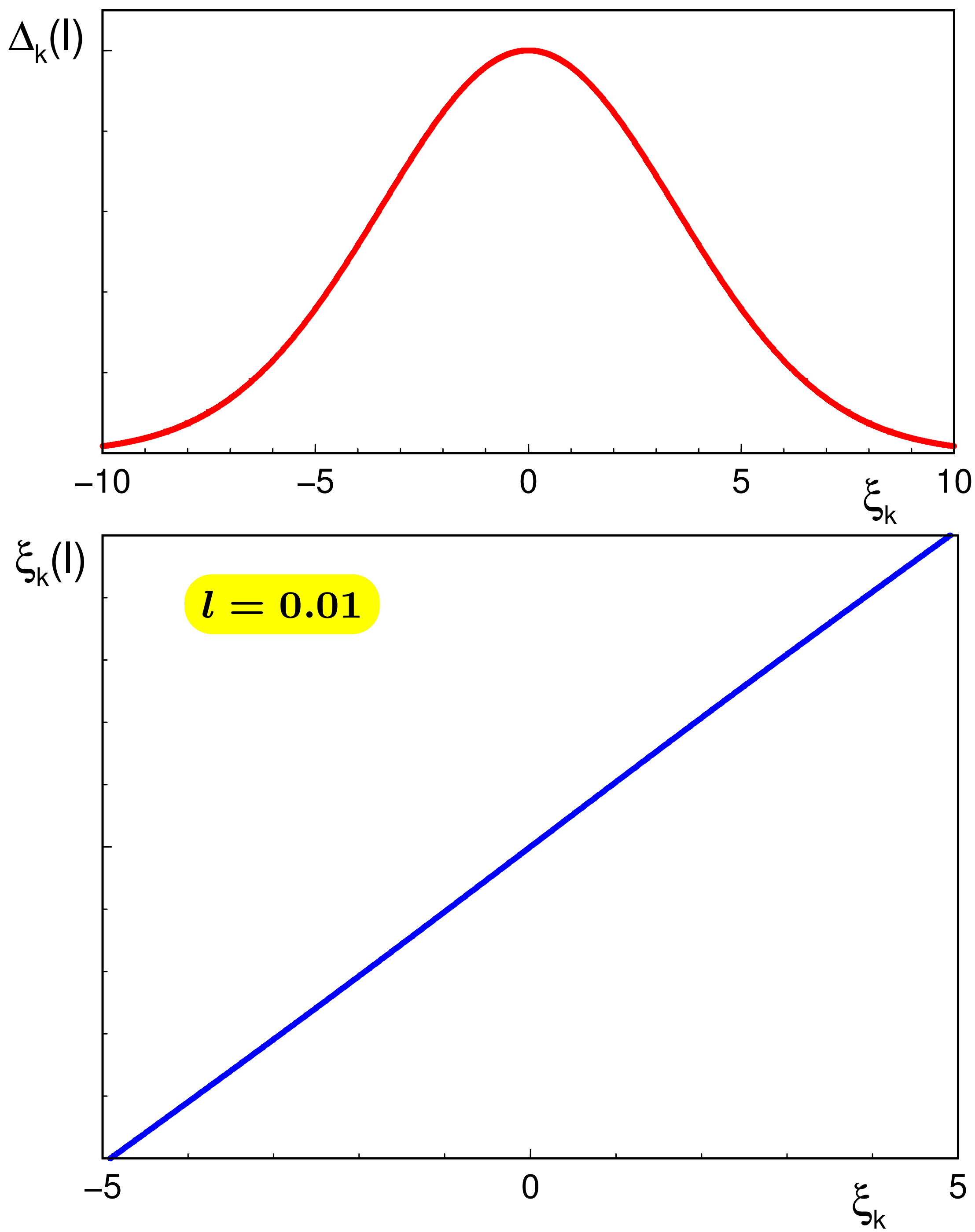
T. Domański, http://xxx.lanl.gov/cond-mat/0602236.



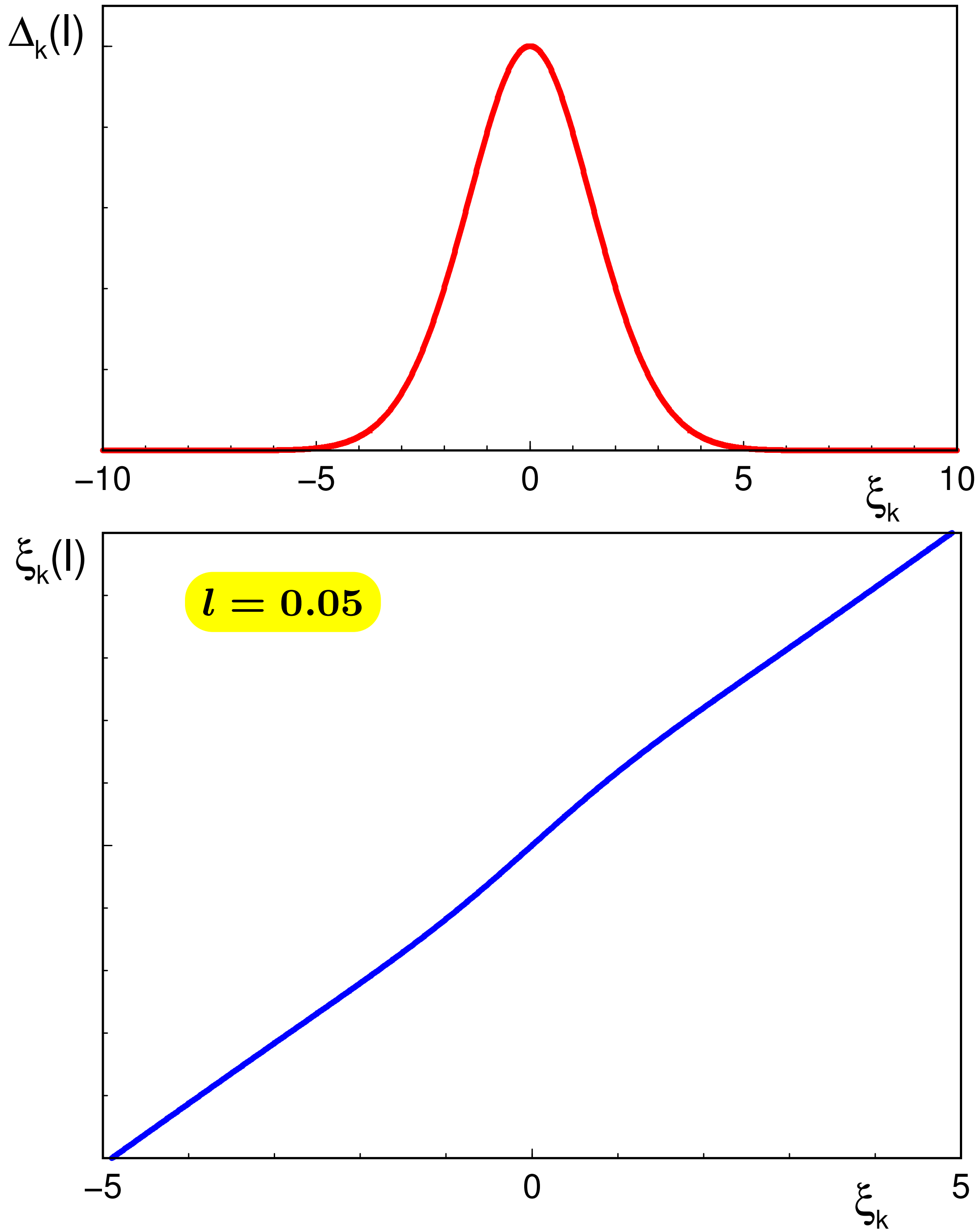
$\Delta_k(l)$
–10
–5
0
5
10
ξ_k
$\xi_k(l)$
$l = 0$
–5
0
5
ξ_k



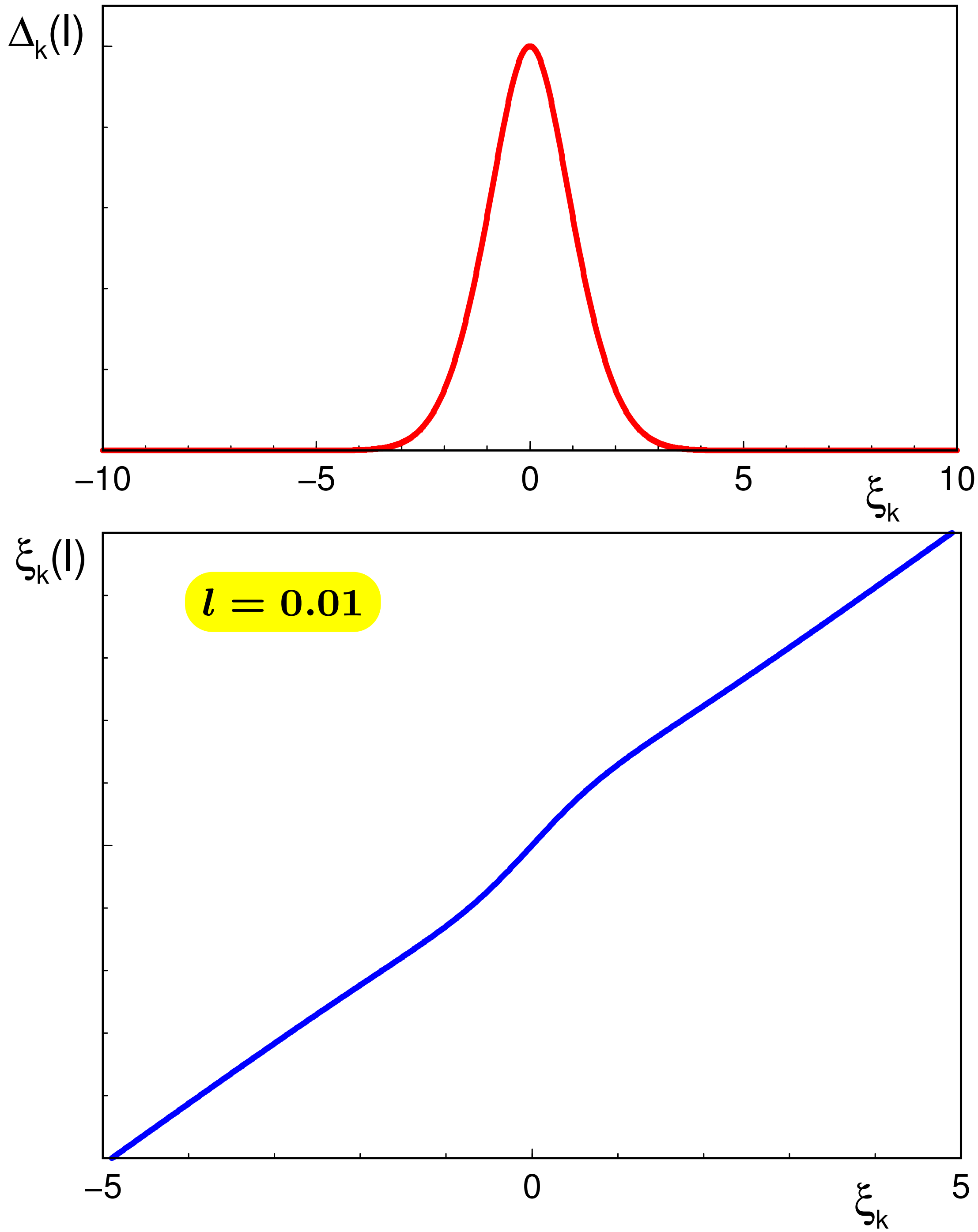
Δk(l)
−10
−5
0
5
10
ξk
ξk(l)
l = 0.001
−5
0
5
ξk



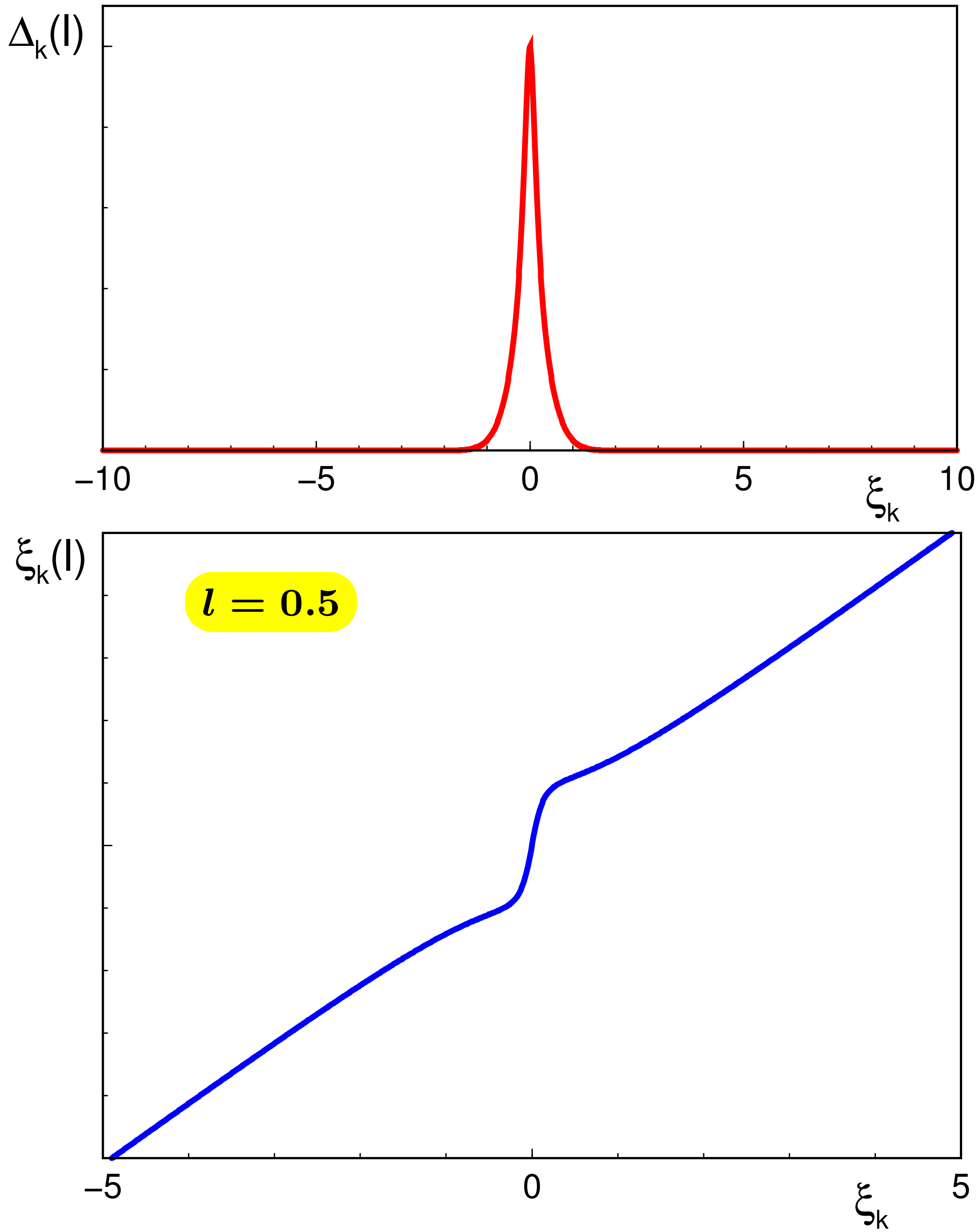
$\Delta_k(l)$
−10
−5
0
5
10
ξ_k
$\xi_k(l)$
$l = 0.01$
−5
0
5
ξ_k



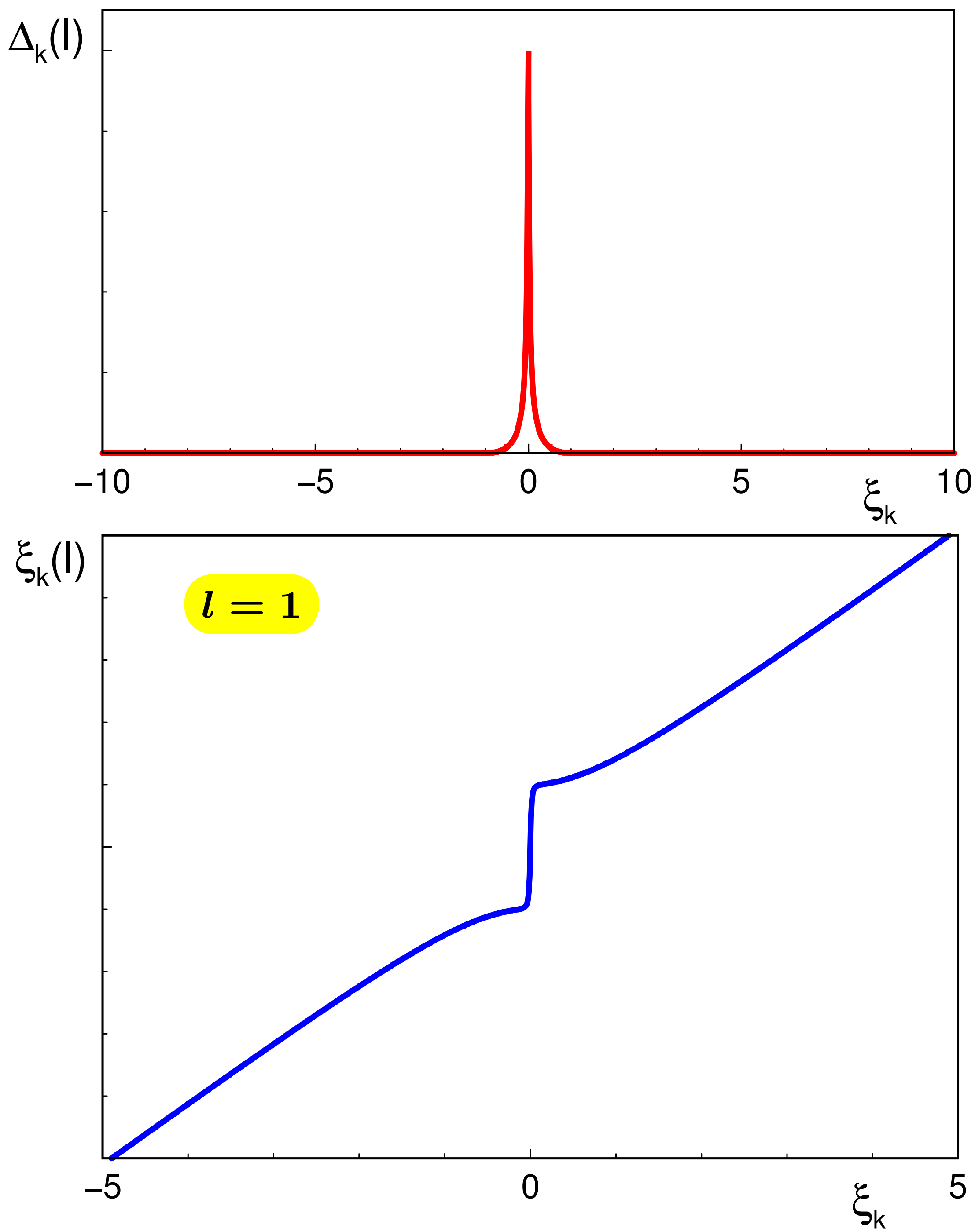
$\Delta_k(l)$
−10
−5
0
5
10
ξ_k
$\xi_k(l)$
$l = 0.05$
−5
0
5
ξ_k



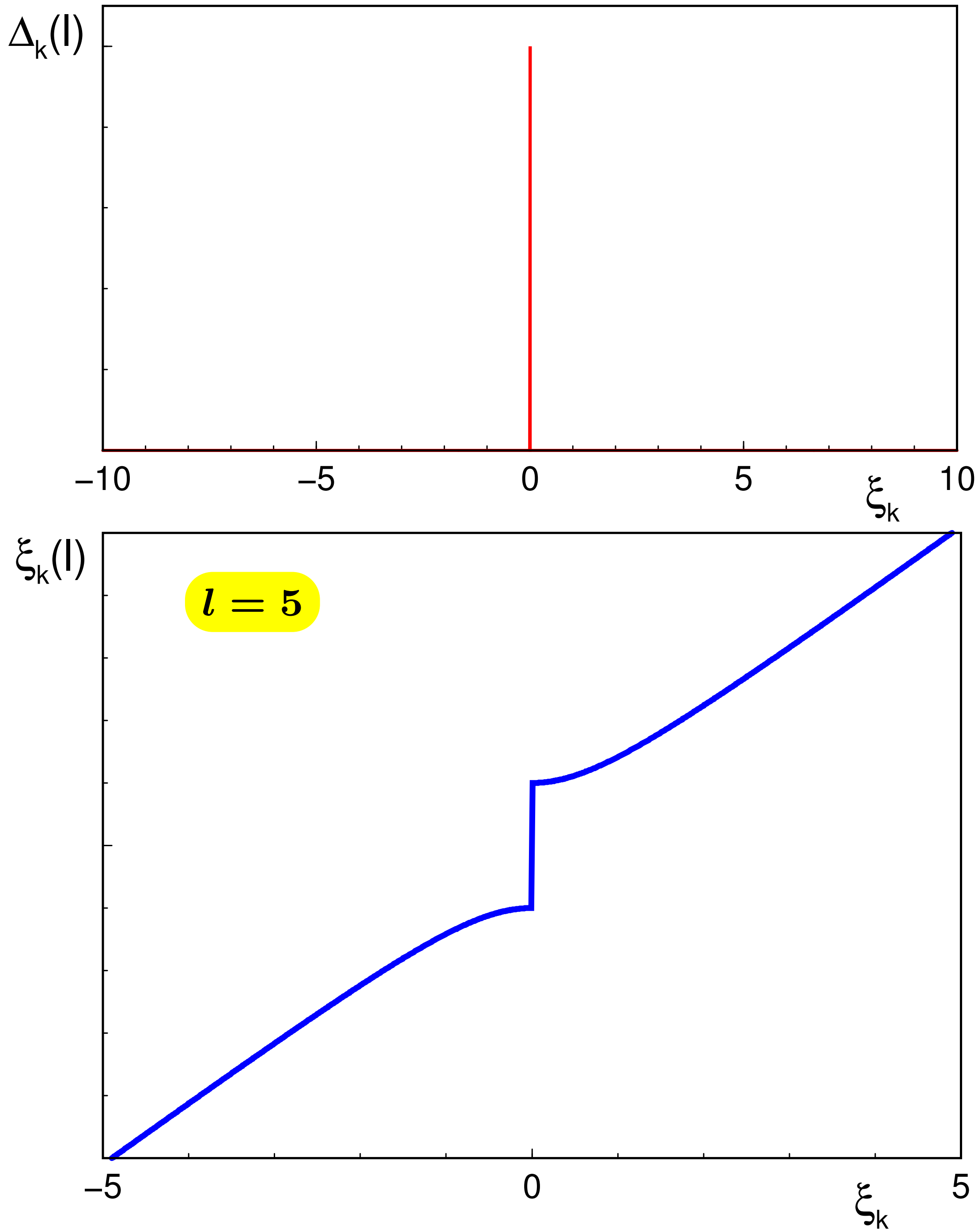
$\Delta_k(l)$
–10
–5
0
5
10
ξ_k
$\xi_k(l)$
$l = 0.01$
–5
0
5
ξ_k



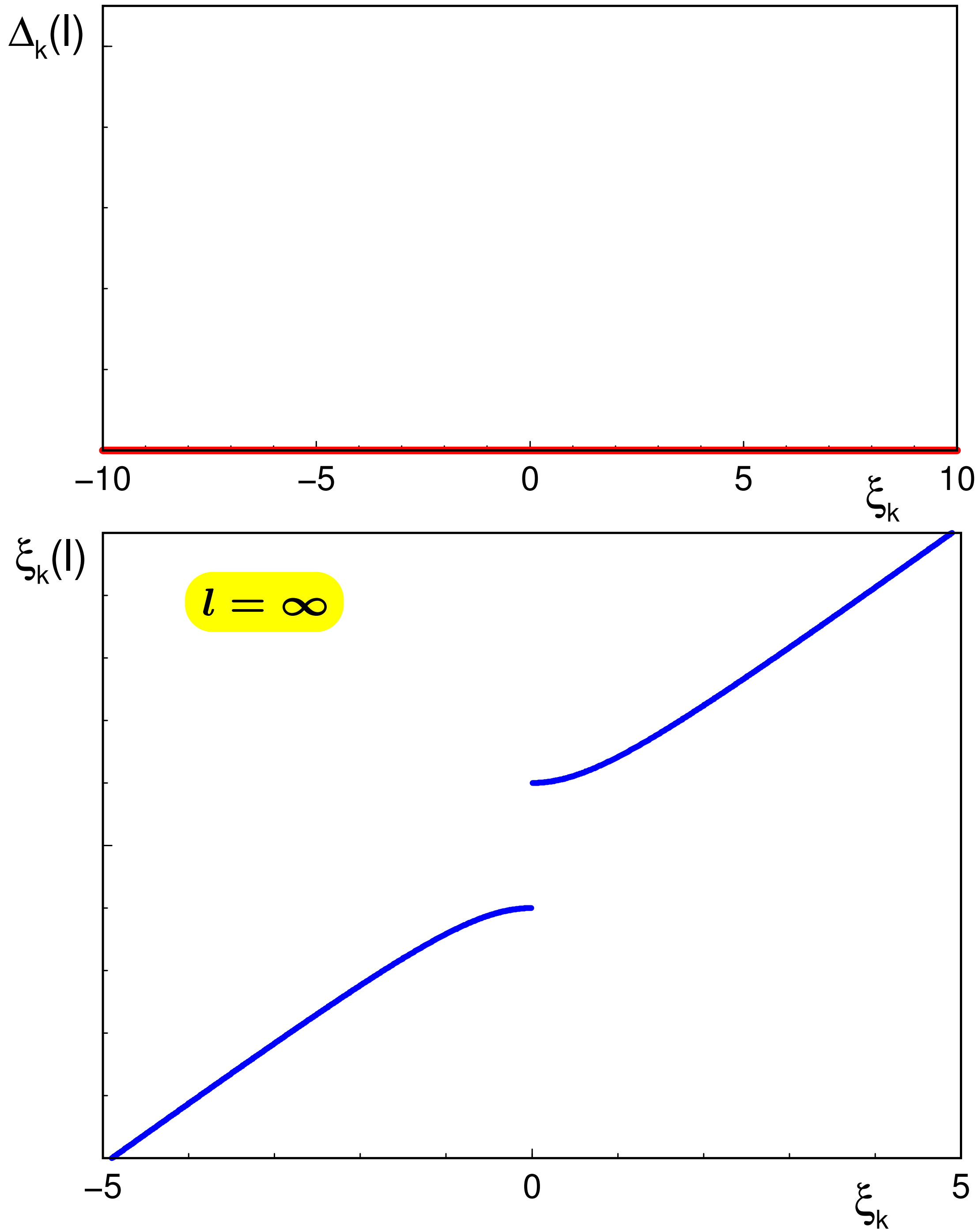
$\Delta_k(l)$
−10
−5
0
5
10
ξ_k
$\xi_k(l)$
$l = 0.5$
−5
0
5
ξ_k



$\Delta_k(l)$
−10
−5
0
5
10
ξ_k
$\xi_k(l)$
$l = 1$
−5
0
5
ξ_k



Δk(l)
–10
–5
0
5
10
ξk
ξk(l)
l = 5
–5
0
5
ξk



$\Delta_k(l)$
−10
−5
0
5
10
ξ_k
$\xi_k(l)$
$l = \infty$
−5
0
5
ξ_k

6. Applications

6.2. Boson-fermion model: a challenging problem

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$$
\begin{aligned}
H &= \sum_{\mathbf{k}\sigma} \left(\varepsilon_{\mathbf{k}} - \mu\right) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \left(E_{\mathbf{q}} - 2\mu\right) b^{\dagger}_{\mathbf{q}} b_{\mathbf{q}} \\
&+ \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q}} v_{\mathbf{k},\mathbf{q}} \left(b^{\dagger}_{\mathbf{q}} c_{\mathbf{k},\downarrow} c_{\mathbf{q}-\mathbf{k},\uparrow} + \text{h.c.} \right)
\end{aligned}
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$$+ \frac{1}{\sqrt{N}} \sum_{\mathbf{k},\mathbf{q}} v_{\mathbf{k},\mathbf{q}} \left(b^{\dagger}_{\mathbf{q}} c_{\mathbf{k},\downarrow} c_{\mathbf{q}-\mathbf{k},\uparrow} + \text{h.c.} \right)$$

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The BF model is not solvable exactly.

Outline of the procedure

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Hamiltonian at $0 < l < \infty$

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$$\hat{H}_F(\infty) + \hat{H}_B(\infty) \; + \; \mathbf{0}$$

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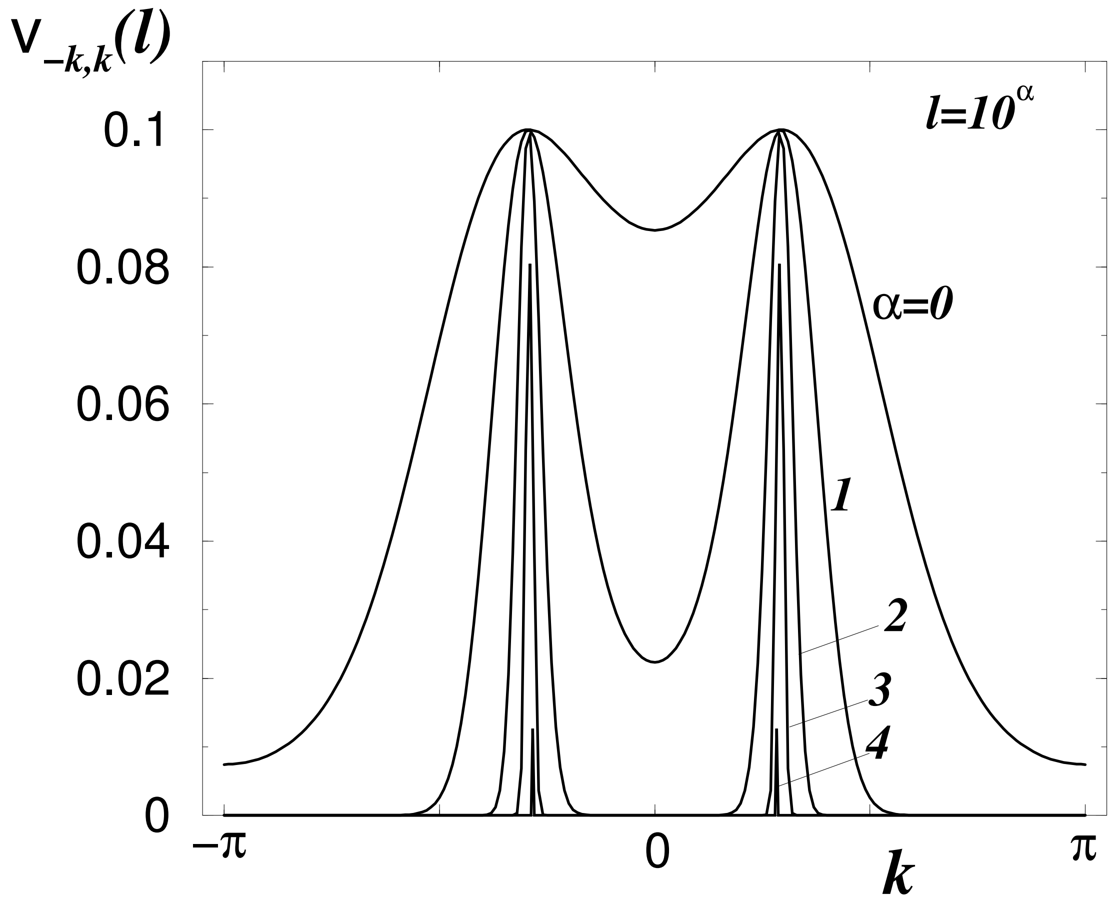
T. Domański and J. Ranninger, Phys. Rev. **B 63**, *134505 (2001).*

Flow of the boson-fermion coupling $v_{-\mathbf{k},\mathbf{k}}(l)$.



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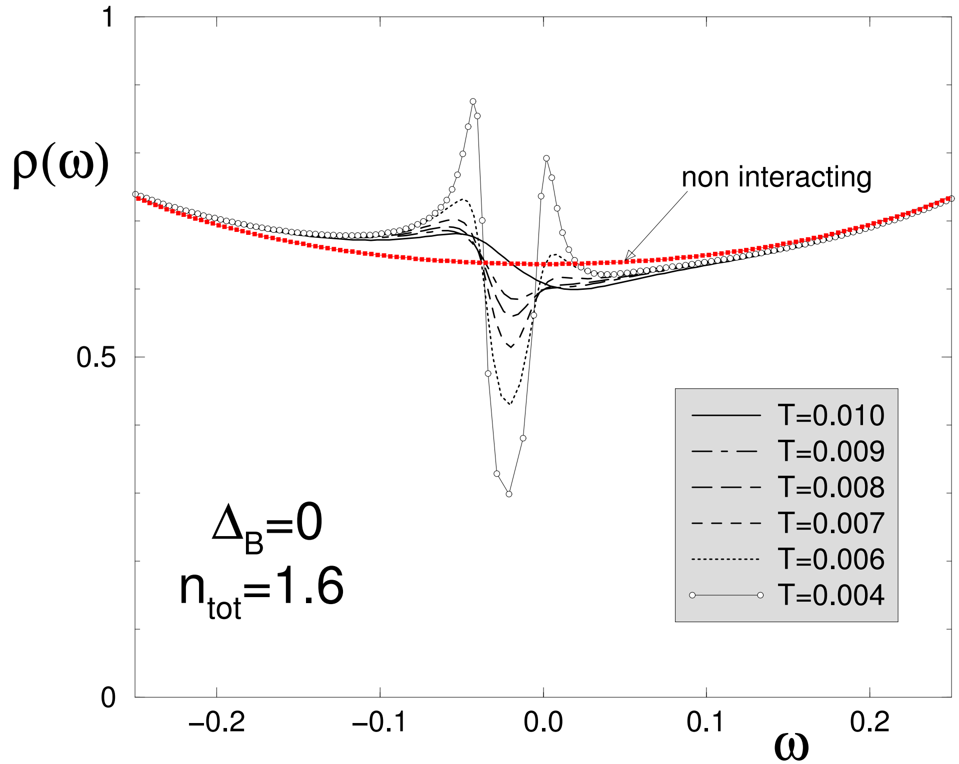
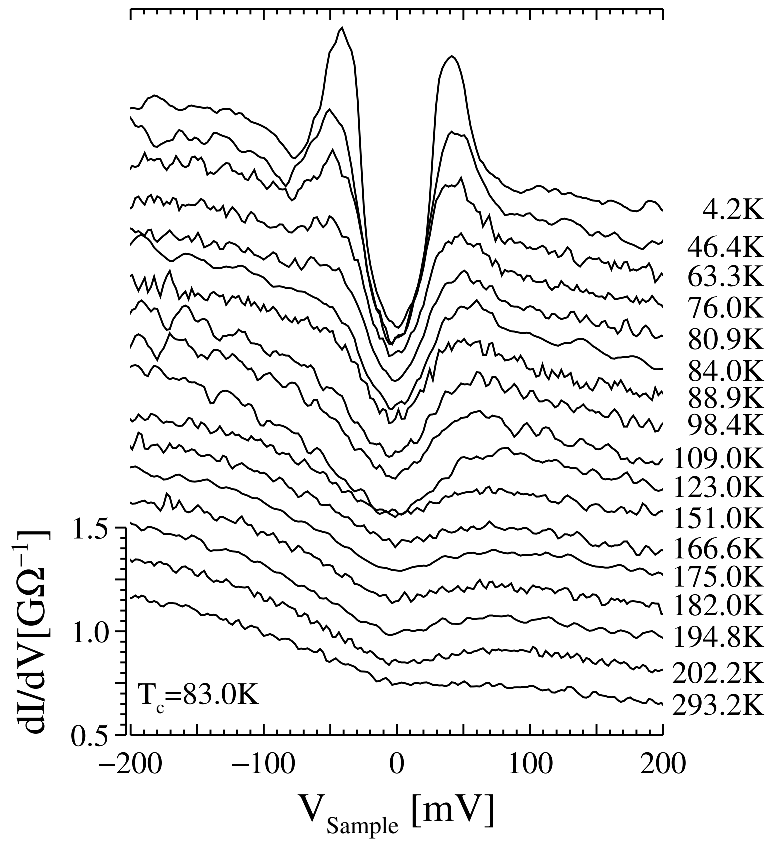


Near the Fermi energy there forms either a true gap (for $T < T_c$) or a pseudogap (for $T > T_c$), the latter being a precursor of the phase transition.

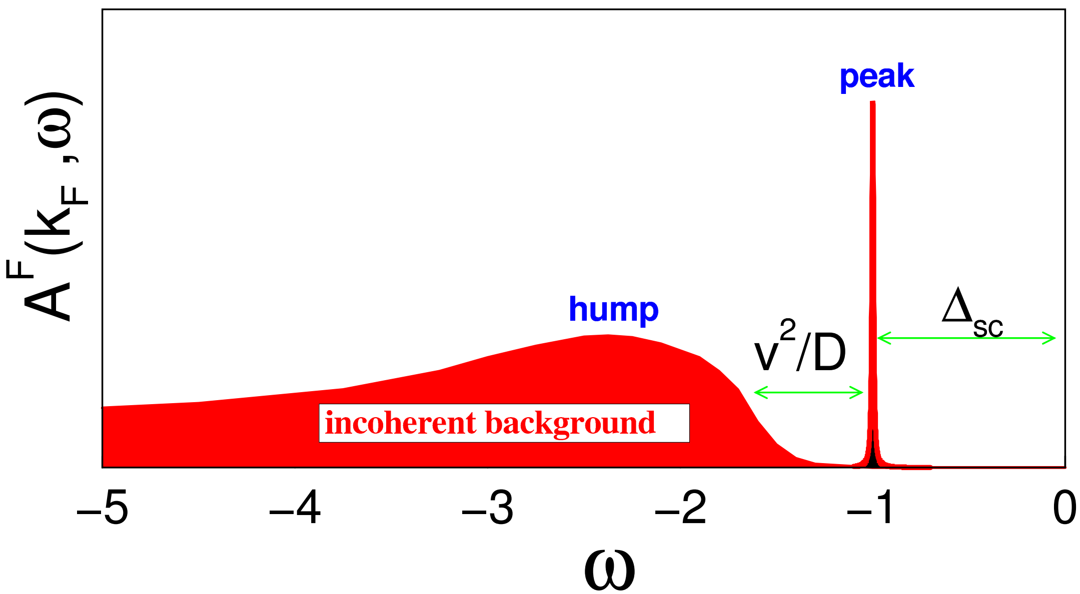
T. Domański & J. Ranninger, Physica C **387**, *77 (2003).*



STM conductance of cuprates for tempertures below T_c.

Ch. Renner et al, *Phys. Rev. Lett.* **80**, *149 (1998).*

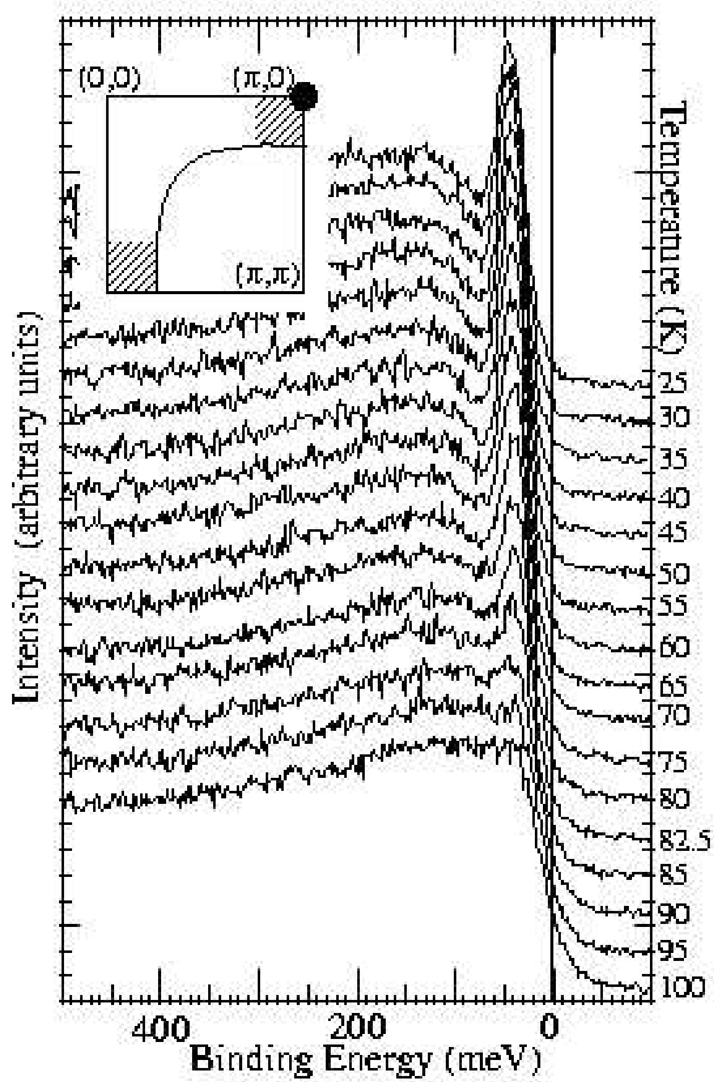
ARPES intensity for $T < T_c$



Schematic view of the spectral function in the antinodal direction for temperatures $T < T_c$ obtained using the boson-fermion model .

T. Domański and J. Ranninger, Phys. Rev. B **70**, *184513 (2004).*

Experimental data



A.G. Loeser, Z.-X. Shen et al, *Phys. Rev. B* **56**, *14185 (1997).*

Concuding remarks

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