Lublin, 7 XI 2006

Description of a transition into the superconducting state

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Outline

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/ pairing in the many-body systems /

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- **Path integral formulation**
  / the saddle-point solution, Gaussian corrections /
- **Renormalization Group technique**
  / the idea of scaling /
- **Recent RG extentions**
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I. Introduction

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Very often formation of the fermion pairs goes hand in hand with **superconductivity/superfluidity** but it needs not be the rule.

Strategy

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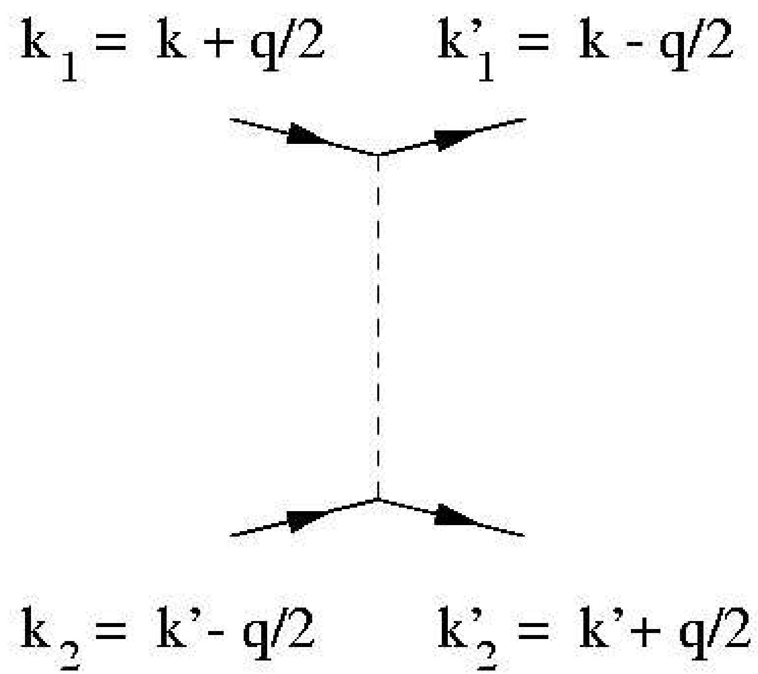
Our objective is to study the system of interacting fermions



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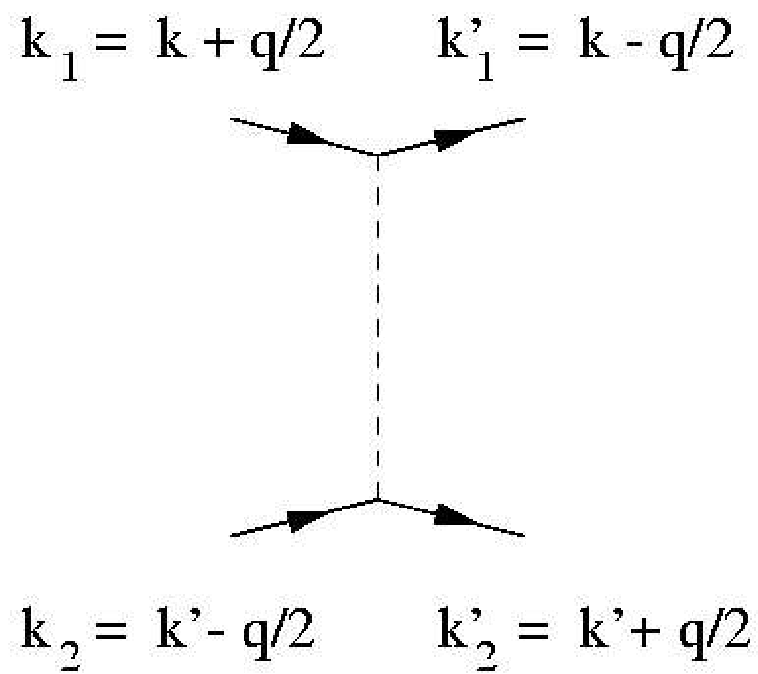

$$
\begin{aligned}
\hat{H} &= \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \mu) \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} \\
&+ \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \sum_{\sigma,\sigma'} g_{\mathbf{k},\mathbf{k}',\mathbf{q}} \hat{c}^{\dagger}_{\mathbf{k}'+\frac{\mathbf{q}}{2},\sigma} \hat{c}^{\dagger}_{\mathbf{k}-\frac{\mathbf{q}}{2},\sigma'} \hat{c}_{\mathbf{k}+\frac{\mathbf{q}}{2},\sigma'} \hat{c}_{\mathbf{k}'-\frac{\mathbf{q}}{2},\sigma}
\end{aligned}
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Pairing interactions

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The momentum representation:

$$\hat{H} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \; \hat{c}^{\dagger}_{\mathbf{k}\uparrow} \; \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \; \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow}$$

where $V_{\mathbf{k},\mathbf{k}'} < 0$ (at least for some $\mathbf{k}$, $\mathbf{k}'$ states)

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The real space representation:

$$\hat{H} = \sum_{i,j} \sum_{\sigma} t_{i,j} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \sum_{i,j} V_{i,j} \; \hat{c}^{\dagger}_{i\uparrow} \; \hat{c}_{i\uparrow} \; \hat{c}^{\dagger}_{j\downarrow} \hat{c}_{j\downarrow}$$

with attractive potential $V_{i,j} < 0$

II. Path integral formulation

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Thermodynamic properties such as the total energy, specific heat, pressure *etc* can be derived from the partition function defined as

$$\mathcal{Z} = \mathrm{Tr}\left\{ e^{-\beta \hat{H}} \right\}$$

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It is convenient to express the partition unction $\mathcal{Z}$ in terms of the path integrals over Grassmann variables

$$\mathcal{Z} = \int D[c, c^*] \;\; e^{-S}$$

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Formally they are eigenvectors of $\hat{c}$ and $\hat{c}^\dagger$ operators

$$\begin{aligned} \hat{c}\,|c\rangle &= c\,|c\rangle \\ \langle c^*|\,\hat{c}^\dagger &= \langle c^*|\,c^* \end{aligned}$$

with c and c^* being their eigenvalues (Grassmann numbers).

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In this way the partition function can be expressed as

$$\mathcal{Z} = - \int dc_N^* \, dc_1 \; e^{-c_N^* c_1} \left\langle c_N^* \right| e^{-\beta \hat{H}} \left| c_1 \right\rangle .$$

Time slicing

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We now expand the exponential into a sequence

$$e^{-\beta \hat{H}} = \left(e^{-\Delta\tau\ \hat{H}} \right)^N$$

of the discretized imaginary time $\tau \in \langle 0, \beta \rangle$ where $\Delta\tau = \beta/N$.

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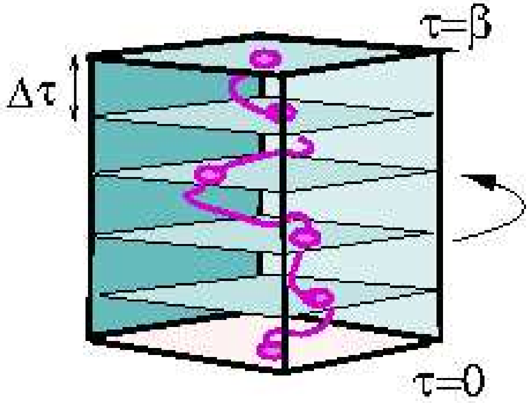

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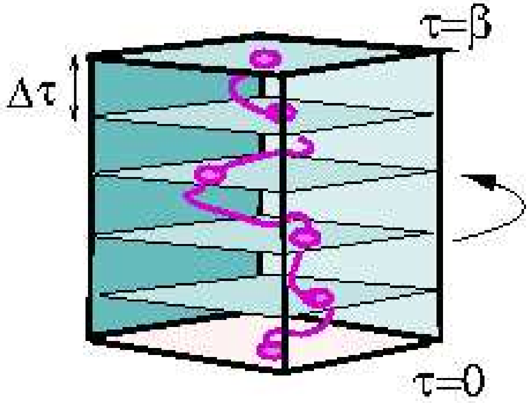

Using the normally ordered Hamiltonian

$$\left\langle c_j^* \right| e^{-\hat{H}\Delta\tau} \left| c_j \right\rangle = e^{c_j^* c_j}\ e^{-\Delta\tau H[c_j^*, c_j]}$$

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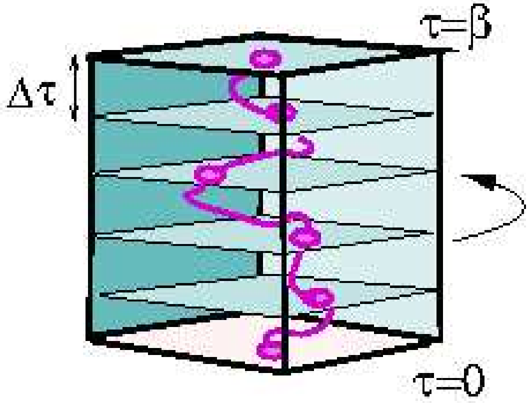

we finally obtain

$$\begin{aligned} \mathcal{Z} &= \int \Pi_{j=1}^{N} dc_j^* \, dc_j \; e^{-S} \\ S &= \sum_{j=1}^{N} \left[c_j^* \, \frac{c_{j+1} - c_j}{\Delta\tau} + H[c_j^*, c_j] \right] \Delta\tau \end{aligned}$$

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Grassmann variables obey the anti-periodic boundary conditions

$$c(\tau + \beta) = -c(\tau), \qquad c^*(\tau + \beta) = -c^*(\tau)$$

The BCS Hamiltonian

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We now apply the path integral formalism to the BCS model

$$\hat{H} = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} \, \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} - g \, \hat{A}^{\dagger} \hat{A}$$

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with the pair operators defined by

$$\hat{A} = \sum_{\mathbf{k}} \hat{c}_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \qquad\qquad \hat{A}^{\dagger} = \sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow}\ \hat{c}^{\dagger}_{-\mathbf{k}\downarrow}$$

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The partition function $\mathcal{Z} = \int D[c^*, c]e^{-S}$ contains the action

$$S = \int_0^{\beta} d\tau \sum_{\mathbf{k}\sigma} c^*_{\mathbf{k}\sigma}(\tau)\ (\partial_\tau + \xi_{\mathbf{k}})\ c_{\mathbf{k}\sigma}(\tau) - g A^*(\tau)A(\tau)$$

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It is convenient to use the following identity

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Substituting it to the partition function $\mathcal{Z} = \int D[\Delta^*, \Delta, c^*, c]\, e^{-S}$

$$S = \int_0^\beta d\tau \sum_{\mathbf{k}\sigma} c^*_{\mathbf{k}\sigma} \left(\partial_\tau + \xi_{\mathbf{k}}\right) c_{\mathbf{k}\sigma} + \Delta A^* + \Delta^* A + \frac{1}{g}\Delta^*\Delta$$

we obtain the action which becomes quadratic in the fermion fields !

Integration over the fermion fields

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The path integral can be now carried out exactly with respect to the Grassmann variables $c_{\mathbf{k}\sigma}$ and $c^*_{\mathbf{k}\sigma}$ giving

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The effective action of the pairing (boson) field is given by

$$S_{eff}[\Delta^*, \Delta] = \int_0^\beta d\tau \left(\frac{\Delta^*(\tau)\Delta(\tau)}{g} + \sum_{\mathbf{k}} \mathrm{Tr}\ \ln\left(\partial_\tau + h_{\mathbf{k}}\right) \right)$$

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where

$$h_{\mathbf{k}} = \begin{bmatrix} \xi_{\mathbf{k}} & \Delta(\tau) \\ \Delta^*(\tau) & -\xi_{\mathbf{k}} \end{bmatrix}$$

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For the case of uniform $\Delta(\tau) = \Delta$ we obtain the determinant

$$\det\left(\partial_\tau + h_{\mathbf{k}}\right) = \Pi_{\mathbf{k}}\left(\omega_n^2 + \xi_{\mathbf{k}}^2 + |\Delta|^2\right)$$

where $\omega_n = (2n+1)\pi\beta^{-1}$ is the Matsubara frequency.

The saddle-point approximation

This problem can be solved exactly either if the pairing field $\Delta(\tau)$ is uniform or almost uniform (including the small Gaussian corrections).

The partition function is related with the Free energy via $\mathcal{Z} = e^{-\beta F}$, so we finally get

$$F = -\frac{1}{\beta} \sum_{\mathbf{k},n} \ln\left(\omega_n^2 + \xi_{\mathbf{k}}^2 + |\Delta|^2\right) + \frac{|\Delta|^2}{g}$$

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Minimizing F with respect to Δ^* we obtain the BCS gap equation

$$\frac{\partial F}{\partial \Delta^*} = 0 = -\sum_{\mathbf{k},n} \frac{\Delta}{\omega_n^2 + \xi_{\mathbf{k}}^2 + |\Delta|^2} + \frac{\Delta}{g}$$

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$$\Delta = g \sum_{\mathbf{k}} \frac{\Delta}{2E_{\mathbf{k}}} \tanh\left(\frac{\beta E_{\mathbf{k}}}{2}\right)$$

where $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta|^2}$.

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1. Normal state $(T \geq T_c)$ .... $a < 0, \quad b > 0$
The minimum occurs at $\Delta = 0$.

2. Superconducting state $(T < T_c)$ .... $a > 0, \quad b > 0$
The minimum moves to $|\Delta|^2 = \frac{a}{2b}(T - T_c)$.

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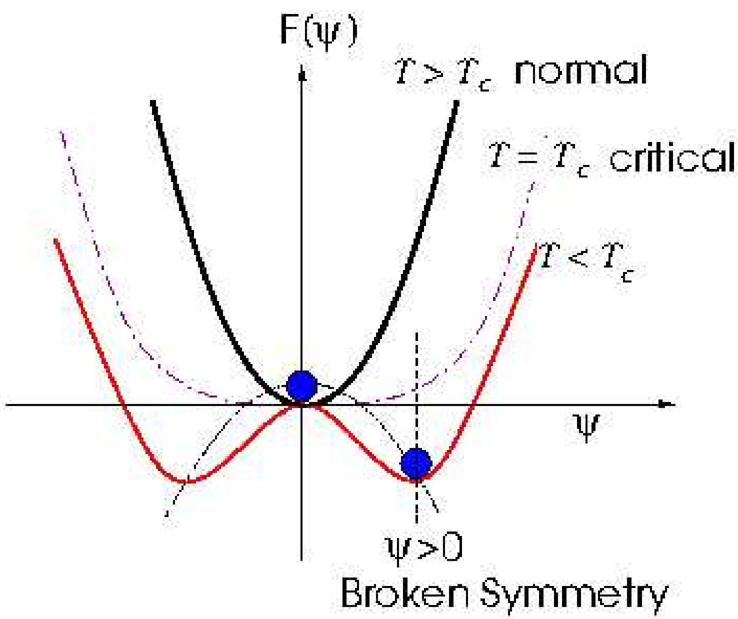

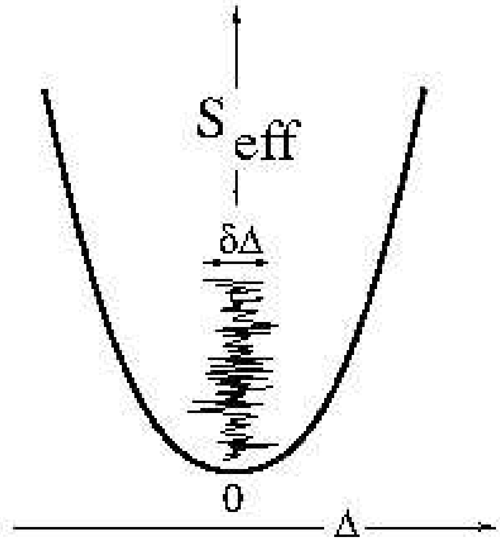

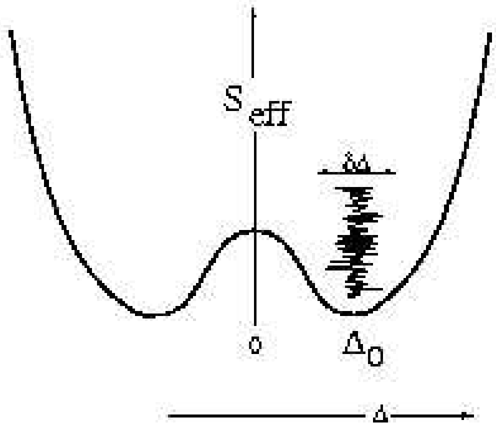

One can also include some fluctuations around the saddle-point.

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$$\mathcal{G}[\chi,\chi^*] = \log\left[\mathcal{Z}^{-1}\int D[c^*,c]e^{-(S+\sum_{\mathbf{k},\sigma} c^*_{\mathbf{k}\sigma}\chi_{\mathbf{k}\sigma}+\chi^*_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma})}\right]$$

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For instance, the two-point Green's function is

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A more specific discussion can be found e.g. in

V.N. Popov,
Functional integrals and collective excitations, Cambridge Univ. Press (1987);
J.W. Negele and H. Orland,
Quantum many-particle systems, Perseus Books (1998).

III. Renormalization Group

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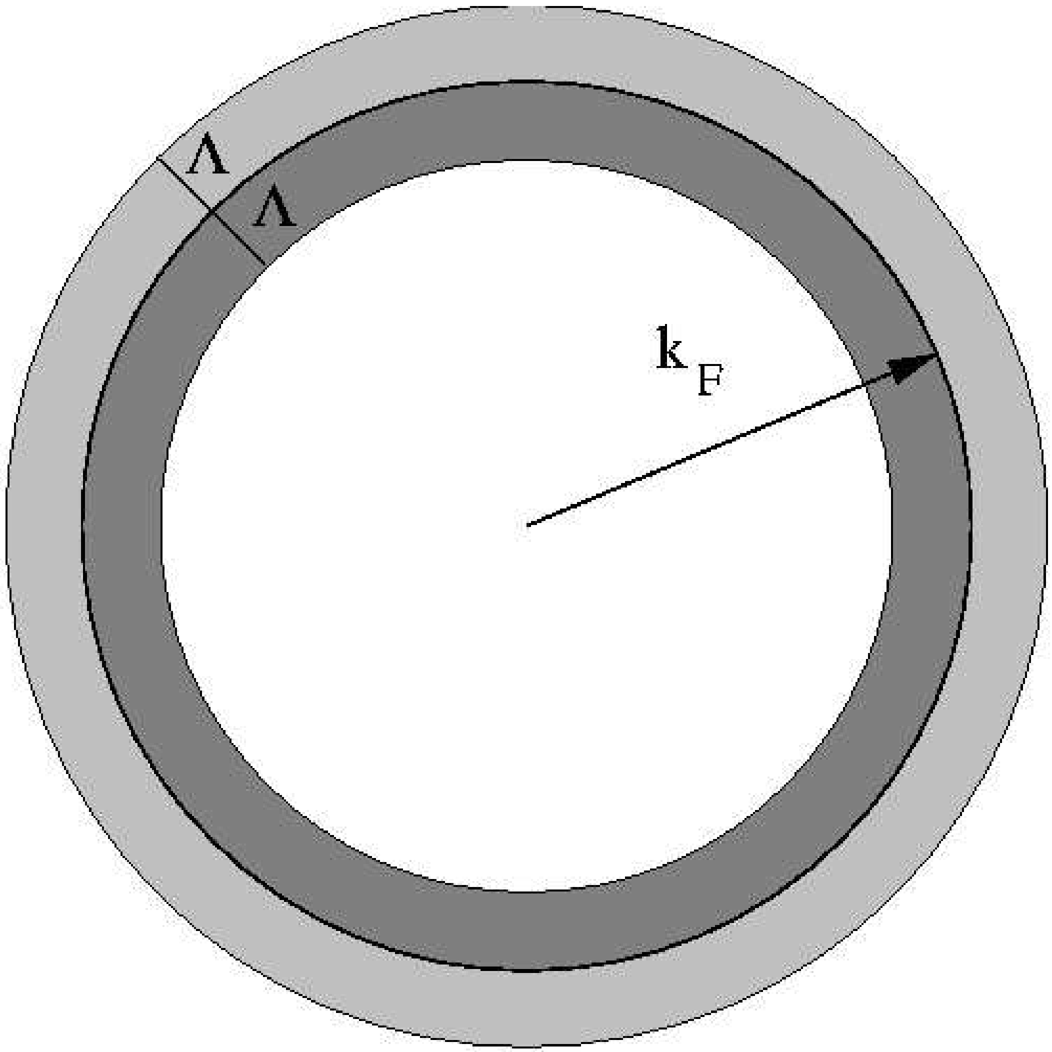
$$e^{-S^{\Lambda}[c^*,c]} = \int D^{>\Lambda}[c^*, c] \; e^{-S[c^*,c]}$$

so that the generating functional becomes

$$\mathcal{G}[\chi, \chi^*] = \log \left[\mathcal{Z}^{-1} \int D^{<\Lambda}[c^*, c] e^{-S^{\Lambda} - \int_k^{<\Lambda} c^*_{\mathbf{k}\sigma}\chi_{\mathbf{k}\sigma} + c_{\mathbf{k}\sigma}\chi^*_{\mathbf{k}\sigma}} \right]$$

Mode elimination in the momentum space:



Fast modes (i.e. fermion fields outside the shell of width 2Λ) are integrated out and the leftover contains only *slow modes* which are relevant for the physically observed properties.

Nobel Prize in Physics 1982

Kenneth Wilson

for his theory of critical phenomena in connection with phase transitions

Remarks on the RG scheme

Upon a succesive decrease of the energy cut-off Λ toward the Fermi energy the high energy excitations are integrated out. This leads simultaneously to:

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⇒ **topology of the Fermi surface might deform**

⇒ **and sometimes even the Fermi surface itself might completely break down !**

In case of the symmetry broken phases the scaling procedure is additionally complicated due to a lower boundary (the energy gap $|\Delta|$).

The conventional RG techniques are blind with respect to the symmetry-broken states which are separated by energy barrier from the symmetric state.

R. Gersch, J. Reiss and C. Honerkamp, Progr. Theor. Phys. (2006).

IV. Recent RG extentions

RG ideas to deal with symmetrry broken states

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1. A small symmetry-breaking component $\mathbf{\Delta(\Lambda_0)}$ is imposed at a certain initial condition Λ_0. Its physical meaning establishes from the flow to the asymptotic fixed point

$$\mathbf{\Delta = \lim_{\Lambda \to 0} \Delta(\Lambda)}$$

M. Salmhofer et al, *Progr. Theor. Phys.* **112**, *943 (2004).*

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2. One introduceds the collective boson fields $\boldsymbol{\Phi}$, $\boldsymbol{\Phi^*}$ via the Hubbard- Stratonovich transformation. Some effective Fermi-Bose theory is then developed using the functional RG equations.

$$\boldsymbol{S = S_0[c, c^*] + S_0[\Phi, \Phi^*] + S_I[c, c^*, \Phi, \Phi^*]}$$

F. Schütz, L. Bartosch, P. Kopietz, Phys. Rev. B **72**, *035107 (2005).*

Continuous unitary transformation

Instead of integrating out the fast modes (high energy sector) one constructs the canonical transformation $\hat{H}(l) = \hat{U}(l)\hat{H}\hat{U}^{\dagger}(l)$ such that:

- Hamiltonian is diagonalized in a series of infinitesimal steps

$$\hat{H} \longrightarrow \ldots \longrightarrow \hat{H}(l) \longrightarrow \ldots \longrightarrow \hat{H}(\infty)$$

  with l being a continuous parameter

- evolution of the Hamiltonian is governed by **the flow equation**

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

  where formally $\hat{\eta}(l) = -\hat{U}(l)\, \partial_l \hat{U}^{\dagger}(l)$.

F. Wegner, Annalen der Physik **3***, 77 (1994).*

Comparison to the usual RG method

Similarities:

- diagonalization of the high energy states occurs mainly during the first part of the transformation
- the low energy states are diagonalized at the very end of transformation

Roughly speaking, one can draw the following relation to the Wilson's numerical RG method:

$$\frac{1}{\sqrt{l}} \longleftrightarrow \Gamma$$

Differences:

Throughout the continuous canonical transformation one keeps track of the slow and high energy modes, therefore their mutual feedback effects can be analyzed.

Practical choice

For Hamiltonians with the following structure

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

one can choose

$$\hat{\eta}(l) = \left[\hat{H}_0(l), \hat{H}_1(l)\right]$$

and then

$$\lim_{l\to\infty} \hat{H}_1(l) = 0$$

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).

1. Heating up exercise

The bilinear Hamiltonian:

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

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

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

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$$\begin{aligned}
\partial_l \ \xi_{\mathbf{k}}(l) &= 4\xi_{\mathbf{k}}(l) \ |\Delta_{\mathbf{k}}(l)|^2 \\
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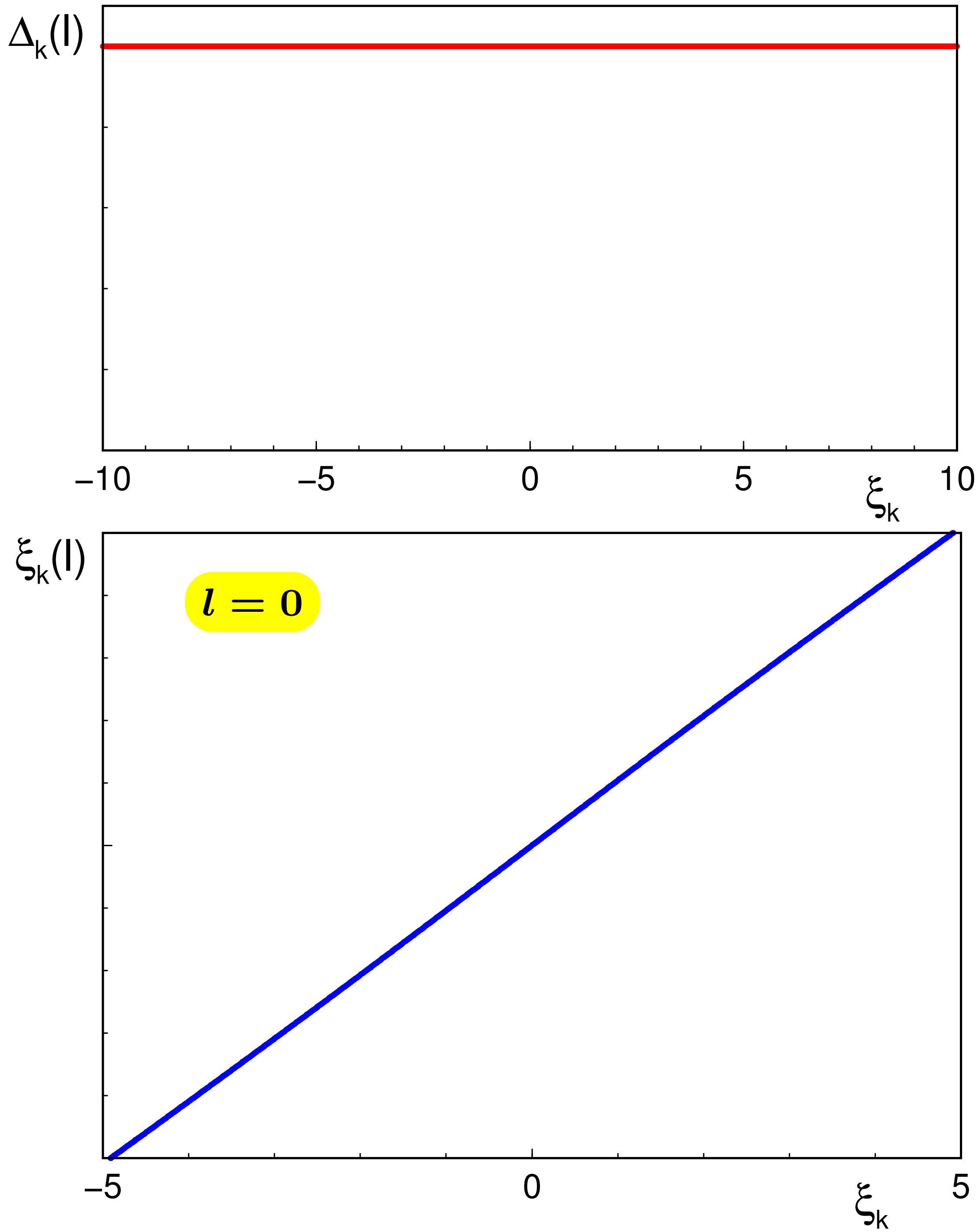
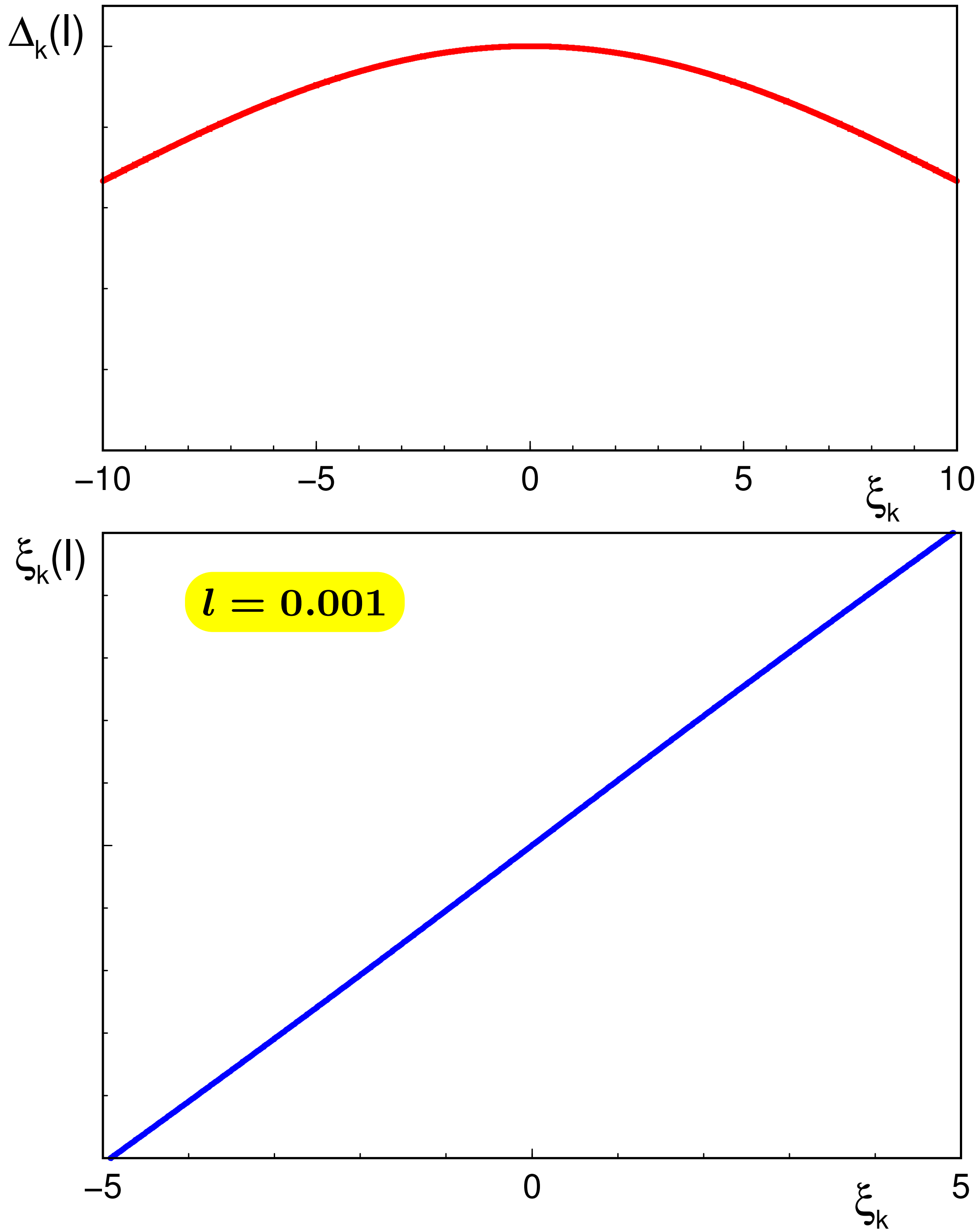
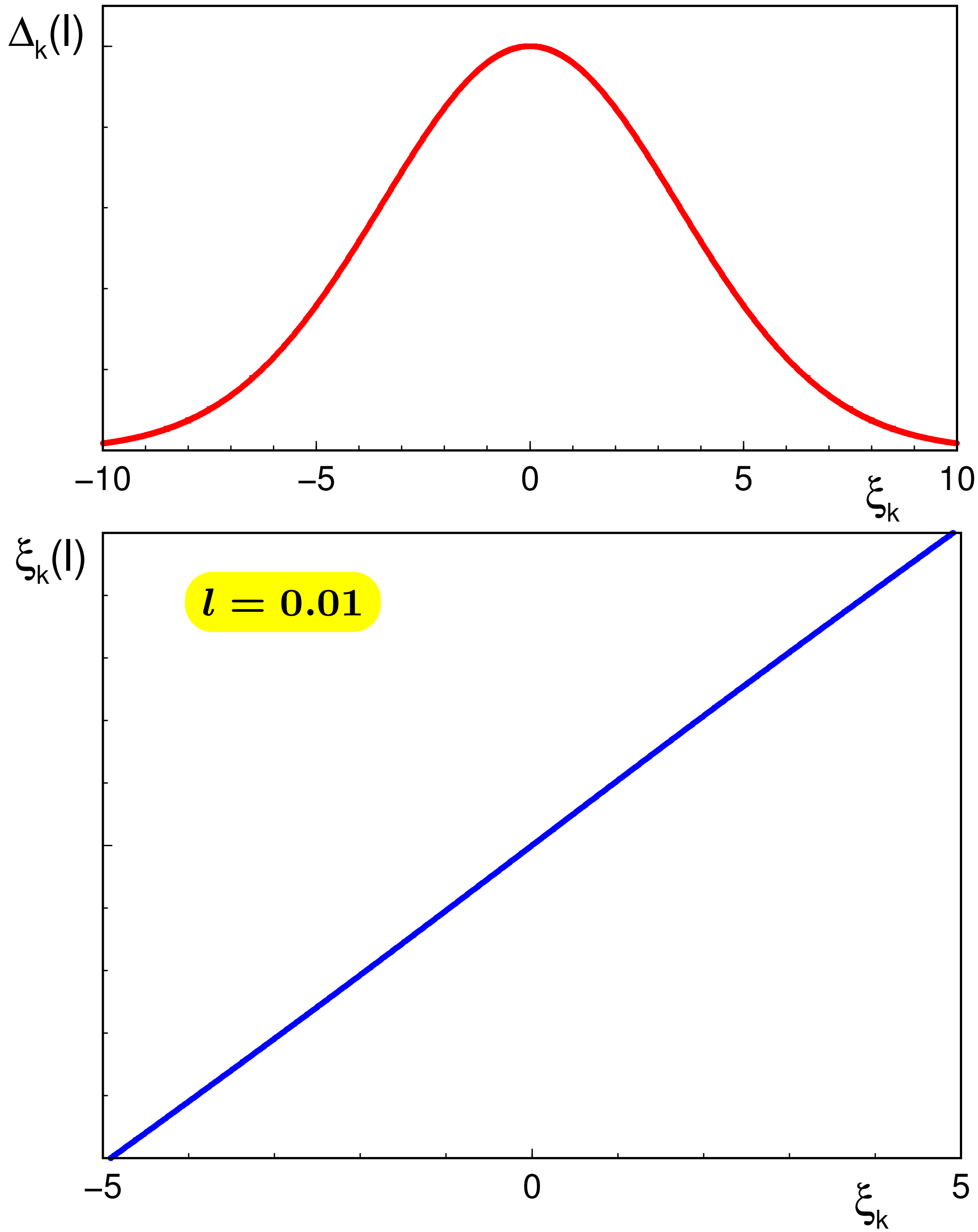
T. Domański, cond-mat/0602236 (to be published).



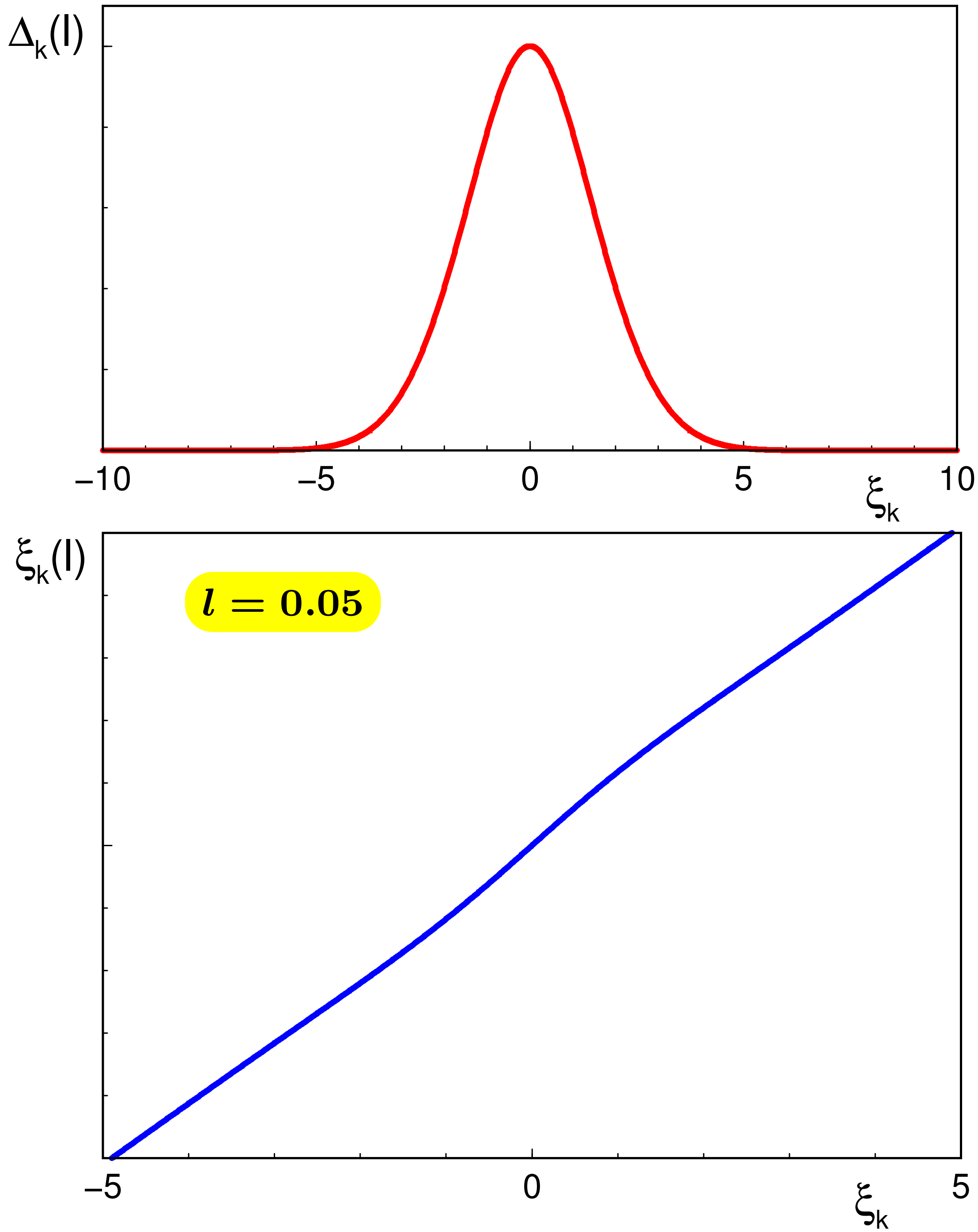
$\Delta_k(l)$
−10
−5
0
5
10
ξ_k
$\xi_k(l)$
$l = 0$
−5
0
5
ξ_k



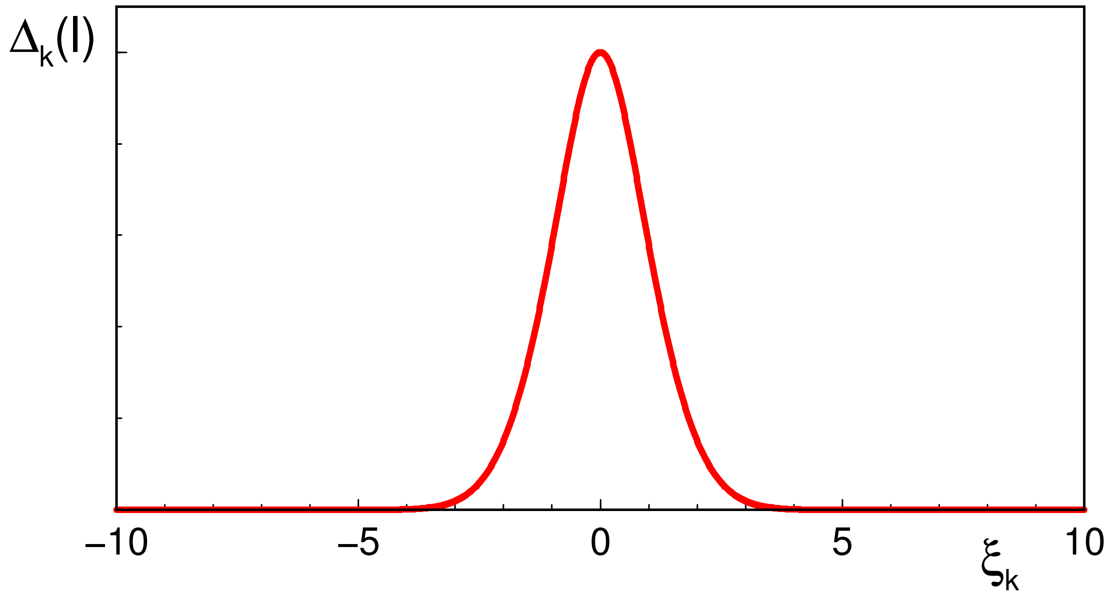
$\Delta_k(l)$
−10
−5
0
5
10
ξ_k
$\xi_k(l)$
$l = 0.001$
−5
0
5
ξ_k



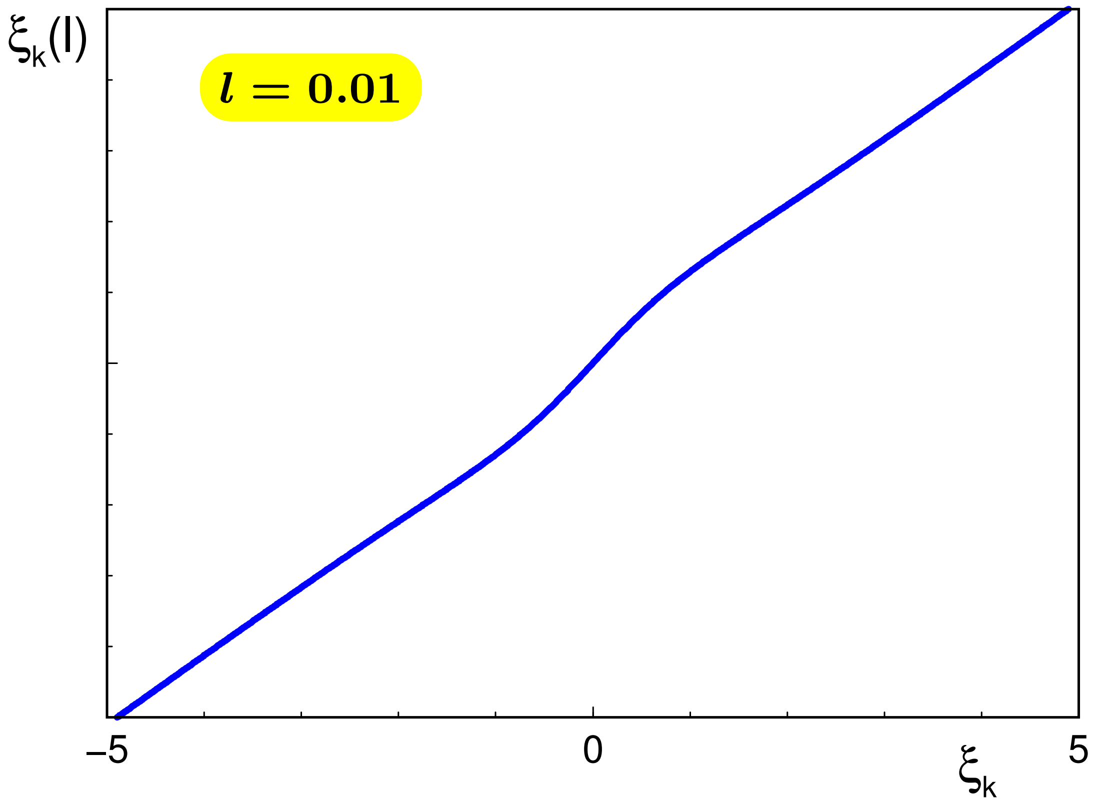
Δ_k(l)
−10
−5
0
5
10
ξ_k
ξ_k(l)
l = 0.01
−5
0
5
ξ_k



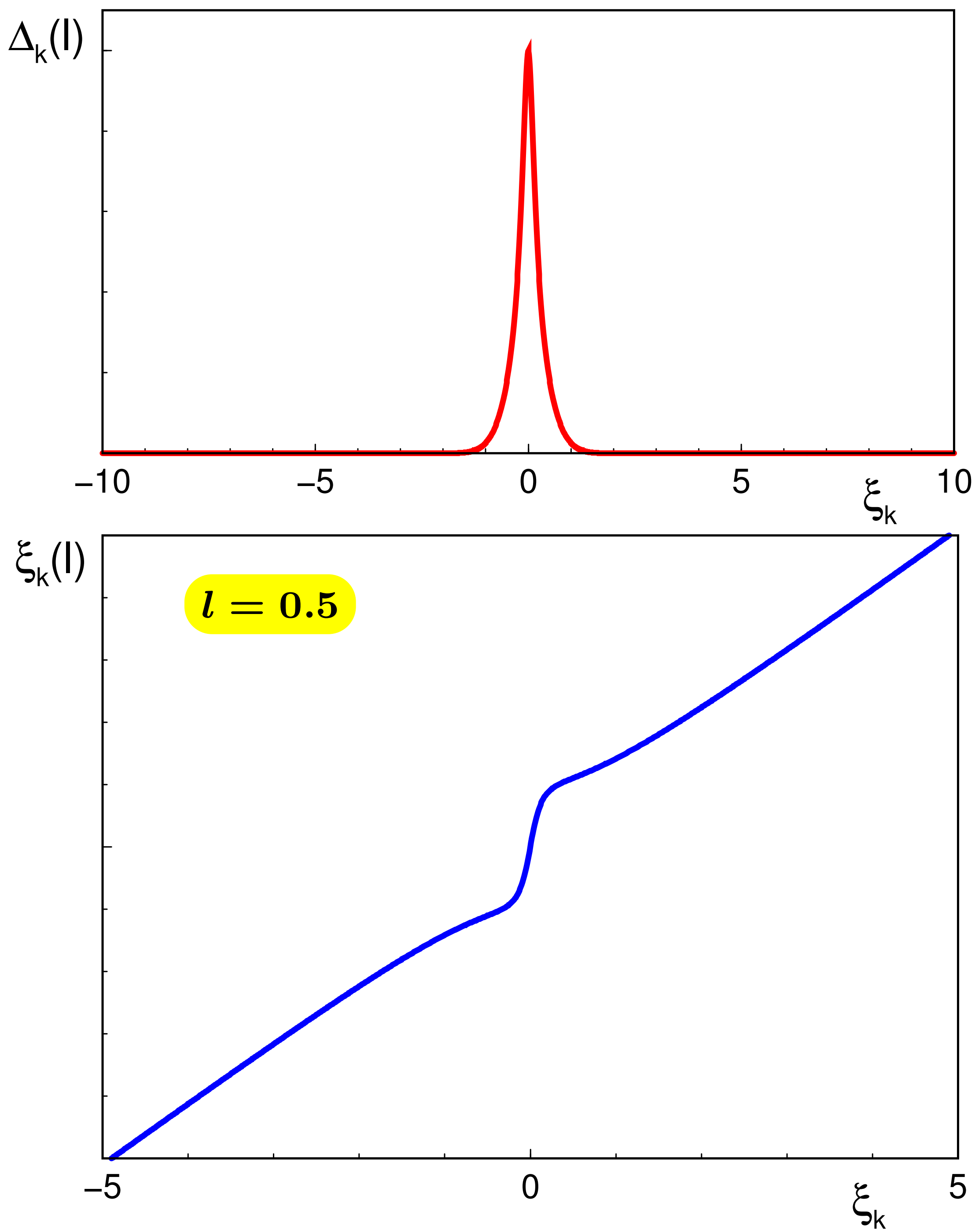
$\Delta_k(l)$
−10
−5
0
5
10
ξ_k
$\xi_k(l)$
$l = 0.05$
−5
0
5
ξ_k



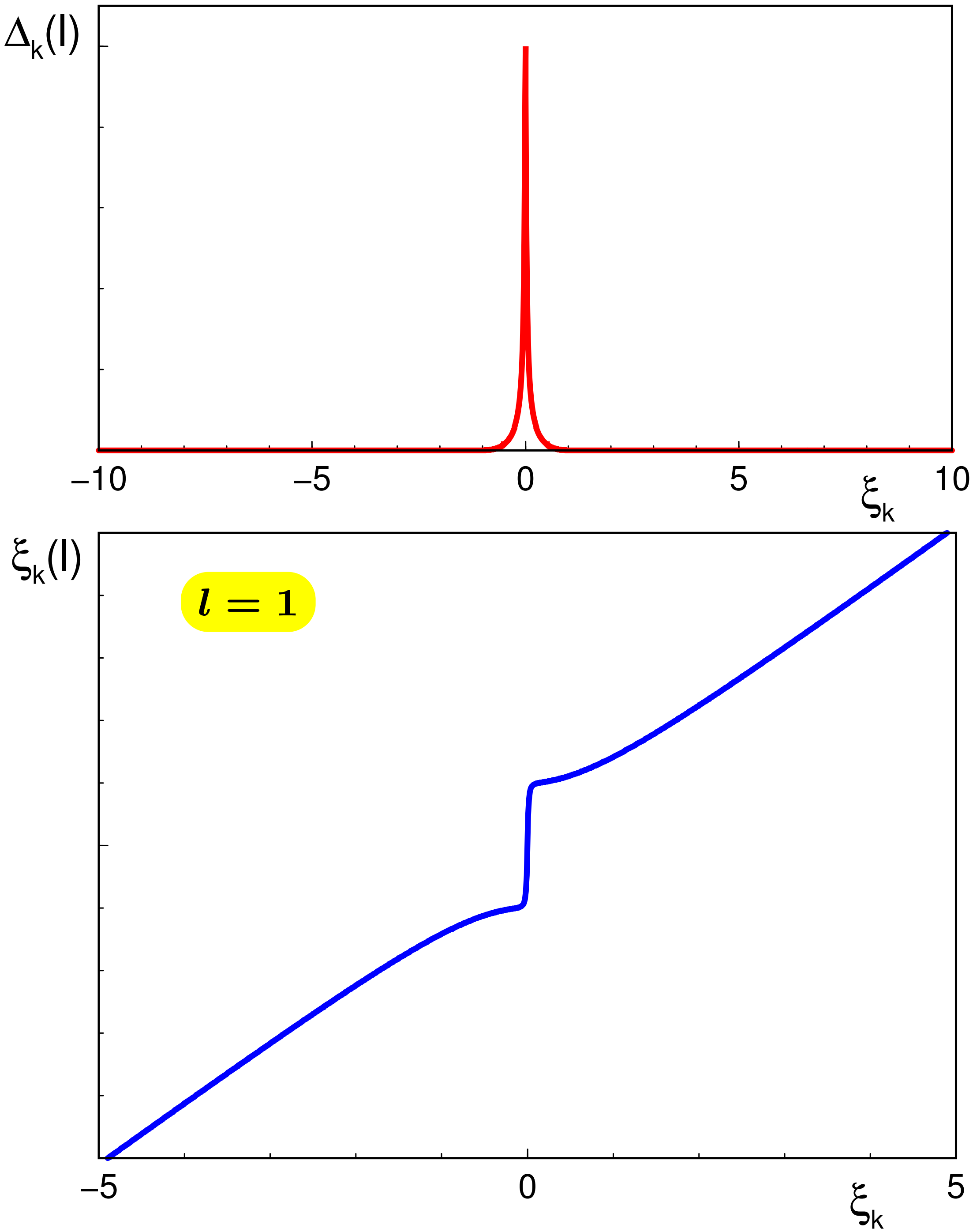
Δk(l)
−10
−5
0
5
10
ξk



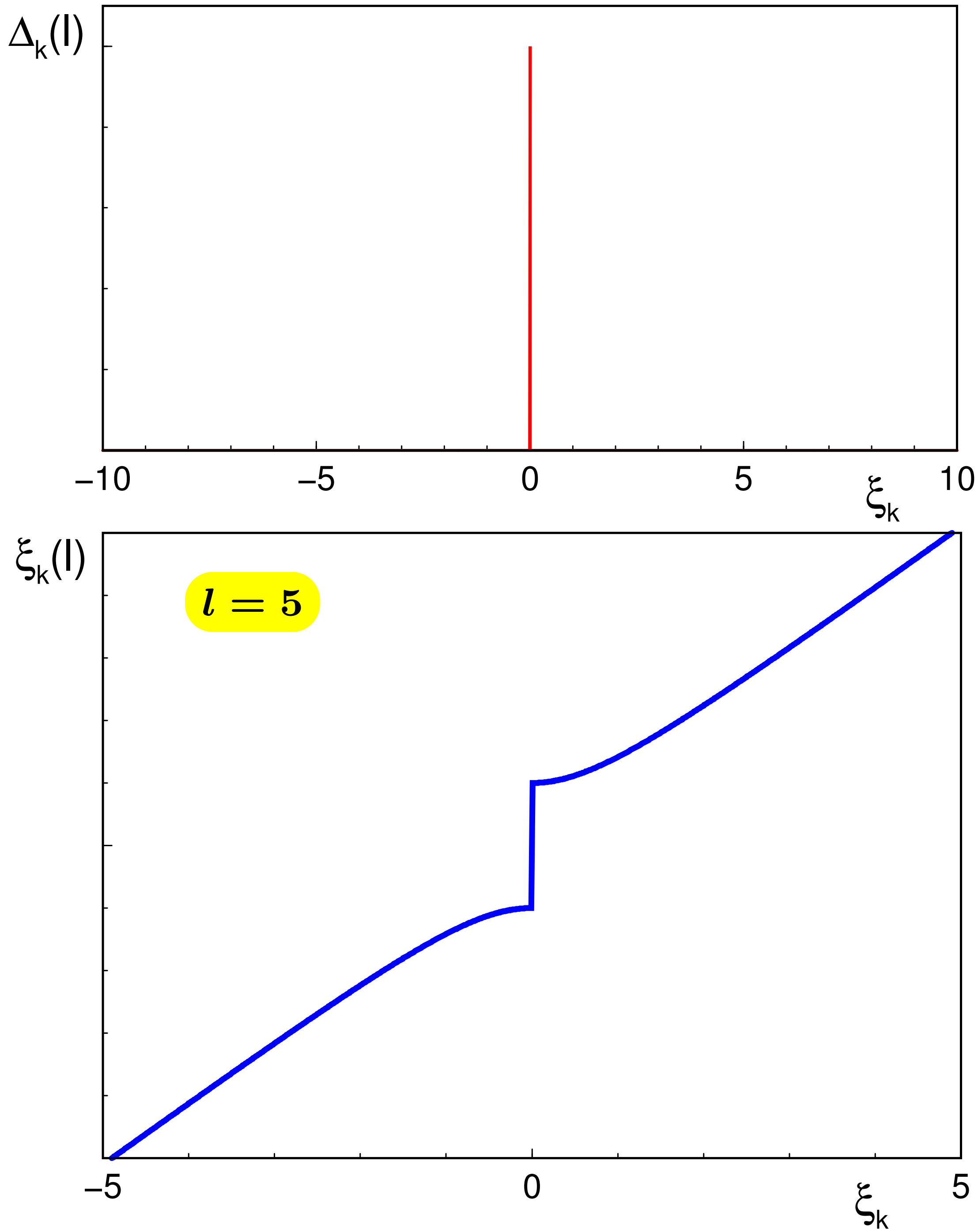
ξk(l)
l = 0.01
−5
0
5
ξk



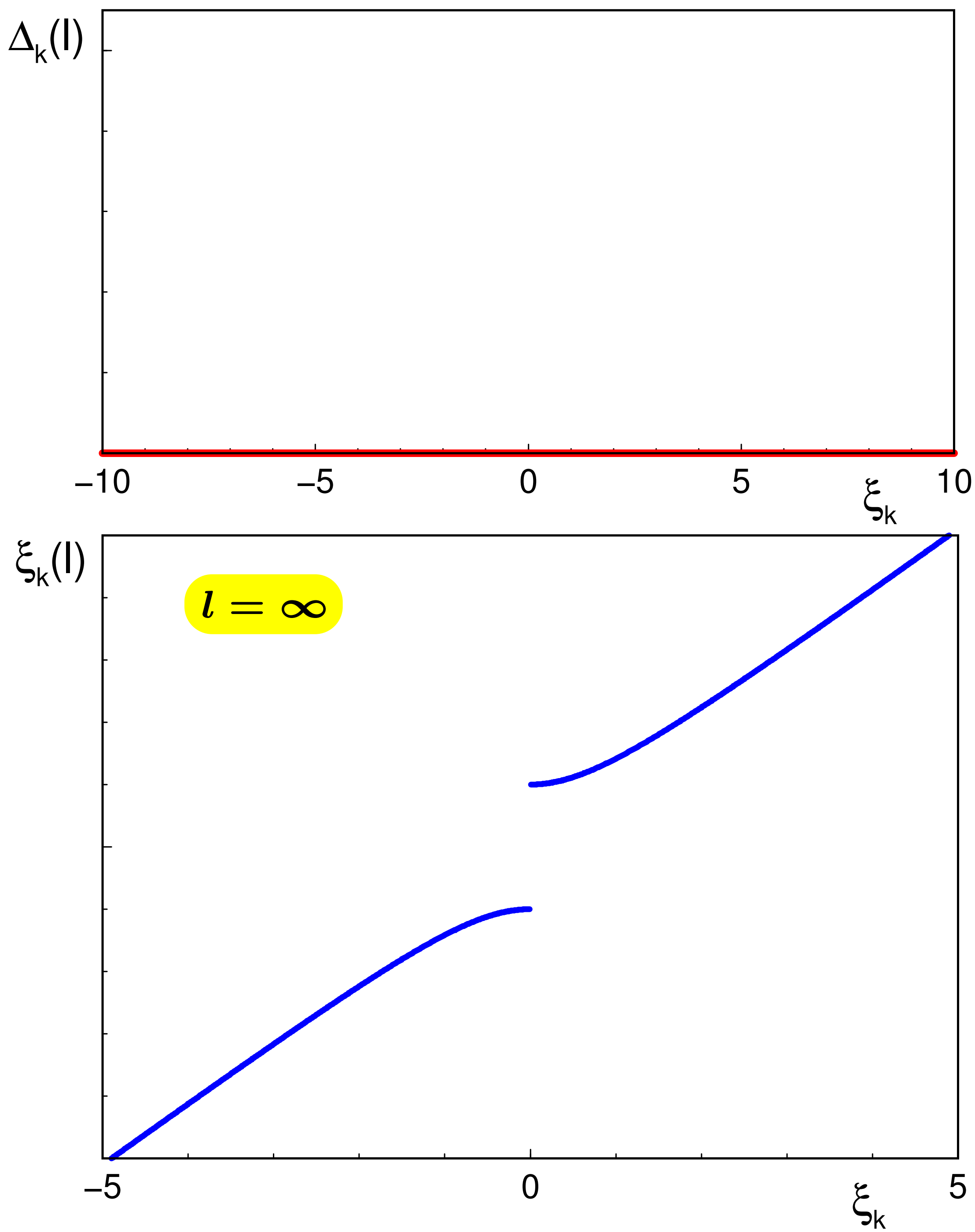
$\Delta_k(l)$
−10
−5
0
5
10
ξ_k
$\xi_k(l)$
$l = 0.5$
−5
0
5
ξ_k



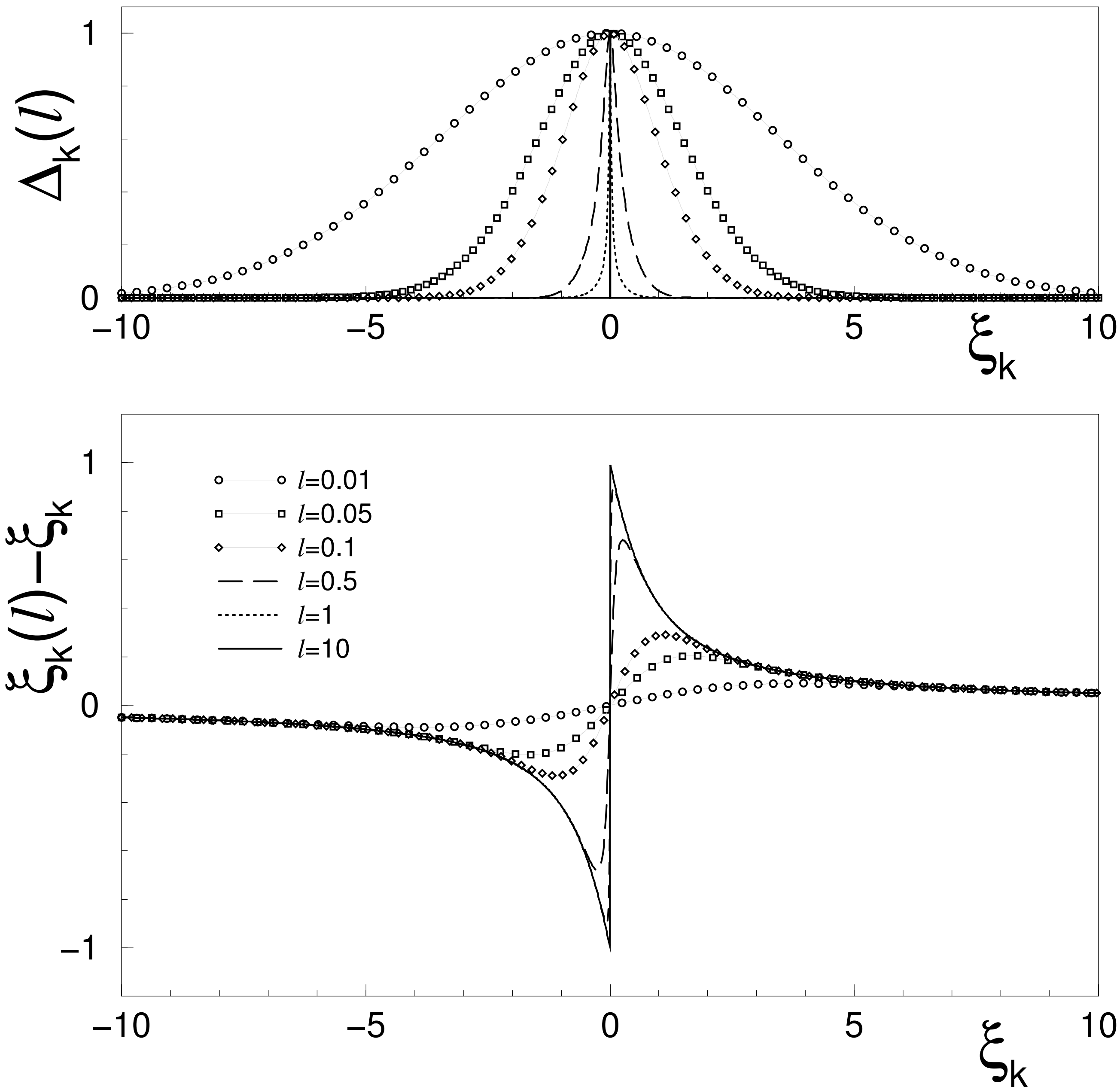
Δk(l)
−10
−5
0
5
10
ξk
ξk(l)
l = 1
−5
0
5
ξk



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



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



Renormalization of $\Delta_{\mathbf{k}}(l)$ *and* $\xi_{\mathbf{k}}(l)$ *during the* flow.

2. The real challenge

Boson-fermion model

$$
\begin{aligned}
H &= \sum_{\mathbf{k}\sigma} (\varepsilon_{\mathbf{k}} - \mu)\, c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} (E_{\mathbf{q}} - 2\mu)\, 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]
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Such Hamiltonian is obtained by elliminating the two-body interactions via the Hubbard-Stratonovich transformation

$$\sum_{\mathbf{k}'} c^{\dagger}_{\mathbf{q}-\mathbf{k}',\uparrow}\, c^{\dagger}_{\mathbf{k}',\downarrow} \longrightarrow b^{\dagger}_{\mathbf{q}}$$

a) Outline of the procedure

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In order to study the many-body effects we construct

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Hamiltonian at $\mathbf{0 < l < \infty}$

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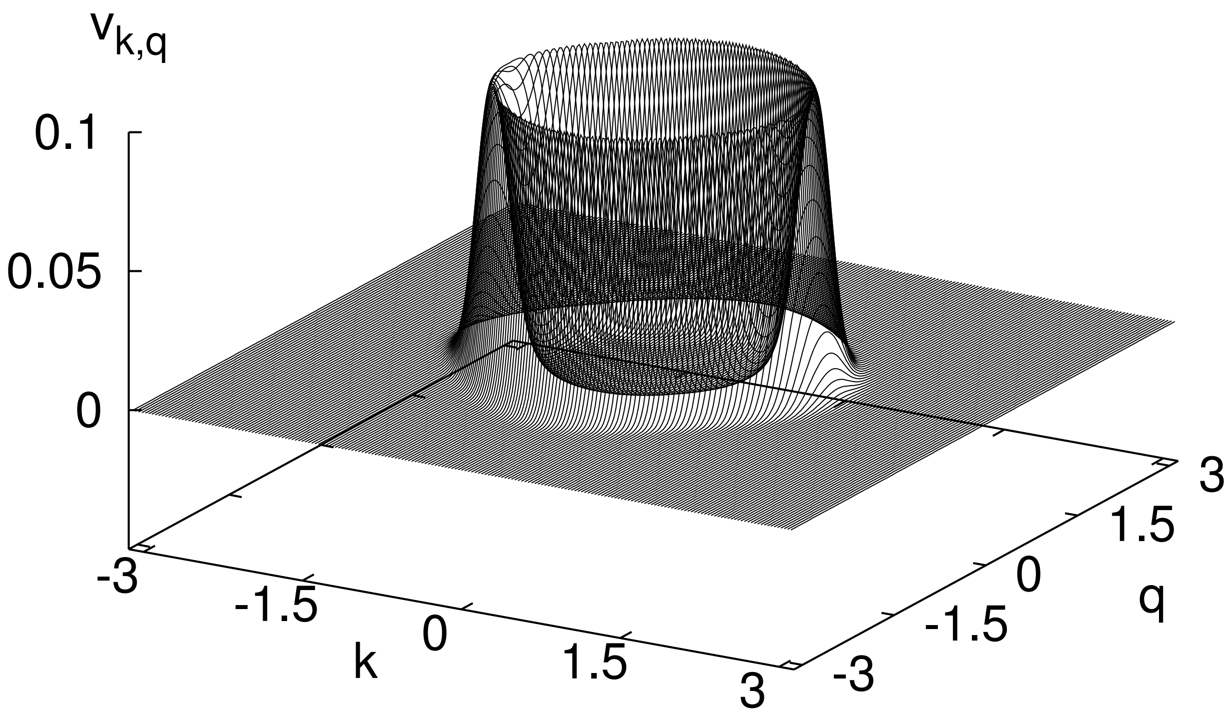
Hamiltonian at $l = \infty$

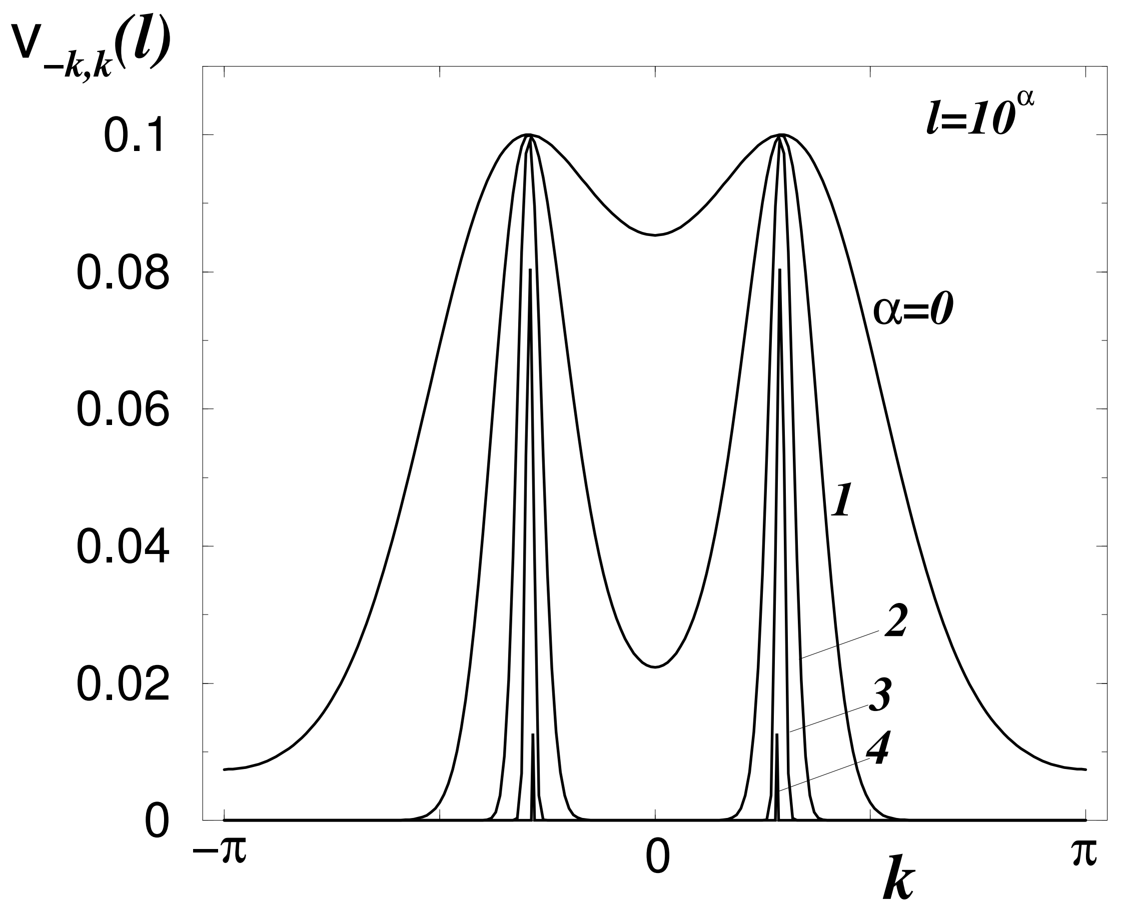
$$\hat{H}_F(\infty) + \hat{H}_B(\infty)$$

The boson-fermion coupling $v_{\mathbf{k},\mathbf{q}}(l)$ during the flow.



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

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



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

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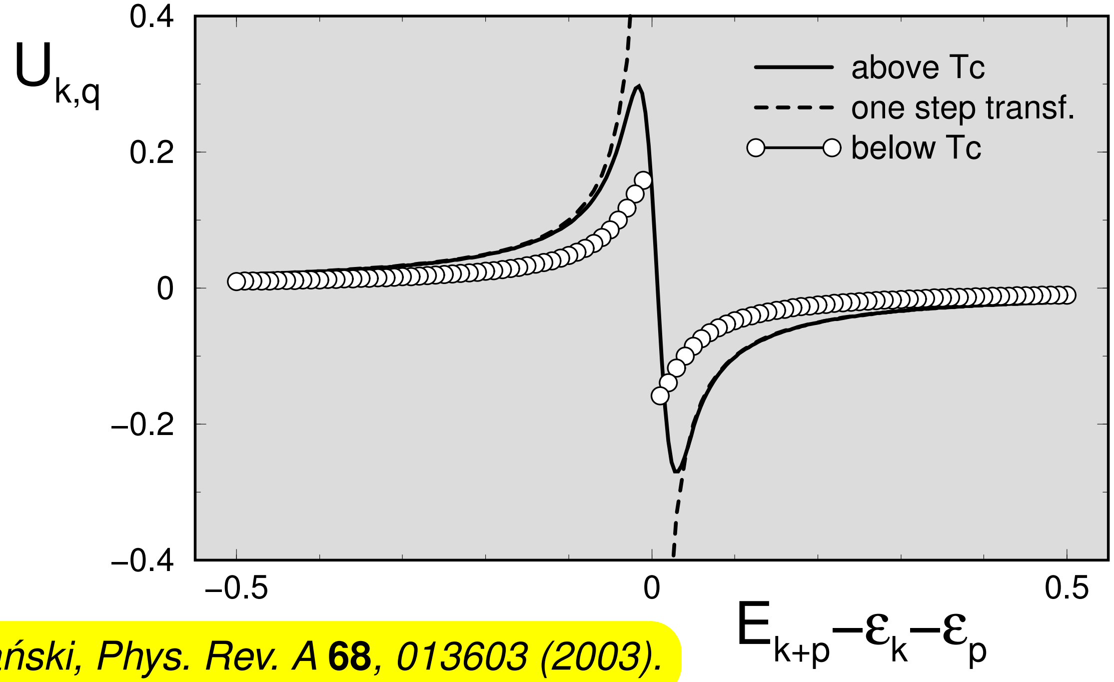
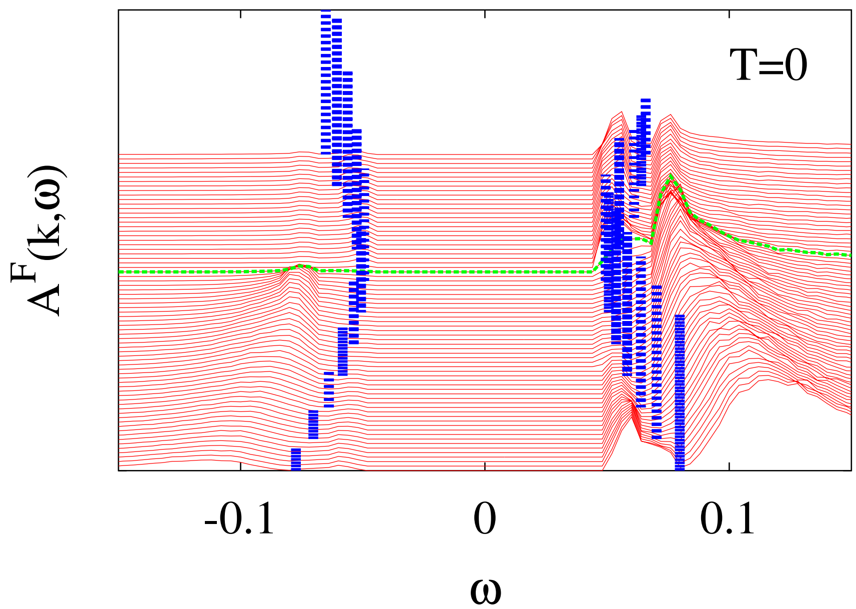


T. Domański, Phys. Rev. A **68**, *013603 (2003).*

c) The single particle spectrum

Bogoliubov-like spectrum

$T < T_c$

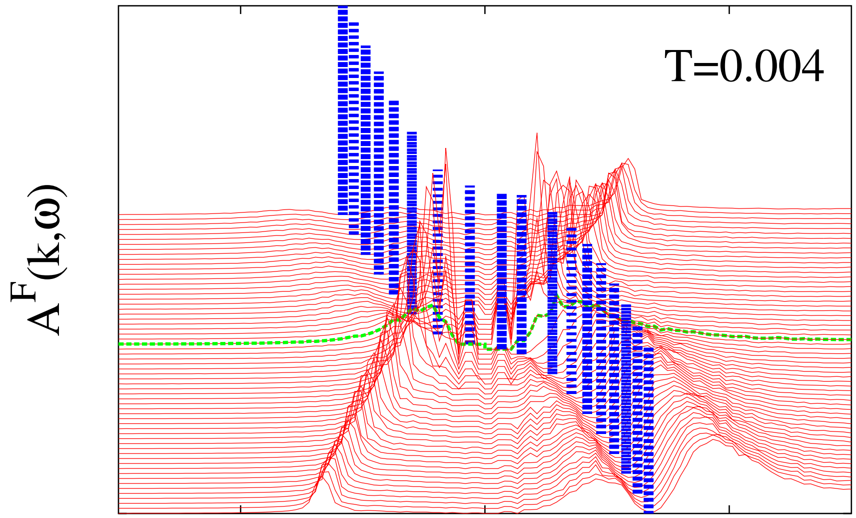


Below the critical temperature T_c there exist two branches of the excitations at energies $\omega = \pm\sqrt{(\varepsilon_{\mathbf{k}} - \mu)^2 + \Delta_{sc}^2}$ (like in the BCS theory).

T. Domański and J. Ranninger, Phys. Rev. Lett. **91**, *255301 (2003).*

Bogoliubov-like spectrum

$T < T^*$



*Pasing through T_c the Bogoliubov-type spectrum survives but one branch (*the shaddow*) gets damped. Physically it means that fermion pairs no longer have an infinite life-time.*

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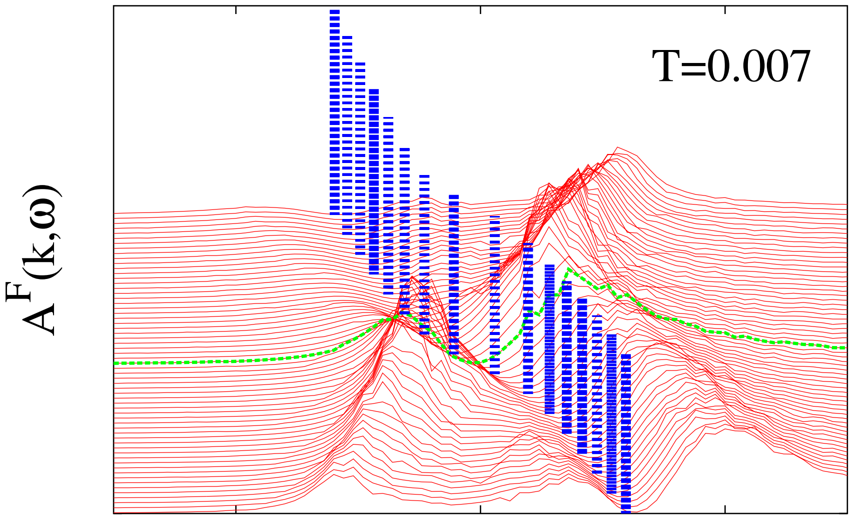

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Bogoliubov-like spectrum

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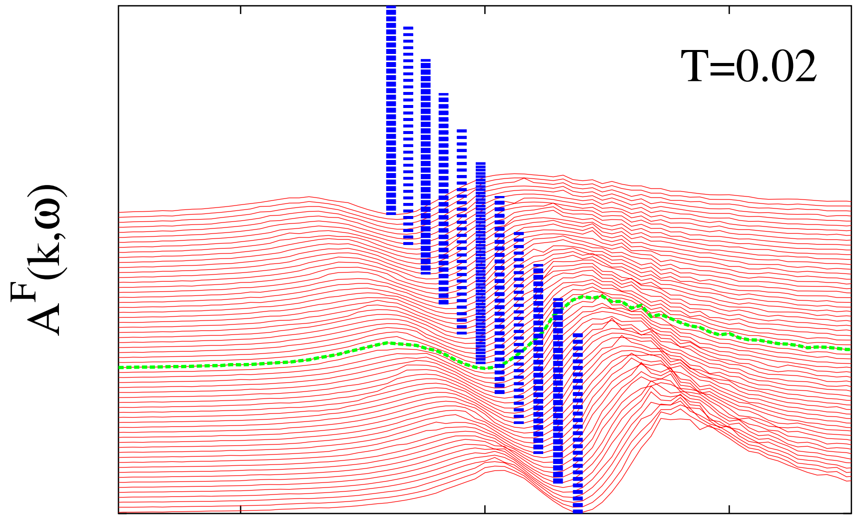

For temperatures far above T_c the Bogoliubov modes are completely gone. There remains only one well established single quasiparticle peak without a gaped dispersion.

T. Domański and J. Ranninger, Phys. Rev. Lett. **91**, *255301 (2003).*

d) Collective phenomena

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Investigating the correlation function of the fermion pairs

$$\left\langle \sum_{\mathbf{k}} c_{\mathbf{k}\downarrow}(\tau) c_{\mathbf{q}-\mathbf{k}\uparrow}(\tau) \sum_{\mathbf{k}'} c^{\dagger}_{\mathbf{q}-\mathbf{k}'\uparrow}(\tau') c^{\dagger}_{\mathbf{k}'\downarrow}(\tau') \right\rangle$$

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we found that the corresponding spectral function

$$\mathcal{N}_{\mathbf{q}} \, \delta\left(\omega - \tilde{E}_{\mathbf{q}}\right) + \mathcal{A}^{inc}_{\mathbf{k}}(\omega)$$

consists of:

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- and the incoherent background $\mathcal{A}^{inc}_{\mathbf{k}}(\omega)$.

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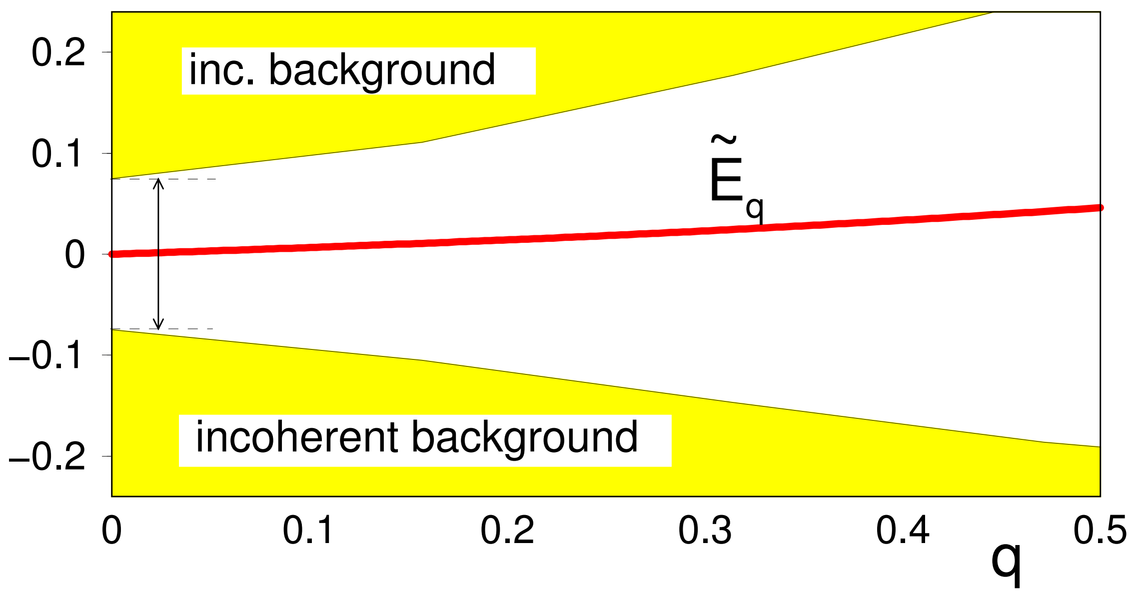
consists of:

- the quasiparticle peak at $\omega = \tilde{E}_{\mathbf{q}}$
- and the incoherent background $\mathcal{A}^{inc}_{\mathbf{k}}(\omega)$.

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

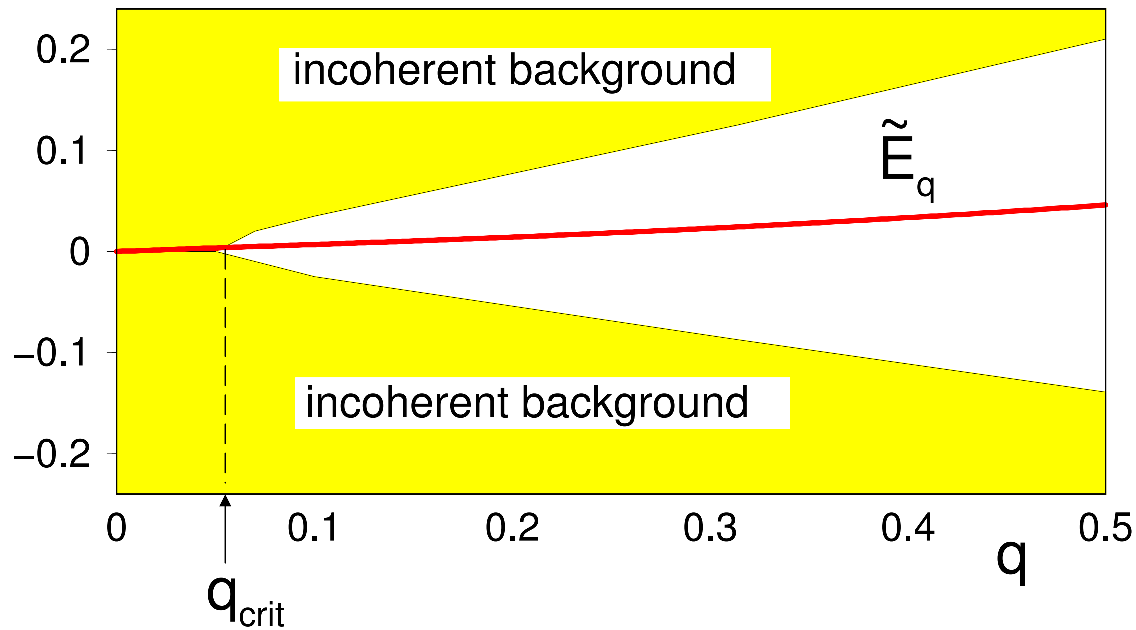
The pair spectrum for $T < T_c$



The quasiparticle peak is well separated from the incoherent background and, in the limit $\mathbf{q} \to \mathbf{0}$, has a characteristic dispersion $\tilde{E}_{\mathbf{q}} = c\,|\mathbf{q}|$. This Goldstone mode is a hallmark of the symmetry broken state.

Such a unique situation could be observed in the case of ultracold fermion atoms, otherwise the Coulomb repulsions lift this mode to the high plasmon frequency.

The pair spectrum for $T^* > T > T_c$



Above the transition temperature (for $T > T_c$):

- *the qusiparticle peak overlaps at small momenta with the incoherent background,*
- *for $\mathbf{q} \to \mathbf{0}$ the Goldstone mode disappears,*
- *remnant of the Goldstone mode is seen above $\mathbf{q}_{crit}$.*

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Quantum fluctuation phenomena are typical for all superconductors/superfluids besides the extremely large Cooper pairs.