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Concepts

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Summary: concepts, tools, and procedures to know

Concepts and Tools

- **Weakly excited systems in matter behave as if they were a set of independent damped harmonic oscillators:** the frequency ω_{ij} is related to the energy needed to excite the state and the relaxation time τ describes the state lifetime, hampered by interactions with the surroundings.
- **The average power dissipated by an external force acting on a medium provides information on the induced fluctuations, in particular on frequencies and damping of the modes in the system, or else its excitations.** The link is provided by the imaginary part of the response function, that is in turn connected to the dielectric function. This is how most measurements do work.
- **The dielectric function $\varepsilon(\omega) = E_{ex}(\omega)/E(\omega)$, essentially measures the capacity of the medium of screening the acting external field.**
- The real part of the dielectric function drives the propagation of radiation and the imaginary part determines absorption phenomena.
- Propagation and absorption behaviors are related to each other. Mathematically, through the Kramers-Kronig relations.

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- **The characteristic behaviors of materials can be probed by observing the response of the system to external disturbances:** these are conveniently chosen of the type, frequency and wavelength suited to excite a time and/or space fluctuation about the average value of that given property. The way the system responds, reveals information on interactions, statistics, and dimensionality. The temperature dependence of response coefficients is determined by the microscopic interaction driving the scattering event, as well as by statistics and dimensionality.
- When slowly-varying external disturbances act on the material, conditions of local thermodynamical equilibrium can be considered in the sample, that are set in by the high collision rate on the scale of external disturbance variations. This is the collisional or hydrodynamic regime.

Summary: concepts, tools, and procedures to know

Concepts and Tools

- **In quantum world statistics automatically introduces a correlation due to exchange. To this, a correlation originated by the interaction between the particles is to be added.**
- Exchange has negligible effects whenever the single-particle wavefunctions are not overlapped and is quite effective when the particle wavefunctions are delocalized, as in crystals and especially in metals.
- The quantity $ng(\mathbf{r},\mathbf{r}')$ can be viewed as the particle density which would be observed when sitting on the particle at position $\mathbf{r}$.
- The density profile $n_{xc}(\mathbf{r},\mathbf{r}')$ can be viewed as a hole that is dug in by exchange and correlation processes between the system particles, leading to screening of the interactions.

- **The adimensional parameter $r_s = r_0/a_b$ measuring the system density can be identified also with the system coupling strength.**
- **The excess energy due to exchange and correlations modifies both potential and kinetic energy. This is a purely quantum effect, whatever the statistics of the particles might be.**
- Inclusion of the exchange term works to keep the electrons far apart because of the Pauli exclusion principle and therefore lowers the energy. This effect is expected to become progressively negligible while the density lowers.
- In metals spatial correlation effects are relevant and are to be treated to some extent together with the spin correlations.
- Exchange and correlation effects are connected to screening. The quantity ε_0 is a measure of the number N_i of induced charges contained within the screening sphere with radius R_s. In an insulator $N_i < Z$, whereas in metal $N_i = Z$ implying $\varepsilon_0 \rightarrow \infty$ and $R_s \rightarrow \infty$.

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- **The response function measures the change of a given observable as a consequence of the action of an external perturbation coupling to the same observable or to a different one to which it is correlated. Mathematically, a response function (the imaginary part of it) is in essence the equilibrium average on the commutator at different times between the operator related to the observable and the operator related to the quantity to which the external disturbance couples. By this means, a non-equilibrium property is related to an equilibrium property.**

- The dynamical structure factor (is a correlation function and) measures the intensity of the scattered probe (particle or radiation) after this has impinged on the sample material and exchanged (lost or picked up) energy and momentum with (to or from) the excitations of the system. Ratios between the intensities of Brillouin (finite frequency) to Rayleigh (elastic, zero frequency) peaks yield information on thermodynamic derivatives such as specific heats. Widths of the peak yield information on transport coefficients (see Appendix below).
- The imaginary part of the response function measures the dissipated power of the probe into the sample
- The response function is characterized by space and time symmetries are built in the system.
- Structure factor and imaginary part of the response function at finite temperature are related to each other: the dissipated power of the probe on the sample provides information on the (spontaneous) fluctuations of the excited observable and thus on the system structure.
- Sum rules are exact expressions composed from n-th frequency moments of the imaginary response function - thus of commutators with the Hamiltonian - which help setting benchmarks to approximated response functions.
- Variables which are associated with the densities of conserved quantities (particle or spin density and related currents, energy,…) are almost time independent when the conserved quantities vary slowly in space: the time Fourier transforms of their spatial integrals - i.e. the k=0 part of the spatial Fourier transform - are proportional to a delta-function in frequency.
- Under these conditions, their behavior is governed by hydrodynamic laws. Thus, the equations of hydrodynamics and the associated thermodynamic and transport behavior described by transport coefficients, can be deduced from theoretical calculation or experimental measurement of the long-wavelength, low-frequency correlations functions (performing the limits in appropriate order).

- The poles of the frequency and momentum-dependent response function represent the frequencies and damping constants of the normal modes (excitations) of the system (e.g. sound velocity and its attenuation). Modes are of two types: propagating modes (e.g. a density fluctuation propagates as an ordinary sound waves) and diffusive modes (e.g. an entropy fluctuation spreads out diffusively by a random walk process)
- The residues represent the effectiveness of external disturbances in setting up these modes. In particular,

  a) in the k-limit in which the frequency goes to zero first and then k goes to zero, the response function yields the static susceptibilities which are thermodynamic derivatives of the conserved quantities with respect to their conjugated variables (e.g. magnetization with respect to magnetic field)

  b) in the omega-limit in which the wave number goes to zero first and then frequency does, the expression for the response function reduces to a constitutive equation relating the current of a conserved quantities (e.g. pressure that is the current of the momentum) to the gradient of the conjugate variable (e.g. fluid velocity or vector potential)

  c) the real part of the coefficient relating these two latter quantities is the corresponding transport coefficients: thus transport coefficients can be obtained both from the poles (e.g. as diffusion coefficients) and from the residues of the response function (e.g. as viscosities). These is the content of Kubo relations

- If the number of conservation laws is - say - N, the number of thermodynamics correlation functions is N^2, and N^2 is the number of thermodynamic second derivatives - like compressibility and other susceptibilities like spin susceptibility - and N^2 transport coefficients. The number of independent terms is smaller whenever symmetry properties exist.
- Microscopic hydrodynamic (Navier-Stokes for normal fluids) equations can thus be obtained by combining together the following exact relations and comparing them with the low frequency and wave number expressions of the response functions:

- conservation laws relating the time derivative of the quantity (for normal fluid: particle density, current density, energy) to the divergence of the corresponding current (for normal fluid: particle-current density, generalized pressure, or stress tensor, and energy-current density)
- galilean transformation, zero-force and zero-torque laws

- **constitutive relations, that are expansions of the current densities to first order in gradients of the local conjugated generalized forces (velocity field representing the analogue of a vector potential which might trigger transverse currents, temperature and pressure). In essence, the constitutive equations relate the current of a conserved quantity (those just listed above) to their:**

  a) non-dissipative part (density times velocity field for the particle density, pressure for the stress tensor, velocity field times energy density plus pressure for the energy current) because of galilean transformation, and

  b) dissipative part driven by the gradient/divergence of the conjugate variable dictated by zero-force (momentum conservation) and zero-torque (angular momentum conservation) laws, via fluid viscosities (velocity field for the stress tensor via the bulk and shear viscosities, temperature for the energy current via the heat conductivity). So for example, an energy current can be produced by a nonzero average velocity field carrying energy and/or pressure, but also by a temperature gradient (even if the average velocity is zero). Note that particle-density current is driven only by non-dissipative terms (thus, no pressure and no temperature gradients via related viscosities), nor the energy-density current involves pressure gradient-driven terms, because of zero-force theorem
- **thermodynamic relations, connecting the gradient of local generalized forces (like pressure or temperature in normal fluids) to the remaining variables (like local particle and energy density), via thermodynamic derivatives connected to frequencies of excitations (e.g. speed of sound) and their damping**

Procedures

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- **Given H with external perturbation acting on a selected observable, express the space and time/momentum and frequency fluctuation of the observable out of equilibrium in terms of the real-time response function. In particular:**
- **- Single out the real and imaginary time parts of the response**
- **- Identify the imaginary part with dissipation**
- **- Relate the following quantities: response function-dynamical structure factor-pair correlation function**
- **Relate imaginary part of response function and dynamical structure factor at finite temperature (fluctuation-dissipation theorem)**
- **Relate system properties to the response function: screened potential, correlation energy, pressure and compressibility [Ch. 5.6 Mahan and/or Ch. 2 Kadanoff+Baym]**
- **Calculate sum rules**
- **Calculate the response function in Random Phase Approximation by equation of motion method and corresponding dielectric function [Ch. 5.5.B Mahan]**
- **Write hydrodynamic equations by combining conservation laws, constitutive relations, thermodynamic relations, galilean transformations, zero-force and zero-torque theorems [Ch. 4 Forster and/or P.C. Martin]**
- **Link phenomenological viscosities, transport coefficients, diffusion constants, frequencies and damping of excitation modes, and thermodynamic derivatives with k- and frequency-limiting behaviors of response functions (via Kubo relations and thermodynamic sum rules)**

Proposed exercises

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- **Properties of response functions and connections with pair correlation function and structure factor**

1. **Problems 9 and 10 page 494 Ch. 5 of Mahan II edition**
2. **Problems 3 to 8 pages 127-128 Ch. 6 of Kittel II rev. edition [solutions in Appendix]**

- **Calculate RPA response and/or dielectric functions and its extensions**

1. **Study the paper**
   Journal of Physics: Condensed Matter Volume 6 Number 42
   S Conti *et al* 1994 *J. Phys.: Condens. Matter* 6 8795 doi:10.1088/0953-8984/6/42/011
   Dielectric response of the degenerate plasma of charged bosons in static-local-field approximations
   S Conti, M L Chiofalo and M P Tosi
   From <http://iopscience.iop.org/0953-8984/6/42/011>
2. **Examples in Ch. 5.1-5.4 of Iadonisi, Cantele, Chiofalo and Problems with solutions 5.1-5.5 therein**
3. **Use the RPA for a fermion system at very low temperature to determine zero and first sound collective excitations [e.g. Ch. 7.4 of Kadanoff and Baym]**

- **Sum rules**

1. **Study the paper**
   Journal of Physics: Condensed Matter Volume 8 Number 12
   M L Chiofalo *et al* 1996 *J. Phys.: Condens. Matter* 8 1921 doi:10.1088/0953-8984/8/12/007
   Sum rules for density and particle excitations in a superfluid of charged bosons
   M L Chiofalo, S Conti and M P Tosi
   From <http://iopscience.iop.org/0953-8984/8/12/007>
2. **Problems 16. and 17. page 495 Ch. 5 of Mahan II edition**

- **Connection with microscopic hydrodynamics**

1. **Study the example of spin diffusion in either Ch. 2 of Forster or (preferable) Sec. C of P.C. Martin**

Appendix

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that is, the attenuation of ultrasonic shear waves. This exhibits the predicted non-hydrodynamic behavior, which is plotted schematically in Fig. 16.

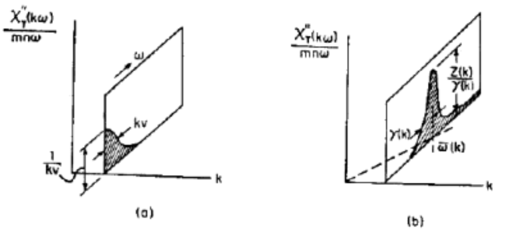

Fig. 16. Behavior of $\chi_T''(k\omega)$ in the non-hydrodynamic regime for the same systems shown in Fig. 15. (a) For the weakly interacting gas the behavior is like that of a free gas: Gaussian, with a width proportional to the thermal velocity v and the wavenumber k. In terms of a mean free time τ the hydrodynamic width $Dk^2 \sim v(v\tau k)\,k$ overestimates the result in the non-hydrodynamic ($kv\tau \gg 1$) regime. A parametric Lorentzian fit to $\chi_T''(k\omega)$ of the form discussed in the text therefore requires $\tau^{-1}(k) \approx \tau^{-1}(0) + kv$. (b) For the isotropic solid, phonons persist in the non-hydrodynamic regime but their damping is also smaller than hydrodynamics predicts; the strength of the phonon peak may be substantially reduced by anharmonic effects with "many-phonon" contributions giving the remainder of the sum rule.

D. Correlations of Conserved Quantities, Particularly the Density

The examples we quoted in the previous section are discussed in a paper by Kadanoff and myself[26]. Also discussed in that paper are the corresponding formulas for the remaining hydrodynamic parameters – the energy and density. Of these correlation functions, the one that is most easily accessible to measurement is the density correlation function. In these lectures we will not have time to go through the hydrodynamic analysis which leads to predictions for the density correlation function like those obtained for χ_T and χ_{MM} in Section C. Instead we shall content ourselves with quoting the results for χ_{nn} and commenting on their experimental significance.

Before doing so, however, let us merely state the generalization its derivation entails. The chief new feature is the necessity for treating simultaneously the conservation laws for all densities whose currents depend phenomenologically on common density gradients, and which therefore lead to coupled linearized hydrodynamic equations. Because of this coupling, the correlation functions of a particular density, like those for a particular coupled oscillator in Section A, exhibit several normal modes with varying strength.

In the thermodynamic discussion of a fluid we would encounter difficulties if we tried to describe a two component system using only the laws

of mass and energy conservation and the associated thermodynamic description, or if we tried to describe a one component fluid as we describe a photon gas, using only the law of energy conservation and not specifying the mass density. Likewise, in a ferromagnet, it would be inadequate to employ an ensemble in which the magnetization direction is unspecified. For each system an ensemble must be employed which stipulates all conserved quantities. Only when they are all taken into account, and experimentally controlled, will measurements give well defined results with small fluctuations and correlations have finite range. Correlations in a ferromagnet extend over large distances; it is only when the direction of magnetization is stipulated that the remaining correlations have finite range, and experimental results microscopic significance.

When the ensemble is described by a certain number of conservation laws, say n, the number of thermodynamic correlation functions is of order n^2. Correspondingly, there are about n^2 thermodynamic second derivatives (like compressibilities and susceptibilities) and a similar number of irreversible or Onsager coefficients. The number of independent terms is actually somewhat smaller because of a number of symmetry properties[27]. A general discussion of thermodynamics, both reversible and irreversible must take account of these thermodynamic cross derivatives and terms like thermal diffusion coefficients which relate currents of one conserved quantity to derivatives of another. It must also be concerned with the effect on the frequency and damping of the n "hydrodynamic normal modes" like sound propagation in which oscillations of the various conserved quantities participate. For example, it is the coupling of density and energy fluctuations which leads to the replacement of the Newton sound velocity $c^2 = (dp/dmn)_T$ by the Laplace sound velocity $c^2 = (dp/dmn)_s$. Likewise, it is this coupling which leads to a temperature diffusivity $D = \varkappa/mnc_p$ in place of $\varkappa/mnc_v$, and to an attenuation of longitudinal sound by thermal conduction, as well as by longitudinal viscosity. Specifically, the frequencies of the two coupled longitudinal normal modes in a fluid are given approximately by

$$\omega^2 - c_i^2k^2 + iD_ik^2\omega = 0 \tag{1}$$

where, in terms of the bulk viscosity ζ, the shear viscosity η, the thermal conductivity $\varkappa$, the specific heats at constant pressure c_p, and volume, c_v, we have

$$mc_1^2 = \left(\frac{dp}{dn}\right)_s; \qquad D_1 = \frac{\zeta + (4\eta/3)}{mn} + \frac{\varkappa}{mn}\left(\frac{1}{c_v} - \frac{1}{c_p}\right), \tag{2}$$

and

$$c_2^2 = 0; \qquad D_2 = \frac{\varkappa}{mnc_p}. \tag{3}$$

The quantity s is the entropy per unit mass.

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[In superfluids, apart from dissipative terms the corresponding equations[28] are

$$m(c_1^2 + c_2^2) = \frac{mTn_s}{n_n}\frac{s^2}{c_v} + \left(\frac{dp}{dn}\right)_s$$

$$mc_1^2c_2^2 = \frac{Tn_s}{n_n}\frac{s^2}{c_v}\left(\frac{dp}{dn}\right)_T$$

where n_s is the superfluid density and $n_s + n_n = n$.]

The comparison of hydrodynamics and correlation functions to which we alluded above then gives

$$\chi''_{nn}(k\omega) = n\left(\frac{\partial n}{\partial p}\right)_T\left[\frac{D_2k^2\omega[1-(c_v/c_p)]}{\omega^2+(D_2k^2)^2} + \frac{D_1k^4\omega c_1^2(c_v/c_p)}{(\omega^2-c_1^2k^2)^2+(D_1k^2\omega)^2}\right]$$
$$- n\left(\frac{\partial n}{\partial p}\right)_T\frac{D_2k^2\omega(\omega^2-c_1^2k^2)[1-(c_v/c_p)]}{(\omega^2-c_1^2k^2)^2+(D_1k^2\omega)^2}, \qquad (4)$$

$$\chi''_{n\varepsilon}(k\omega) = T\left(\frac{\partial n}{\partial T}\right)_p\left[\frac{D_2k^2\omega}{\omega^2+(D_2k^2)^2} - \frac{D_1k^2\omega(\omega^2-c_1^2k^2)}{(\omega^2-c_1^2k^2)^2+(D_1k^2\omega)^2}\right]$$
$$+ \frac{\varepsilon+p}{n}\chi''_{nn}(k\omega), \qquad (5)$$

and

$$\chi''_{\varepsilon\varepsilon}(k\omega) = \frac{mnc_pTD_2k^2\omega}{\omega^2+(D_2k^2)^2} + 2\frac{\varepsilon+p}{n}\chi''_{n\varepsilon}(k\omega) + \left(\frac{\varepsilon+p}{n}\right)^2\chi''_{nn}(k\omega) \qquad (6)$$

where ε is the energy density.

In the low wave number-low frequency limit, the correlation function composed of the transverse component of the momentum exhibits a diffusion structure with diffusivity, $D_T = \eta/mn$, given by the viscosity divided by the mass density. The correlation functions above also have a diffusion structure but here the diffusivity is the thermal diffusivity, $D_2 = \varkappa/mnc_p$. They also exhibit the damped sound wave propagation. The total weight of χ''_{nn}/ω is $n(\partial n/\partial p)_T$ of which a proportion $(1 - c_v/c_p)$ comes from the diffusion process and a proportion c_v/c_p comes from the sound propagation.

Note once more that the hydrodynamic analysis is only correct in the limit as $k \to 0$. Thus, for example χ_T behaves asymptotically in ω as $i\eta k^2/\omega$ (which vanishes as $k \to 0$), while rigorously χ_T behaves like ω^{-2} for all k.

Eq. (4) is an old and famous result derived in 1934 by Landau and Placzek[29] and depicted in Fig. 17. Indeed, using equation (4) we can determine by measuring $\chi''_{nn}(k\omega)/\omega$, for small k and small ω,

$$n\left(\frac{\partial n}{\partial p}\right)_T, \frac{c_p}{c_v}, \frac{\varkappa}{mnc_p}, \frac{\zeta + (4\eta/3)}{mn}. \qquad (7)$$

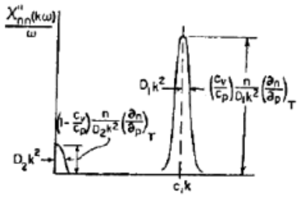

Fig. 17. The characteristic Landau-Placzek expression for $\chi''_{nn}(k\omega)/\omega$ involves a Brillouin doublet ($\omega = \pm c_1k$) and a central peak. The widths give the damping of these modes; the total intensity is given by $n(\partial n/\partial p)_T$ and is exhausted by the two peaks whose relative intensities are (c_v/c_p) and $[1 - (c_v/c_p)]$ respectively. The central peak would be replaced by a central doublet in a superfluid.

In addition since $\pi^{-1}\int d\omega\, \omega\chi''_{nn}(k\omega) = mnk^2$ we could determine mn. If we also measure $\chi''_{nn}(k\omega)/\omega$ for large k, so that we have the instantaneous correlation function

$$\tilde{S}_{nn}(k, t = 0) = \int \frac{2\hbar\omega}{1 - e^{-\beta\hbar\omega}}\frac{\chi''_{nn}(k\omega)}{\omega}\frac{d\omega}{\pi} \qquad (8)$$

we can also determine in a classical system with a known interaction potential, the energy and pressure, and therefore the specific heat. The quantity $(\partial n/\partial T)_p$ can be determined by measuring $\chi''_{n\varepsilon}$ as a function of T, and the only remaining parameter, η, can be determined, as we saw in Sec. C from $\chi''_T(k\omega)$.

To state this result more theoretically: all thermodynamic and hydrodynamic parameters of a classical fluid as well as most other measurable properties can be determined by measuring (experimentally) or calculating (theoretically) the function $\chi''_{n(\varepsilon)}(k\omega)$ or $S_{n(\varepsilon)}(k\omega)$. (In a quantum fluid, a measurement of the specific heat and pressure would also be necessary, since the kinetic energy density and kinetic pressure are not just $\frac{3}{2}nkT$ and nkT.)

The function $\chi''_{nn}(k\omega)/\omega$ is an even function. Therefore $S_{nn}(k\omega)$ is approximately even (i.e. it is even when $\hbar\omega \ll kT$). The function $\chi''_{nn}(\omega)/\omega$ therefore has two peaks at $\omega = \pm c_1k$ (a Brillouin doublet) and a central peak.

Also, since

$$\frac{c_v}{c_p} = \left[1 + \frac{T}{mn^2c_v}\left(\frac{dp}{dT}\right)_n^2\left(\frac{\partial n}{\partial p}\right)_T\right]^{-1} \qquad (9)$$

at low temperatures, the central peak is vanishingly small. Typically it behaves at $(T/T_{\text{Debye}})^4$ for small T. At $T = 0$, the doublet in χ'' at $\omega = \pm ck$ (with $(dp/dn)_T = mc^2$ and $\omega\chi''_{nn}(k\omega) = nk^2\pi|\omega|\delta(\omega^2 - c^2k^2)/m$) exhausts

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in the long wavelength limit the sum rules

$$\lim_{k\to 0}\int \frac{\chi''_{nn}(k\omega)}{\omega}\frac{d\omega}{\pi} = n\left(\frac{dn}{dp}\right)_T$$

and

$$\int \chi''_{nn}(k\omega)\omega\frac{d\omega}{\pi} = \frac{nk^2}{m}. \tag{10}$$

The opposite extreme occurs at the critical point of a fluid. Then $(\partial n/\partial p)_T = \infty$ so that the area under $\chi''_{nn}(k\omega)$ becomes infinite. The great preponderance of this area comes from the central peak, the area under the Brillouin peaks remaining relatively constant. Although the area under the central peak increases and its tail tends to swamp the Brillouin peaks its half width, which depends on $\varkappa/mnc_p$, is reduced because c_p is increased. The behavior of the correlation function in this region has been the subject of intensive study recently[30]. Likewise the behavior in critical mixtures, which also show increased scattering and slowed diffusion, has been recently investigated. (See Fig. 18.)

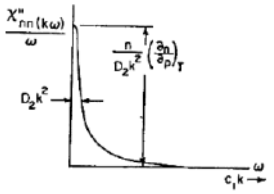

Fig. 18. The same Landau-Placzek formula when $n(\partial n/\partial p)_T \to \infty$ near a critical point and $D_2 \to 0$.

Implicit in the above discussion has been the assumption that the behavior near T_c is dominated by the zero in $(\partial p/\partial n)_T$. While this assumption is born out, $(\partial p/\partial n)_T \sim (T - T_c)^\gamma$ where $\gamma \sim 1.3$; it is not unity as it would be in simple theories. Likewise, it appears that while $\varkappa$ and c_v are not regular at T_c, they do not diverge very strongly. The experimental evidence seems to indicate that $c_v \sim (T - T_c)^{-\alpha}$ where $\alpha \sim .1$, $\varkappa \sim (T - T_c)^{-\lambda}$ where λ lies between .1 and .7 but the results are not definitive. The weak singularities may also affect the position of the Brillouin peaks near T_c, (the velocity of sound), but the attenuation, and the dominance of the central peak makes this difficult to discuss.

Like the function $\chi_T(kz)$ we discussed earlier, the function χ_{nn} and the related function $\chi_L(kz)$

$$m^2z^2\,\chi_{nn}(kz) = k^2\chi_L(kz) - nmk^2 \tag{11}$$

may be studied outside of the hydrodynamic regime, that is, for $\omega\tau \gg 1$ and $kl \gg 1$. In a rare gas, the transition occurs for relatively small k. For larger k the behavior is again free-gas like. In particular

$$\frac{\chi''_{nn}(k\omega)}{\omega} = \left[\frac{\pi}{2}\right]^{\frac{1}{2}}\frac{n\beta}{kv}\exp\left[-\frac{1}{2}\left(\frac{\omega}{kv}\right)^2\right] \tag{12}$$

For the rare gas it is possible to interpolate between these limits using the Boltzmann equation with different force laws, and various other approximations. In Figs. 19–21, are plotted theoretical curves showing how the transition takes place.[32] Also plotted for comparison are some experimental studies in the Brillouin region and the transition region.[33]

In an isotropic solid one can also study $\chi''_L(k\omega)/\omega$ in the nonhydrodynamic regime, and, at sufficiently high frequencies, one finds behavior of the same form indicated for $\chi''_T(k\omega)/\omega$. Actually the situation is considerably more complicated; there are various regimes[34] depending on the curvature of $c^2_\infty(k)$ with k^2 as well as on the parameters $\omega\tau$ and $\hbar\omega/kT$.

There is also a particularly interesting domain in the isotropic solid when the temperature is low so that the phonon picture is approximately valid and the non-momentum conserving umklapp processes unimportant. Under these circumstances, a kind of hydrodynamic picture is applicable for $\omega\tau_u >> 1$, in which the energy current (which is essentially, the momentum density times c^2) is conserved. One then has, when $\omega\tau << 1$, essentially a gas of phonons in the hydrodynamic limit.[35] For this gas of phonons the pressure is $\frac{1}{3}$ the energy density so that we may write

$$\frac{\partial\varepsilon}{\partial t} = -\nabla\cdot\mathbf{j}^\varepsilon = -\nabla\cdot c^2\,\mathbf{g} = -\nabla^2\frac{c^2}{3}\varepsilon. \tag{13}$$

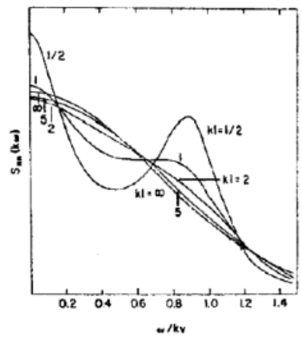

Fig. 19. $S_{nn}(k\omega)$ for various values of wave number k times mean free path, l.

Concepts

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Summary: concepts, tools, and procedures to know

Concepts and Tools

- **In quantum world statistics automatically introduces a correlation due to exchange. To this, a correlation originated by the interaction between the particles is to be added.**
- Exchange has negligible effects whenever the single-particle wavefunctions are not overlapped and is quite effective when the particle wavefunctions are delocalized, as in crystals and especially in metals.
- The quantity $ng(\mathbf{r},\mathbf{r}')$ can be viewed as the particle density which would be observed when sitting on the particle at position $\mathbf{r}$.
- The density profile $n_{xc}(\mathbf{r},\mathbf{r}')$ can be viewed as a hole that is dug in by exchange and correlation processes between the system particles, leading to screening of the interactions.

- **The adimensional parameter $r_s = r_0/a_b$ measuring the system density can be identified also with the system coupling strength.**
- **The excess energy due to exchange and correlations modifies both potential and kinetic energy. This is a purely quantum effect, whatever the statistics of the particles might be.**
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- In metals spatial correlation effects are relevant and are to be treated to some extent together with the spin correlations.
- Exchange and correlation effects are connected to screening. The quantity ε_0 is a measure of the number N_i of induced charges contained within the screening sphere with radius R_s. In an insulator $N_i < Z$, whereas in metal $N_i = Z$ implying $\varepsilon_0 \to \infty$ and $R_s \to \infty$.

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- **On quite general grounds, Hoehnberg and Kohn theorem states that a one-to-one correspondence exists between the density $n(\mathbf{r})$ of an interacting system and the external potential $V_e(\mathbf{r})$ acting on it.**
- According to the Kohn and Sham scheme, the interacting system can be mapped onto an equivalent and effective non-interacting one, characterized by an effective single-particle potential.
- DFT and response or dielectric function theories are strictly connected: DFT effective and xc potentials calculated at the local density are related to the response function of the real system and to a Kohn and Sham response function built up from fictitious single-particle orbitals.
- $V_{xc}(\mathbf{r})$ is a good approximation for the xc energies and the DFT results are in general more accurate and realistic than those obtained within Hartree-Fock calculations.
- **A unified theoretical framework exists to treat the dynamics of a weakly inhomogenous normal and super-fluids, that is derived from a formulation of DFT in terms of currents and with the use of general considerations such as Galileian invariance, conservation laws and time-reversal symmetries. Explicit calculation of the microscopic current response in the homogeneous system leads to equations of motion for the currents that are formally equivalent to Navier-Stokes equations for a normal fluid and to Landau two-fluids equations for superfluids.**

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Procedures

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- **Write Local Density Approximation for the nonlocal Hartree-Fock exchange potential [Iadonisi, Cantele, Chiofalo p. 620]**
- **Write closed set of Kohn-Sham equations, given H**
- **Write the analogue of Kohn-Sham equations in the case of current-density functional theory**
- **Write Navier-Stokes equations from current-density functional theory [Vignale, Ullrich, Conti, PRL 79, 4878 (1997) see** http://arxiv.org/pdf/cond-mat/9706306.pdf**]**

Proposed exercises

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- **Quick Questions, Examples, and Problems 6.2-6.5 and 6.8-6.11 with solutions in Ch. 6 of Iadonisi, Cantele, Chiofalo [ICC]**
- **Study the papers on applications of either DFT or TDDFT to different systems:**

1. **Ullrich and Vignale, Time-dependent current density functional theory for the linear response of weakly disordered systems**
   From <http://arxiv.org/pdf/cond-mat/0201483.pdf>
2. **Dowload Baym and Pethick, Ground-state properties of magnetically trapped BEC Rubidium gas, http://arxiv.org/pdf/cond-mat/9508040.pdf. Use eq. (4) or (12) therein as approximations for the equilibrium densities of a BEC of Rubidium atoms in a harmonic trap, and calculate within LDA expressions for the energy per particle of the inhomogeneous gas and the compressibility**
3. **P. Pedri (Orsay), S. De Palo (Trieste), E. Orignac (ENS-Lyon), R. Citro (Salerno), M. L. Chiofalo (SNS Pisa)**
   Collective excitations of trapped one-dimensional dipolar quantum gases.
   Journal-ref: Phys. Rev. A 77, 015601 (2008) http://arxiv.org/pdf/0708.2789.pdf
4. **S. De Palo, E. Orignac, R. Citro, M. L. Chiofalo, The low-energy excitation spectrum of one-dimensional dipolar quantum gases. Journal-ref: Phys. Rev. B 77, 212101 (2008)**
   http://arxiv.org/pdf/0801.1200.pdf
5. **ML Chiofalo, SJJMF Kokkelmans, J. Milstein, M. Holland, Signatures of resonance superfluidity in a quantum Fermi gas, http://arxiv.org/pdf/cond-mat/0110119.pdf**

Concepts

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- **Dictionary between Green's functions and response functions. In particular:**

1. **Single- G_1 [two- G_2]particles Green function describe the propagation of a disturbance once one single [two particles in sequence (add two and remove two, add and remove two +add and remove two,…)] is [are] added or removed to or from the system at equilibrium. Similar concepts hold for higher-order GF (from now on only G_1 and G_2 are considered)**
2. **G_1 and G_2 satisfy the same boundary condition in imaginary time, which leads to the definition of advanced and retarded Green's function, to the analogue of the fluctuation-dissipation theorem, and the definition of the single-particle and two-particles spectral functions as the Fourier transforms, from time to frequency domain, of the imaginary part of the response function**
3. **In the case of free particles, the single-particle spectral function A(ω)~δ(ω) is a delta in frequency/energy and the two-particle spectral function is zero. In the interacting case, the two-particle spectral function Γ(ω) represents the microscopic expressions for the finite width of the lorentzian-shaped (no longer delta-function shaped) single-particle spectral function of a damped harmonic oscillator, as driven by dissipation (damping) processes**
4. **Information contained in the Green's functions:**
   -- The single-particle spectral function A(ω) represents the weight with which the average occupation number f(ω) of the normal mode with energy ω enters the particle-number counting
   -- A(1±f)/Af=$e^{-\beta(\omega-\mu)}$ is the detailed-balance principle
   -- From the partition function Z=tr[$e^{-\beta(H-\mu N)}$]=$e^{\beta P\Omega}$, the average energy <H>=ΩFT[(ω+p^2/2m)f(ω)A(ω)/2], the average number of particles $\beta N=\partial \ln Z/\partial\mu$ and average density n containing A(ω), the pressure P from $\mathrm{n}=\partial\,\mathrm{P}/\partial\mu|_{\beta\Omega}$ and the correlation energy from $\partial \ln Z/\partial\lambda=-\beta<V>$ can be easily calculated. In essence, once A(ω) and Γ(ω) are known

- **An imaginary-time response function can be defined , whose Fourier transform in frequency domain corresponds to the real-time response function, where the corresponding spectral function is the difference between the advanced and retarded components of the frequency-FT of the imaginary-time Green's function**
- **The single-particle Green's function satisfies a self-consistent equation of motion, whereas the G_2**
  appearing in this equation can be replaced in terms of G_1, since schematically an out-of-equilibrium Green;s function can be defined in the presence of a perturbing external potential U coupling e.g. to the density, so that the functional derivative relation ±iδG_1/δU=i[G_2-G_1G_1] holds in terms of the external potential U coupling to the density (in this case, generalizable to other situations).
- **Approximations for G_2 allow to solve for G_1, calculate the response, and from the response calculate the transport properties, as long as it has been done within the response-function theory. More efficiently, a technique to consistently derive approximations for G_1 is by iteration: in the self-consistent equation formulated only in terms of G_1 , the non-interacting G_0 is first introduced, from which a new single-particle G is calculated and updated, and so on. This technique can be visualized in terms of diagrams expanding in powers of the interparticle interaction potential V.**
- **Alternatively, the concept of self-energy Σ=$G_0^{-1}-G^{-1}$ is introduced, which contains all the information on interactions and which satisfies the usual boundary conditions as the Gs. In essence, Γ(ω)=$\Sigma^{>}(\omega)\pm\Sigma^{<}$(ω) (the plus and minus signs for Bose and Fermi particles) relates the two-particle spectral function to the advanced and retarded self-energy, in much the same way as A(ω)=$\mathrm{G}^{>}(\omega)\pm\mathrm{G}^{<}$(ω) relates the single-particle spectral function to the advanced and retarded single-particle Green's function. $\Sigma^{<}$(ω) represents the collision rate after adding a particle to the system. Finally A(ω)=Γ(ω)/[(ω-E(p)-Re Σ(ω))^2+Γ(ω)^2/4]**
- **Finally, average particle, current, and energy densities can be defined in terms of Green's**

functions with corresponding conservation laws in the slowly-varying variable limit: the conservation laws of hydrodynamics are recovered as a hierarchy of side-to-side functionally differentiated equations, stemming from the lowest-order one, that is the continuity equation.

Procedures

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- **Derive the boundary condition for Green's functions and self-energies**
- **Express the physical observables in terms of spectral functions**
- **Write the equation of motion for G_1 both in terms of G_2 and in terms of Σ**
- **Operate the iteration procedure to derive approximations for G via functional differentiation**
- **Express approximation in terms of diagrams**
- **Link imaginary- and real-time Green's functions**
- **Express conserved particle, current, and energy densities in terms of Green's function G_1**

Proposed exercises

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- **Study the following examples from Haken, Quantum Field Theory of Solids. An introduction, North Holland (1976)**

complex ε-plane. Regarded as a function of ε, function (38.18) has a pole in the complex ε- plane. This pole consists of a real part ε_k and an imaginary part composed of the reciprocal of the life-time $-\gamma$ (see figure 56). In this way we arrive at the basic interpretation: the pole (or perhaps the poles) of the

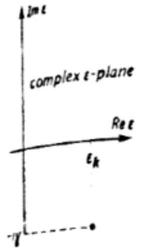

Fig. 56
The poles of the Green's function $G_k(\varepsilon)$ **in the complex** ε **(energy) plane.**

Green's function $G_k(\varepsilon)$ determines the energy and lifetime of the particle in interaction with its surroundings. As these interactions may lead to a completely new excited state, which has little to do with the original state of a particle, we refer to "quasi-particles" in this case. In fact this concept may even be taken further. For there are cases (e.g. plasmons, cf. §27), where it is not necessary to add a particle to the system to create excited states that have all the appearances of a particle moving through the system. We came across the simplest example in §8, i.e. the phonon which moves through the lattice as an excitation quantum.

Let us briefly see how to define $G_k(t)$ directly, without having to go all the way round *via* the Fourier transform of the original Green's function $G(x, t)$. Let us assume that this happens *via*

$$G_k(t) = -i\langle \Phi | T a_k(t) a_k^+(0) \Phi \rangle \tag{38.19}$$

The proof is easy if we expand $\psi^+(x, t)$, $\psi(x, t)$ as a series of plane waves, e.g.

$$\psi(x, t) = \sum_k a_k(t) \frac{1}{\sqrt{V}} e^{ikx}$$

The separate steps in this calculation are left as an exercise for the reader.

§ 39 Examples of equations for Green's functions and their solution

This section will contain two examples to show what equations for Green's functions look like and what approximations usually have to be made

in order to solve them.

The first case is that of the many-electron problem in a solid and the second that of the interaction of an electron with lattice vibrations and thus especially to the polaron.

Example 1. The equation for the Green's function for the many-electron problem. Our aim is to obtain an equation for the Green's function defined in the spatial representation by $G(x, t; x', t') = -i\langle \Phi | T\psi(x, t)\psi^+(x', t')\Phi\rangle$ (see (38.10)). The simplest method consists of applying the equation of motion for the annihilation operator $\psi(x, t)$. We have already derived the equation of motion for the annihilation operator, in §16, for the case of an example of the Hamiltonian operator of the many-electron problem (see equation (A16.15)). So as not to have too many terms, and also to take account of the translation-invariance of the problem from the start, we shall leave out the lattice potential $V(x)$ and assume this to be justified in the light of the effective mass method (cf. §18). Thus we base our argument on the following equation of motion

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = \left\{ -\frac{\hbar^2}{2m^*} \Delta \right\} \psi(x, t) + \int \psi^+(x'', t) \frac{e^2}{|x'' - x|} \psi(x'', t) \psi(x, t) d^3x'' \tag{39.1}$$

Let us multiply this equation (39.1) from the right by the operator $\psi^+(x', t')$, apply the time-ordering operator T from the left, and form the expectation value with respect to a state Φ (which we need not yet specify more closely). We then obtain

$$i\hbar \langle \Phi | T \frac{\partial \psi(x, t)}{\partial t} \psi^+(x', t') \Phi \rangle = -\frac{\hbar^2}{2m^*} \Delta_x \langle \Phi | T \psi(x, t) \psi^+(x', t') \Phi \rangle + \int \frac{e^2}{|x'' - x|} \langle \Phi | T \psi^+(x'', t) \psi(x'', t) \psi(x, t) \psi^+(x', t') \Phi \rangle d^3x'' \tag{39.2}$$

To obtain an equation for the Green's function, we must, of course, take the d/dt outside the expectation value. This actually conceals a slight difficulty which can easily cause us problems. So as not to fall into this trap, we write $G(x, t; x', t')$ in a way that expresses the T operator in terms of an

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"ordinary" c-number function. To this end we use the step function $\Theta(t-t')$, which is defined as follows

$$\Theta(t-t')=\begin{cases}1 & \text{for} \quad t>t' \\ 0 & \text{for} \quad t<t'\end{cases} \tag{39.3}$$

Then the T product may also be formulated as

$$T\psi(x,t)\psi^+(x',t')=\psi(x,t)\psi^+(x',t')\Theta(t-t')\mp \\ \mp\psi^+(x',t')\psi(x,t)\Theta(t'-t) \tag{39.4}$$

The minus sign applies to Fermi operators ψ, the plus sign to Bose operators.

As comparison with the definition of a T operator shows (see (38.6), (38.7)) (39.4) and (38.6), (38.7) do in fact agree. To obtain a rule for taking the derivative of G with respect to time, let us form the expectation value on both sides of (39.4) with respect to Φ, multiply by $-i$, and differentiate with respect to time t:

$$\frac{\partial}{\partial t}G(x,t;x',t')=-i\Big\{\langle\Phi|\frac{\partial\psi(x,t)}{\partial t}\psi^+(x',t')|\Phi\rangle\Theta(t-t')\mp \\ \mp\langle\Phi|\psi^+(x',t')\frac{\partial\psi(x,t)}{\partial t}|\Phi\rangle\Theta(t'-t)+ \\ +\langle\Phi|\psi(x,t)\psi^+(x',t')|\Phi\rangle\frac{\partial}{\partial t}\Theta(t-t')\mp \\ \mp\langle\Phi|\psi^+(x',t')\psi(x,t)|\Phi\rangle\frac{\partial}{\partial t}\Theta(t'-t)\Big\} \tag{39.5}$$

Using the T operator, the first two terms in (39.5) may be written in the form

$$-i\langle\Phi|T\frac{\partial\psi(x,t)}{\partial t}\psi^+(x',t')|\Phi\rangle \tag{39.6}$$

To transform the last two expressions in (39.5), we will use the fact, well known from mathematics, that the derivative of the step function is the δ-function:

$$\frac{\partial}{\partial t}\Theta(t-t')=\delta(t-t') \\ \frac{\partial}{\partial t}\Theta(t'-t)=-\delta(t-t') \tag{39.7}$$

After regrouping, the last two sums in (39.5) then take the following form:

$$-i\langle\Phi|\{\psi(x,t)\psi^+(x',t')\pm\psi^+(x',t')\psi(x,t)\}|\Phi\rangle\delta(t-t') \tag{39.8}$$

But the expression in the curly brackets in (39.8) is the anticommutator (Fermi) or the commutator (Bose) of ψ and ψ^+. As it is followed by the function $\delta(t-t')$, we may equate the two times t and t'. In line with the usual commutation relations (13.8) or (12.15), this reduces the expression between the curly brackets to an ordinary delta function $\delta(x-x')$. As, on account of the normalization of Φ, the remaining expectation value $\langle\Phi|\Phi\rangle$ is equal to one, (39.8) takes the simple form

$$-i\delta(x-x')\delta(t-t') \tag{39.9}$$

Combining the first two terms of (39.5), given by (39.6), and the last two terms of (39.5), given by (39.9), we finally obtain

$$\frac{\partial}{\partial t}G(x,t;x',t')=-i\langle\Phi|T\frac{\partial\psi(x,t)}{\partial t}\psi^+(x',t')|\Phi\rangle- \\ -i\delta(x-x')\delta(t-t') \tag{39.10}$$

Let us now return to the original equation (39.2). Multiplying this on both sides by $(-i)$ and inserting (39.10) into its left-hand side, we obtain the final equation

$$i\hbar\frac{\partial}{\partial t}G(x,t;x',t')=\hbar\delta(t'-t)\delta(x'-x)-\frac{\hbar^2}{2m^*}\Delta_x G(x,t;x',t')- \\ -i\int\frac{e^2}{|x''-x|}G(x'',t;x'',t-0;x,t;x',t')d^3x'' \tag{39.11}$$

Here we have used the abbreviation

$$G(x_1,t_1;x_2,t_2;x_3,t_3;x_4,t_4) \\ =\langle\Phi|T\psi^+(x_1,t_1)\psi(x_2,t_2)\psi(x_3,t_3)\psi^+(x_4,t_4)\Phi\rangle \tag{39.12}$$

As the time-ordering operator has been used in equation (39.11), but as equal values of time $t_1=t_2=t$ should really be used, $t-0$ has been taken as one of the arguments, so that the correct order of the operators ψ^+,ψ is maintained. Equation (39.11) represents rather a blow to anyone who thought that the use of Green's functions had solved the problem. We originally wanted to derive an equation for the Green's function $G(x,t;x',t')$. But we have succeeded only partially as we were forced to introduce a more complicated Green's function, i.e. (39.12). For this we have to derive a further equation, which is, of course, perfectly feasible. This new equation, however, contains a Green's function with 6 operators. The method may be continued *ad lib*, producing a whole hierarchy of equations whose solution is no simpler than that of the original problem. We must, therefore, turn to approximations. Before discussing the latter, we shall consider a case which can be solved exactly.[1]

Free particles without Coulomb interaction. In this case the last term of equation (39.11) vanishes, so that the equation takes the following form:

$$\frac{\partial G(x,t;x',t')}{\partial t} = \frac{i\hbar}{2m^*}\Delta_x G(x,t;x',t') - i\delta(t-t')\delta(x-x') \qquad (39.13)$$

As the inhomogeneity $\sim \delta(t-t')\delta(x-x')$ depends only on the difference between the co-ordinates, we put

$$G = G(x-x', t-t') \qquad (39.14)$$

To solve (39.13), let us write G as a Fourier integral:

$$G(x-x', t-t') = \frac{1}{(2\pi)^2}\iint \tilde{G}(k,\varepsilon)\, e^{ik(x-x')-i\varepsilon(t-t')} d^3k\, d\varepsilon \qquad (39.15)$$

Let us also expand $\delta(t-t')\delta(x-x')$ into a Fourier series

$$\delta(t-t')\delta(x-x') = \frac{1}{(2\pi)^4}\iint e^{ik(x-x')-i\varepsilon(t-t')} d^3k\, d\varepsilon \qquad (39.16)$$

We substitute both expressions into (39.13). Let us recall that

$$\frac{d}{dt}e^{-i\varepsilon t} = -i\varepsilon e^{-i\varepsilon t} \qquad (39.17)$$

$$\Delta_x e^{ikx} = -k^2 e^{ikx} \qquad (39.18)$$

Taking all the terms of (39.13) to the left gives

$$\frac{1}{(2\pi)^2}\iint e^{i(k(x-x')-\varepsilon(t-t'))}\left\{\tilde{G}(k,\varepsilon)\left(-i\varepsilon + \frac{i\hbar}{2m^*}k^2\right) + i\frac{1}{(2\pi)^2}\right\} d^3k\, d\varepsilon = 0 \qquad (39.19)$$

As the exponential functions are linearly independent of one another, the left-hand side of (39.19) can become zero only if the integrand is identically zero. This gives

$$\tilde{G}(k,\varepsilon) = \frac{1}{(2\pi)^2}\,\frac{1}{\varepsilon - \varepsilon_k} \qquad (39.20)$$

where we have written

$$\hbar\varepsilon_k = \frac{\hbar^2 k^2}{2m^*} \qquad (39.21)$$

[1]) Those less familiar with mathematics (especially Fourier transformation and the residue theorem) may safely skip this example and continue on p. 276.

Substituting (39.20) into (39.15) gives us

$$G(x-x'; t-t') = \frac{1}{(2\pi)^4}\iint \frac{e^{ik(x-x')-i\varepsilon(t-t')}}{\varepsilon - \varepsilon_k} d^3k\, d\varepsilon \qquad (39.22)$$

It seems sensible to evaluate this integral by means of the residue theorem. This introduces a difficulty typical of Green's functions: the integrand has a pole at $\varepsilon = \varepsilon_k$, i.e. a singularity on the integration path. To remove this difficulty, one adds an infinitesimally small imaginary quantity $\pm i\gamma$, $\gamma > 0$ to the denominator: $\dfrac{1}{\varepsilon - \varepsilon_k + i\gamma}$. For reasons which will shortly become clear, we shall choose the positive sign. Let us consider

$$\int_{-\infty}^{\infty} \frac{e^{-i\varepsilon\tau} d\varepsilon}{\varepsilon - \varepsilon_k + i\gamma} \qquad (\tau = t - t') \qquad (39.23)$$

To be able to use the residue theorem, we have to close the contour of integration at infinity, and the integrand should make zero contribution there.

1) for $\tau = t - t' > 0$ we shall close it over the lower half-plane, as then $Im\,\varepsilon < 0$, i.e. the real part of the exponent in (39.23) $Re\{-i\varepsilon\tau\} < 0$ (see figure 57). The pole at $\varepsilon = \varepsilon_k - i\gamma$ lies within the surrounding contour. The residue theorem then gives

$$\oint \frac{e^{-i\varepsilon\tau} d\varepsilon}{\varepsilon - \varepsilon_k + i\gamma} = -2\pi i e^{-i\varepsilon_k\tau - \gamma\tau} \underset{\gamma\to 0}{=} -2\pi i e^{-i\varepsilon_k\tau} \qquad (39.24)$$

2) for $\tau = t - t' < 0$ we must close the integration path over the upper half-plane. As no pole is surrounded by the contour, the residue theorem gives $\oint = 0$.

Thus we have satisfied the condition

$$G(x,t;x',t') = 0 \quad \text{for} \quad t < t' \qquad (\text{see } (38.2)) \qquad (39.25)$$

From the method of integration (choice of sign for $i\gamma$) one can see that equation (39.13) does *not* include condition (39.25), but that this must be added expressly. Using (39.24) and (39.25), we obtain

$$G(x-x'; t-t') = \begin{cases} \dfrac{-i}{(2\pi)^3}\displaystyle\int e^{ik(x-x')-i\varepsilon_k(t-t')} d^3k & t > t' \\ = 0 & t < t' \end{cases} \qquad (39.26)$$

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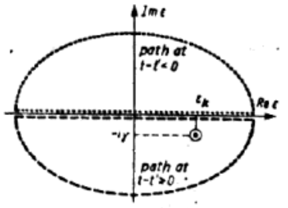

Fig. 57 Applying the residue theorem.

Let us now compare our result (39.26) with (38.1) and (38.2). This shows complete agreement (so long as we bear in mind that in §38 we used a Fourier series, and that here we used a Fourier integral: this is solely a question of the region of normalization, and it has nothing to do with the physical principles or the formalism). In spite of this agreement, our problem still contains a stumbling block (see exercise 1).

But now let us return to our general equation (39.11) with Coulomb interaction:

The Hartree approximation. To solve equation (39.11) we shall need to make some approximations typical of the theory of Green's functions and completely equivalent to the original Hartree approximation (or the slightly more general Hartree-Fock approximation). For we shall resolve the Green's function referring to 4 operators into a product of simple Green's functions of the form (Hartree approximation)

$$G(x_1, t_1; x_2, t_2; x_3, t_3; x_4, t_4) = \pm G(x_2, t_2; x_1, t_1) G(x_3, t_3; x_4, t_4) \quad (39.27)$$

or, in abbreviated form:

$$G(1, 2; 3, 4) = \pm G(2, 1) G(3, 4) \quad (39.28)$$

The upper sign applies to Fermi operators ψ^+, ψ, the lower one to Bose operators. Let us substitute approximation (39.28) into equation (39.11). Bearing in mind that

$$\begin{aligned} G(x, t-0; x, t) &= \pm i \langle \Phi | \psi^+(x, t) \psi(x, t) | \Phi \rangle \\ &= \pm i \varrho(x, t) \quad (\varrho(x, t) \text{ particle density}) \end{aligned} \quad (39.29)$$

we obtain

$$\begin{aligned} i\hbar \frac{\partial G(x, t; x', t')}{\partial t} &= \left\{ -\frac{\hbar^2}{2m^*} \Delta_x + e^2 \int d^3x'' \frac{\varrho(x'', t)}{|x - x''|} \right\} G(x, t; x, t') + \\ &+ \hbar \delta(t - t') \delta(x - x') \end{aligned} \quad (39.30)$$

The operator in the curly brackets on the right-hand side of equation (39.30) is of the form:

kinetic energy + potential energy of a charge e in the field of the charge distribution $e\varrho(x, t)$.

This can be solved by an iterative method very similar to the Hartree method: we specify $\varrho(x, t)$, then use equation (39.30) to calculate G, derive a new value of ϱ from it using equation (39.29), etc.

The Hartree-Fock method. Here we use the following approximation:

$$G(1, 2; 3, 4) = \pm G(2, 1) G(3, 4) - G(3, 1) G(2, 4) \quad (39.31)$$

We leave it to the reader to substitute approximation (39.31) into (39.11) in a manner analogous to that of the Hartree method and to discuss the resulting equation.

Example 2. Interaction of a particle with lattice vibrations. While in the last example we considered Green's function in configuration space, we shall now derive the equations of motion of the Fourier transform of the Green's function. We are thus looking for an equation for the Green's function $G_k(t)$ defined by (38.19). In principle we may proceed in a manner very similar to that used in example 1, starting with the corresponding equations of motion in the Heisenberg picture. For the case of interaction between an electron and the lattice vibrations we have already derived the equation of motion for the phonon operators in §16. Similarly we may formulate equations of motion for the electron operators. Since we shall shortly need to use all these equations, they are given here for simplicity in their explicit form:

$$\dot{a}_k = -i\varepsilon_k a_k - i \sum_w g_w^* a_{k-w} b_w - i \sum_w g_w b_w^+ a_{k+w} \quad (39.32)$$

$$\dot{b}_w = -i\omega_w b_w - i \sum_k g_w a_k^+ a_{k+w} \quad (39.33)$$

$$\dot{b}_w^+ = i\omega_w b_w^+ + i \sum_k g_w^* a_{k+w}^+ a_k \quad (39.34)$$

Equation (39.32) is the obvious starting point for the derivation of an equation for the Green's function. To this end we multiply both sides of (39.32) from the right by $a_{k'}^+(t')$ and from the left by the time-ordering operator T as well as by $-i$.

Finally we shall find the expectation value with reference to a state Φ; we hall use the vacuum state for Φ. We then obtain

$$\frac{dG_{kk'}}{dt} = -i\varepsilon_k G_{kk'} - i\delta_{kk'}\delta(t-t') - \sum_w g_w^* G_{k-w,w,k'} - \sum_w g_w G'_{w,k+w,k'}$$

where we have written (39.35)

$$G_{kk'} = -i\langle\Phi|\,Ta_k(t)a_{k'}^+(t')\,\Phi\rangle \qquad (39.36)$$

$$G_{k-w,w,k'} = \langle\Phi|\,Ta_{k-w}(t)b_w(t)a_{k'}^+(t')\,\Phi\rangle \qquad (39.37)$$

$$G'_{w,k+w,k'} = \langle\Phi|\,Tb_w^+(t)a_{k+w}(t)a_{k'}^+(t')\,\Phi\rangle \qquad (39.38)$$

The fact that function (39.36) arises is, of course, just what we should want. On the other hand, we have once again been forced to introduce new Green's functions, i.e. (39.37) and (39.38). We could now try to resolve the functions (39.37) and (39.38) into products of simpler Green's functions, e.g.

$$G_{k-w,w,k'} = \langle\Phi|\,Ta_{k-w}(t)a_{k'}^+(t')\,\Phi\rangle\langle\Phi|b_w(t)\Phi\rangle \qquad (39.39)$$

It can, however, easily be proved (see Exercise 2) that, for the vacuum state Φ_0, (39.39) vanishes identically. This would imply that the particle moves only as a free particle, as the additional terms in (39.35) describing the coupling between particle and lattice field are identically zero. The example shows clearly how easy it is to make mistakes in the use of Green's functions, and that we need a considerable "feel" for the physics of the situation when using them. There are in fact cases in the literature where the wrong approximations have been made, particularly with regard to the way factorization has been carried out. The last thing we want to do is to frighten readers, and we only wish to show that with a little care we get the right answer. To this end we shall now derive equations for the Green's functions (39.37) and (39.38). Let us differentiate (39.37); then we find that

$$\frac{d}{dt}G_{k-w,w,k'} = \langle\Phi|\,\frac{dT}{dt}a_{k-w}(t)b_w(t)a_{k'}^+(t')\,\Phi\rangle + \qquad (39.40)$$
$$+\langle\Phi|\,T\dot{a}_{k-w}(t)b_w(t)a_{k'}^+(t')\,\Phi\rangle +$$
$$+\langle\Phi|\,Ta_{k-w}(t)\dot{b}_w(t)a_{k'}^+(t')\,\Phi\rangle$$

Here the expression dT/dt has a purely symbolic meaning. It is meant to indicate that the order of t and t' has to be observed during the differentiation and that this results in an additional term. We shall derive this additional term in Exercise 3. It follows that

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$$\frac{dT}{dt}a_{k-w}(t)b_w(t)a_{k'}^+(t') = \delta(t-t')[a_{k-w}(t)b_w(t),\, a_{k'}^+(t)]_+$$
$$= \delta(t-t')b_w(t)\delta_{k',k-w} \qquad (39.41)$$

Apart from the first term in (39.40), which we have just stated explicitly in (39.41), two further terms appear in (39.40). To calculate these we shall substitute the right-hand sides of (39.32) and (39.33) for $\dot{a}$ and $\dot{b}$ respectively. This gives the following expression

$$\frac{d}{dt}G_{k-w,w,k'} = \mathrm{I} + \mathrm{II} + \mathrm{III} \qquad (39.42)$$

where the individual terms are given by

$$\mathrm{I} = \delta(t-t')\delta_{k',k-w}\langle\Phi|b_w(t)\Phi\rangle \qquad (39.43.\mathrm{I})$$

$$\mathrm{II} = \langle\Phi|\,T\{-i\varepsilon_{k-w}a_{k-w} - i\sum_{w'} g_{w'}^* a_{k-w-w'}b_{w'} \qquad (39.43.\mathrm{II})$$
$$-i\sum_{w'} g_{w'}b_{w'}^+ a_{k-w+w'}\}_t b_w(t)\cdot a_{k'}^+(t')\,\Phi\rangle$$

$$\mathrm{III} = \langle\Phi|\,Ta_{k-w}(t)\{-i\omega_w b_w - i\sum_{k''} g_w a_{k''}^+ a_{k''+w}\}_t a_{k'}^+(t')\,\Phi\rangle \qquad (39.43.\mathrm{III})$$

We will show in Exercise 2 that (39.43.I) vanishes. (39.43.II) contains 3 different expressions between the curly brackets. The first may be written in the form

$$-i\varepsilon_{k-w}G_{k-w,w,k} \qquad (39.44)$$

The second expression in the curly brackets contains a phonon annihilation operator $b_{w'}$, which later meets a second phonon annihilation operator. Thus phonon annihilation takes place twice. The annihilation process is connected each time with a coupling factor g_w. If we restrict ourselves to the lowest approximation in the term $\sim g_w^2$, this expression may be left out. The expression deriving from the last term in the curly brackets also vanishes, as the operator b_w^+ gives zero when acting on Φ_0 to the left (see exercise 2). The whole expression (39.43.II), therefore, reduces to (39.44). Lastly, let us consider expression (39.43.III) and again consider the expression in the curly brackets. Apart from the factor $-i\omega_w$, the first term again gives rise to the Green's function (39.37). Let us now look at the second term in (39.43.III) which consists of a sum over operators of the form

$$a_{k-w}(t)a_{k''}^+(t)a_{k''+w}(t)a_{k'}^+(t') \qquad (39.45)$$

Using the usual commutation relation for Fermi particles we may reverse the order of the first two operators, obtaining

$$\delta_{k'',k-w}a_{k''+w}(t)a_{k'}^{+}(t') - a_{k''}^{+}(t)a_{k-w}(t)a_{k''+w}(t)a_{k'}^{+}(t') \quad (39.46)$$

Let us remind ourselves that (39.45) and (39.46) are acting on the vacuum state, and now let us consider the effect of the second term in (39.46) on Φ_0. First of all an electron is created. Then, however, two electrons must be annihilated; as, however, only one is present, applying the corresponding operator to Φ_0 must give zero. Expression (39.45) has thus been reduced to the first part of expression (39.46) and contains only the two electron operators that appeared in the original definition of $G_{kk'}$. These somewhat involved arguments show that expression (39.43.III) reduces to

$$(39.43.\text{III}) = -i\omega_w G_{k-w,w,k'} + g_w G_{kk'} \quad (39.47)$$

Let us now summarize our result. We have derived an equation for $G_{k-w,w,k'}$ given by (39.42). Evaluation of the separate expressions I, II, III leads to the following final result

$$\frac{d}{dt} G_{k-w,w,k'} = -i(\varepsilon_{k-w} + \omega_w) G_{k-w,w,k'} + g_w G_{kk'} \quad (39.48)$$

It might seem that we still had an equally tedious task ahead of us if we wished to derive the corresponding equation of motion for (39.38). But it can be shown, in a manner analogous to that used in exercise 2, that (39.38) vanishes, at least for a state which no longer contains any phonons.

$$G'_{w,k+w,k'} \equiv 0 \quad (39.49)$$

Our task, of finding a closed system of equations for Green's functions, is complete. Using results (39.48) and (39.49), we may write these two types of equation as follows:

$$\frac{dG_{k,k'}}{dt} = -i\varepsilon_k G_{kk'} - i\delta_{kk'}\delta(t-t') - \sum_w g_w^* G_{k-w,w,k'} \quad (39.50)$$

$$\frac{d}{dt} G_{k-w,w,k'} = -i(\varepsilon_{k-w} + \omega_w) G_{k-w,w,k'} + g_w G_{kk'} \quad (39.51)$$

To solve equations (39.50), (39.51), it seems appropriate, by analogy with the method we used to solve the equation for the force-free particle (39.13), to resort to Fourier transformation. This will be discussed in more detail in Exercise 5, but we shall first show by a different and more direct method that an electron in interaction with lattice vibrations really can be described in terms of a new displaced energy and a damping constant. Let us here restrict ourselves to $t > t'$ and to $k = k'$. In this case equation (39.50)

contains the inhomogeneity $\sim \delta(t-t') = 0$, and (39.50), (39.51) represent a system of homogeneous linear equations with constant coefficients. It is well known that to solve a system of equations of this load, we substitute exponential functions for the unknown functions:

$$G_{k,k} = C_k e^{(-i\varepsilon-\gamma)t} \quad (39.52)$$

$$G_{k-w,w,k} = D_{k,w} e^{(-i\varepsilon-\gamma)t} \quad (39.53)$$

where ε, γ, C_k, $D_{k,w}$ are constants to be determined. Substituting (39.52) and (39.53) into (39.50) and (39.51) gives

$$(-i\varepsilon-\gamma)C_k = -i\varepsilon_k C_k - \sum_w g_w^* D_{k,w} \quad (39.54)$$

$$(-i\varepsilon-\gamma)D_{k,w} = -i(\varepsilon_{k-w} + \omega_w) D_{k,w} + g_w C_k \quad (39.55)$$

Equation (39.55) enables us to calculate $D_{k,w}$

$$D_{k,w} = \frac{g_w C_k}{-i\varepsilon - \gamma + i\varepsilon_{k-w} + i\omega_w} \quad (39.56)$$

Substituting this into (39.54), C_k drops out of both sides and we obtain the equation

$$\varepsilon - i\gamma = \varepsilon_k - \sum_w |g_w|^2 \frac{1}{-\varepsilon + i\gamma + \varepsilon_{k-w} + \omega_w} \quad (39.57)$$

Equation (39.57) is an eigenvalue equation for $(\varepsilon - i\gamma)$. Since $(\varepsilon - i\gamma)$ also appears in the summand, it might be difficult to determine $(\varepsilon - i\gamma)$. If we restrict ourselves to small coupling constants $|g_w|^2$, however, then it seems appropriate to solve equation (39.57) by iterative methods. To the zeroth approximation, we may omit the summed terms in (39.57) altogether and then obtain

$$\varepsilon^{(0)} = \varepsilon_k$$
$$\gamma^{(0)} = 0 \quad (39.58)$$

Our next step is to put $\varepsilon = \varepsilon_k$ in the summand. By (39.58), we might be tempted to put $\gamma = \gamma^{(0)} = 0$ but further analysis shows that this leads to contradictions. Let us, therefore, leave γ untouched for the moment, and, by virtue of (39.58), consider the limiting case $\gamma^{(0)} \to 0$:

$$\varepsilon - i\gamma = \varepsilon_k - \lim_{\gamma^{(0)}\to 0} \sum_w |g_w|^2 \frac{1}{-\varepsilon_k + \varepsilon_{k-w} + \omega_w + i\gamma^{(0)}} \quad (39.59)$$

To evaluate the sum in (39.59) further, we shall transform this into an

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integral. We know (cf. (29.27)) that the coupling constants g_w depend on the volume of the crystal V as $g_w \sim 1/\sqrt{V}$. Let us, therefore, put

$$g_w = \frac{1}{\sqrt{V}} g_w^0 \tag{39.60}$$

As the sum is taken over wave vectors, the following relation holds (cf. (30.27))

$$\frac{1}{V} \sum_w = \left(\frac{1}{2\pi}\right)^3 \int \ldots d^3 w$$

Let us evaluate the integral thus formed

$$\frac{1}{(2\pi)^3} \int |g_w^0|^2 \frac{d^3 w}{-\varepsilon_k + \varepsilon_{k-w} + \omega_w + i\gamma^{(0)}} \tag{39.61}$$

for $\gamma^{(0)} \to 0$ using the expression

$$\lim_{\gamma \to 0} \frac{1}{\xi - \xi_0 + i\gamma} = P \frac{1}{(\xi - \xi_0)} - i\pi\delta(\xi - \xi_0) \tag{39.62}$$

where P is the principal value. Substituting (39.61) and (39.62) into (39.59) and separating the real and imaginary parts, we obtain as final result:

$$\varepsilon = \varepsilon_k - \frac{1}{(2\pi)^3} P \int |g_w^0|^2 \frac{1}{-\varepsilon_k + \varepsilon_{k+w} + \omega_w} d^3 w \tag{39.63}$$

$$\gamma = -\pi \frac{1}{(2\pi)^3} \int |g_w^0|^2 \delta(-\varepsilon_k + \varepsilon_{k+w} + \omega_w) d^3 w \tag{39.64}$$

We have already met results (39.63) and (39.64) in the context of perturbation theory. We found for first order perturbation theory that an electron is scattered from the initial state k by interaction with the lattice vibrations – here, more precisely, by the emission of phonons – with a transition probability per second given by expression (39.64). Note that the present case should be considered to be a special one, no thermally excited phonons being present. We also met expression (39.63) in §35, where we calculated the self-energy of the polaron. The present example emphasizes the great advantage of using Green's functions. As we saw in the last section, we really are able to calculate the new energy values and the lifetime of the excited states in one go. Readers who would like to go a little deeper into the problem are recommended to try the following exercises.

Exercises on §39

1. Evaluate (38.10) for free particles, i.e. $\psi \equiv \psi_0$, $\psi^+ \equiv \psi_0^+$ but use the n particle state for Φ. Is $G(x_2, t_2, x_1, t_1) = 0$ still valid if $t_2 < t_1$?

2. Show that $b_w(t)\Phi_0 = 0$ (Φ_0 vacuum state for electrons and phonons).
Hint: Put $b_w(t) = e^{(i/\hbar)Ht} b_w e^{-(i/\hbar)Ht}$ and expand the exponential function on the right into a power series
Pointer: $H\Phi_0 = 0$. Why?
Likewise prove that $\langle \Phi_0 | b_w^+(t) \Phi_0 \rangle = 0$.

3. Prove (39.41).
Hint: Perform the manipulation corresponding to (39.4) and the equations following it.

4. Find the roots of equation (39.75) graphically by determining the points of intersection of the line $f(\varepsilon) = \varepsilon$ with

$$f(\varepsilon) = \varepsilon_k - \sum_w |g_w|^2 \frac{1}{-\varepsilon + \varepsilon_{k-w} + \omega_w}$$

It will be enough to take only a few terms of the sum to illustrate the point.

5. Solve equations (39.50; 51) by Fourier transformation

$$G_{k,k}(t - t') = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} C_k(\Omega) e^{-i\Omega(t-t')} d\Omega \tag{A39.1}$$

$$G_{k-w,w,k} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} D_{k,w}(\Omega) e^{-i\Omega(t-t')} d\Omega \tag{A39.2}$$

Hints: Substituting (A39.1), (A39.2) together with the Fourier representation of the $\delta(t - t')$-function into (39.50), (39.51) leads to the following equations

$$i C_k(\Omega)(\varepsilon_k - \Omega) + \sum_w g_w^* D_{k,w}(\Omega) = -\frac{i}{\sqrt{2\pi}}$$

$$i D_{k,w}(\Omega)(\varepsilon_{k-w} + \omega_w - \Omega) - g_w C_k(\Omega) = 0$$

with the solution

$$C_k = \frac{1}{\sqrt{2\pi}} \frac{1}{f(\Omega)}; \quad f(\Omega) = \Omega - \varepsilon_k + \sum_w |g_w|^2 \frac{1}{-\Omega + \varepsilon_{k-w} + \omega_w}$$

Use the residue theorem to evaluate (A39.1), (A39.2) and prove that the equation for the poles Ω_p: $f(\Omega_p) = 0$ is identical to equation (39.57).

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Concepts

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Ordering and symmetry breaking

- The dynamics of any system of particles/spins is determined by an H that is invariant under transformations in some group *G.* [Examples. For a gas, this group includes time translation and reversal, and the Euclidean group with arbitrary translations+rotations+reflections. For an Heisenberg spin model, this includes time translation and reversal, simultaneous rotations of all spins by arbitrary angle around arbitrary axis]
- At high T, entropy-dominated equilibrium phase is invariant under the same group as H and therefore all nonzero averages <O> are those referring to operators O which are left unaffected by *G.* [Example:in the paramagnetic phase <m>=0 and the magnetization correlation function $C_{mi,mj}(x,x')=3^{-1}\delta_{ij}C_{mi,mj}(|x-x'|)$ and $\lim_{|x-x'|} C_{mi,mj}(|x-x'|)\to 0$].
- Whenever an operator average <ϕ> is not invariant under transformations of the group *G*, a new order appears as described by an "order parameter", <ϕ>. That is the ordered phase breaks the symmetry of H. [Example: in ferromagnetic phase, <m> is invariant under rotations only about an axis parallel or orthogonal to the magnetization, thus with reduced symmetry with respect to the paramagnetic phase. Besides, $\lim_{|x-x'|} C_{mi,mj}(|x-x'|)\to\langle m(x)m(x')\rangle=\langle m\rangle^2\neq 0$].
- Complete description requires to know how <ϕ> transforms under *G.*
- If ordered phase breaks the symmetry of H, this implies that two or more equivalent minima of free energy occur, representing phases which coexist at equilibrium: transformations of the group are those which connect these minima.
- Once <ϕ> is determined, then the statistical-mechanics properties of the system can be calculatedas usual. The trick is to introduce $H_{ext}=-\int d^dx\, h(x)\phi(x)$ in terms of the auxiliary field h(x) coupling to ϕ(x). This trick has a:
  -- Mathematical convenience as it generates all the needed correlation functions by functional differentiation of the partition function, and
  -- Physical significance, as it restricts the statistical ensemble to that corresponding to one of the free energy minima

- Broken symmetries can be either discrete or continuous:

1. Discrete, that is referring to discrete groups with a countable number of elements. Defects might build up, which are of the type of walls and domain, accompanied by kinks and solitons. [Examples: Z_n. The case of Z_2 with the existence of 2 and only 2 equivalent ordered states with order parameter differing only by sign, describes the cases of uniaxial (anti)ferromagnetic order in Ising model, order-disorder transition with order parameter the average difference between densities in ordered and disordered phase, liquid-gas transition (even if it is first order and only average density changes, so that the order parameter is the average difference between the liquid and gas densities). Z_n describes commensurate-incommensurate transitions. See Chaikin and Lubensky]
2. Continuous, that is referring to continuous groups with an uncountable number of elements, such as rotations. At variance with the discrete case, the transition to the new ordered state is accompanied by the appearance of a low-frequency gapless hydrodynamic mode and elastic behavior. Defects which might build up are of topological type such as vortices. [Examples: O_n continuous group of rotations in n D. The case of rotations in 2D, O_2 which is equivalent to U(1) describes the cases of easy-plane (anti)ferromagnets, superfluids, smectic-C and hexatic-B order. O_3 describes the cases of Heisenberg ferromagnetic order and nematic order. O_o Heisenberg antiferromagnetic order and Self-Avoiding-Random-Walk. See Chaikin and Lubensky]

Order and symmetry breaking within a mean-field approach: in essence, the operator driving the new order is replaced by its average

- Bragg-Williams theory has been developed for the Ising transition, with analytical solution for the free energy density as a function of temperature and order parameter, i.e. magnetization
- Landau's idea: construct a free-energy functional that is
  -- invariant under the symmetry group of the disordered phase [e.g. in Ising, would be a functional of the squared magnetization since it has to be invariant under changes of sign in m]
  -- includes the energy cost for deviations from spatial uniformity by means of a term proportional the squared gradient of the non-uniform average order parameter ϕ(x) [validity: slow spatial variations on the scale of interaction range and/or lattice spacings]

-- is expanded in powers of ϕ(x), appropriate to the required symmetry, with temperature-dependent coefficients [validity: ϕ(x) must be small around the critical temperature, so even if it is simpler and preferable than Brag-Williams for second-order transitions, is critical for first-order transitions which are characterized by the discontinous setting of order parameters]

- In general, techniques for developing mean-field theories fall into three categories: variational, mode-mode decoupling, equations of motion

Critical behavior and exponents of physical quantities (all to be intended) close to T_c

- Once the partition function Z and free-energy density f are given, the relevant physical quantities can be determined, along with their behavior in the vicinity of T_c, characterized by critical exponents:

1. Equation of state $\frac{\partial f}{\partial \varphi} = h$ from which ϕ can be determined above and below T_c $\phi \approx (\mathrm{Tc}-\mathrm{T})^{\beta}$
2. Order-parameter susceptibility $\chi = \frac{\partial \varphi}{\partial \mathrm{h}}$, with $\chi \approx |\mathrm{Tc}-\mathrm{T}|^{-\gamma}$
3. Order parameter vs. auxiliary field h: $\phi \approx \mathrm{h}^{1/\delta}$
4. Specific heat $c_v = -T\frac{\partial^2 f}{\partial T^2}$ with associated exponent α (has a jump at Tc)
5. Correlation length ξ, that defines the microscopic length scale over which the fluctuation $\delta\phi(x) = \phi(x) - \langle\phi(x)\rangle$ of the order parameter at x becomes significantly uncorrelated with $\delta\phi(0)$. Since the order parameter correlation function $G(x,0) = \langle\delta\phi(x)\delta\phi(0)\rangle = k_B T\ \chi(x,0)$ and $(\chi^{-1})_{ij}(x,x') = \frac{\delta^2 f}{\delta\varphi_i\varphi_j}$, one has $\xi = (\chi(0)/\chi(q)-1)/q^2$ and $\xi \approx \xi_0 \frac{|\mathrm{T}-\mathrm{Tc}|^{-\nu}}{\mathrm{Tc}}$ and $\chi(x,0;\mathrm{T}\to\mathrm{Tc}) \approx \frac{e^{-|x|/\xi}}{|x|^{d-2}}$ indicating a divergence of the correlation length at Tc
6. Finally, $G(q) \approx D_\infty q^{-(2-\eta)}$
7. All the above can be generalized to multicomponent G_{ij}
8. Within mean field, the exponents can be exactly calculated and turn out to be α=0, $\beta = \frac{1}{2}, \gamma = 1, \delta = 3, \nu = \frac{1}{2}$, η=0

Validity and failure of mean-field description

- Several transitions can be described within a mean-field theory: normal-to-superconductor transition in metals, smectic-A-to-C in liquid crystals, first order liquid-gas, nematic-to-isotropic liquid, and liquid-solid transition. Notice the difference between second-order Ising and first-order liquid-solid/nematic-smectic/liquid gas transitions: in both cases the broken symmetry is discrete, but symmetry under time reversal is different so that Ising must not have odd powers of ϕ in the expansion of f, while the others in general do, which eventually drives the main difference between 2nd and 1st order behavior.
- Mean-field is a valid description until the fluctuations in the order parameter are negligible, that is $\langle(\delta\phi)^2\rangle \ll \langle\phi\rangle^2$, which turns into $(\frac{\xi}{\xi_0})^{d-4} = (\frac{\mathrm{T}-\mathrm{Tc}}{\mathrm{Tc}})^{(4-d)/2} > \frac{A}{\Delta\, \xi_0{}^d} \equiv t_G{}^{(4-d)/2}$ with A a dimension-dependent constant, Δ the jump in the specific heat, ξ_0 the T=0 correlation length, and $t_G \equiv \left|\frac{\mathrm{T}-\mathrm{Tc}}{\mathrm{Tc}}\right|$ the so-called Ginzburg reduced temperature. Now, for d>4 $\xi^{d-4} \to \infty$ as T→Tc and MF is always valid. For d<4, $\xi^{d-4} \to 0$ as T→Tc and MF always fails because of thermal-driven fluctuations, to which quantum correlation-driven fluctuations can add as in reduced dimensions and notably in 1D.
- Smectic A-to-C and normal metal-to-superconducting transitions resist because $t_G \approx 10^{-5}$ and 10^{-16} respectively because of large values of ξ_0

Construction of field theory beyond mean-field

- When MF theory breaks down, one need a more microscopic description of the partition function Z and of free energy functional F[ϕ(x)], which is hared when the length scale set by ξ diverges. One thus resorts to semiphenomenological field theories with the local order parameter treated as a classical continuous field within the concept of coarse graining:
  -- the system is divided into many cells with size much larger than the microscopic length scale and containing sufficiently many particles for statistical purpose
  -- ϕ(x) is averaged over the cell and becomes a classical variable
  -- Z and H are written in terms of this new field, integrating over all possible paths of it in space
  -- alternatively, discrete lattice field theories can be constructed pursuing the same goal: it is a matter of taste which to be used

Renormalization Group Theory

- The Renormalization Group Theory introduced by K. Wilson is a powerful method to calculate critical exponents for non-mean field behaving transitions: it consists of a thinning of degrees of freedom followed by a rescaling of lengths.
- Indeed, critical behavior of different physical quantities can be seen to scale in connected manners, so that not all the critical exponents are independent. Manipulating the homogeneity properties of the various correlation functions, one finds that 2ν=γ, γ=(2-η) ν, the so-called hyperscaling -that is involving the dimension d- relations β=(d-2+η)/2, γ+2=dν, α=2-dν. Eventually, collecting all together, α+2β+γ=2
- These relations are sufficiently closely verified. After calculations by RG or simulational method and/or experimental determination, it generally turns out that
  -- critical exponents depend on d, symmetry and range of interactions but not on form or intensity of interactions
  -- this fact introduces universality classes: as seen from far away, apparently different types of transitions share instead the same critical behavior
  -- for example, in 3D one typically finds α~0, $\beta\sim\frac{1}{3}$, $\gamma\sim\frac{4}{3}$, $\nu\sim\frac{2}{3}$, η~0, with detailed differences driven by symmetry and/or range of interactions
  -- the amplitude of the temperature and field dependence is different above and below the transition: the two amplitude ratios have as well universal behavior, though their variation within the same universality class is more pronounced, so that predictions are more stringent
- Scaling leads to a few essential behaviors. It turns out that, once the gap exponent Δ≡λν=β+γ is defined, along with the reduced temperature t and external field h, one has that
  -- f(t,h)=$|t|^{2-\alpha}X_0\left(\frac{h}{t^{\Delta}}\right)$
  -- ϕ(t,h)=$|t|^{\beta}X_1\left(\frac{h}{t^{\Delta}}\right)$
  -- χ(t,h)=$|t|^{-\gamma}X_2\left(\frac{h}{t^{\Delta}}\right)$
  That is, irrespective of all possible details, the most significant system observables share the same functional dependence on $\left(\frac{h}{t^{\Delta}}\right)$, though with different functions X and different critical exponents. The result can be extended to the case in which the transition is driven by different external fields and might be reached along different paths showing multicritical points. In this case, e.g. f(t,h,g,...)=$|t|^{2-\alpha}X_0\left(\frac{h}{t^{\Delta}},\frac{g}{t^{\Delta g}},\dots\right)$ and so on, with $\Delta_g\equiv\lambda_g$ ν
- The origin of scaling becomes apparent in the Kadanoff construction:
  -- the original lattice is divided into N'=$b^{-d}N$cells centered at a'=ba, with each cell centered at x containing b^d sites so that x'=x/b
  -- the original variable (say, spin) is replaced by a block variable s'(x') referring to the new lattice
  -- the new external field h'(x') thus scales as $h'_\alpha = b^{\lambda_\alpha}h_\alpha$=$b^{d-\omega_\alpha}h_\alpha$and $-2\omega_\alpha$ the exponent with which the correlations in the variable coupled to field h_α behave
  -- re-writing all the functions of the original variable in terms of the new block variable makes the scaling and universal behavior emerge
  -- in momentum representation, the renormalization procedure corresponds to (i) thinning the degrees of freedom by tracing over fields ϕ(q) within a reduced range Λ/b<q<Λ, introding a new Brillouin zone with cutoff Λ/b: removal of the largest q-vectors eliminates the faster field oscillations; (ii) rescaling lenghts via q'=bq in order to revert back to the original BZ-size Λ; (iii) rescaling fields via ϕ(q'/b)=ζϕ'(q') so that faster oscillations are somehow restored
- Notice that λ_α can positive or negative. In the former case the correspondent external field grow after successive rescalings and is said a <u>relevant</u> field, otherwise it dies and it can be considered <u>irrelevant.</u> Irrelevant field do not affect the leading singularity at the critical point, however might give nonzero corrections to them, complicating the determination of critical exponents from e.g. experimental data
- The block variable and rescaling concepts of RG are operated via decimation and renormalization procedure. In essence:
  -- block density matrix is defined with new block parameters, for which recursion relations are set in and solved by iteration until a fixed point is found, that is a value of the parameter which do not change at the next iteration
  -- critical points are described by RG recursion relations
  -- a fixed critical point can be stable (all points flow towards it, thus these points are called basin of attraction) or unstable (its basin of attraction is composed of itself alone) [In e.g. Ising, the stable fixed point describes all the finite temperature behavior, i.e. the paramagnetic phase, whereas the unstable fixed point describes just the T=0 Ising critical point]
  -- a fixed critical point can be stable along some direction and unstable along others
  -- universality comes along since all potentials and/or H in the subspace orthogonal to unstable directions have

the same exponents
-- linearization of recursion relations around unstable critical fixed points yields the same exponents as those describing the scaling of the free-energy density
-- comparison between the two provides critical exponents in terms of the parameters

Procedures

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- **Given a functional form for the free energy, calculate all relevant physical observables and their critical behavior in mean-field**
- **Reduce the number of independent critical exponents via scaling behavior**
- **Derive universal scaling behavior around multicritical points**
- **Operate decimation and renormalization procedure (in 1D, Ising example) with solution of recursion relations and determination of fixed points and critical exponents**

Proposed exercises

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- See Notes, Problems and Solutions by
  Professor Phillip M. Duxbury, Michigan State University, Course
  PHY831: Graduate Statistical Mechanics From <http://www.pa.msu.edu/~duxbury/>
  In particular:
  http://www.pa.msu.edu/~duxbury/courses/phy831/Outline.html

1. Complete Lecture Notes and Problems for Part 4 http://www.pa.msu.edu/~duxbury/courses/phy831/LectureNotesAndProblemsPart4_2012.pdf
2. Complete Solutions to Problems for Part 4 http://www.pa.msu.edu/~duxbury/courses/phy831/Solutions4_2012.pdf

- Problems 4.2 page 209, 5.1 (a) and 5.3 page 283 in Chaikin and Lubensky

- For application to the Ising discrete-symmetry breaking transition: See Notes, Problems and Solutions on these topics by Professor Phillip M. Duxbury, Michigan State University, Course PHY831: Graduate Statistical Mechanics From <http://www.pa.msu.edu/~duxbury/>
  In particular:
  http://www.pa.msu.edu/~duxbury/courses/phy831/Outline.html
  1. Complete Lecture Notes and Problems for Parts 2 and 3
  2. Complete Solutions to Problems for Parts 2 and 3

Concepts

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- Superfluid behavior occurring below a critical temperature, as in, e.g. ^{4}He with $T_c \simeq 2.2$ K, manifests in linear and rotational flows without dissipation, provided that the linear and angular flow velocities be smaller than critical values. Above these threshold values, sound waves and tiny vortex rings or rotons excitations may set in, where the fluid can be dragged along by the walls and slow down.
- The definition of superfluidity can be related to the resistance that a fluid offers to be twisted by transverse, shear external disturbances and, in second place, to longitudinal compressional perturbations. The superfluid carries no entropy, as if it were one single quantum state, as it occurs in Bose-Einstein Condensation (BEC).
- In BEC, a macroscopic occupation of the lowest energy state occurs below a critical temperature, leading to a sort of condensation of bosonic-like particles but in momentum or energy space. The system behaves as if it were one single particle with well defined momentum and energy. While temperature drops down, the De Broglie wavelength becomes infinitely large, so that the kinetic energy of the lowest state drops to zero and the particle wavefunctions hook together extending over all the volume: they have large probability to be at any point in space.
- BEC and superfluidity are related phenomena. However, the density of Bose-Einstein condensed particles is related to the macroscopic occupation of the lowest energy state, whereas the density of superfluid describes the response of the fluid to a twist, that is a transverse probe. Strong interactions introduce a finite probability that non-condensed particles be carried along with the condensate during the superfluid flow and thus affect the occupation of the lowest energy state depleting the condensate: at ideally zero temperature and in homogeneous systems, the whole system is superfluid but not necessarily all of it is Bose-condensed.

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- Superfluidity occurs also in fermionic-like systems, both neutral as in fermionic ^{3}He isotope or charged as with electrons or holes in superconductors: if a sort of pairing mechanism occurs, the fermion pairs can undergo a form of condensation in momentum space below a T_c, by occupying all one and the same ground state while the Pauli exclusion principle would prevent them to do so. Key features of superconductors are zero-resistance behavior, transparency to radiation with frequency below a critical ω_c, exponential behavior of specific heat and thus for activation of thermal excitations, and perfect diamagnetism below T_c.

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- Superconductivity or superfluidity of both bosonic and fermionic-like systems are related phenomena, they all being based on the existence of Bose-Einstein condensed state with wavefunction $\psi(\mathbf{r}) = \sqrt{n_c(\mathbf{r})}e^{i\phi(\mathbf{r})}$ in terms of a condensate density $n_c(\mathbf{r})$ and a global space-dependent phase $\phi(\mathbf{r})$. The superfluid velocity $\mathrm{v_s}$ is dictated by the space gradient of the phase. In a fermion system, the condensate wavefunction becomes the pairing wavefunction $\psi(\mathbf{r}) \to p(\mathbf{r}) \equiv <\psi_\downarrow(\mathbf{r})\psi_\uparrow(\mathbf{r})>$, and corresponding to the situation in which the Bose particle (integer spin) is represented by two paired fermions with opposite spins. Other combinations leading to integer spin are possible, and fermion-pairs wavefunctions do spatially overlap.
- The BCS theory explains superconductivity by assuming that electrons close to the Fermi level are correlated in pairs, so that an energy gap $\Delta(T)$ exists between the ground and the first excited single particle states essentially related to the binding energy of the pair. Since the pairs are highly overlapped in real space though, the gap energy does not coincide with the pair binding energy.
- The dependence of T_c on isotopic species and on vibrational energy supports the idea that the pairing mechanism in conventional superconductors is originated by lattice vibrations. Other pairing mechanisms are expected to be involved in different superconductors, such as the high-T_c ones.
- Whatever the microscopic mechanism might be for the pairing, the BCS theory has shown to be a general framework to treat superconductivity and superfluidity phenomena involving fermionic-like particles, and can be demonstrated to continuously evolve towards the theory of Bose-Einstein Condensation for point-like bosonic particles.

- **The Green's function approach to superfluidity/superconductivity requires the introduction of matrix Green's functions, which include the off-diagonal long-range ordering appropriate to the boson or fermion system under consideration. Using a matrix representation, equations become quite similar to the case of a normal system. But:**

1. **Two self-energies appears, which are related to each other by functional differentiation via the so-called Hugenoltz and Pines theorem, ensuring a gapless**

character of the excitation energies above the ground state. Approximations to the self-energies which satisfy HP theorem are said to be gapless

2. Gapless approximation do not necessarily satisfy even simple conservation laws
3. Therefore, perturbative methods and related diagrammatic techniques must be handled with much care for superfluid/conducting systems

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> • A unified theoretical framework exists to treat the dynamics of a weakly inhomogenous normal and super-fluids, that is derived from a formulation of DFT in terms of currents and with the use of general considerations such as Galileian invariance, conservation laws and time-reversal symmetries. Explicit calculation of the microscopic current response in the homogeneous system leads to equations of motion for the currents that are formally equivalent to Navier-Stokes equations for a normal fluid and to Landau two-fluids equations for superfluids.

- As compared to normal systems, the structure of these equations reflects the same conservation laws, galileian invariance, zero-force and -torque theorems. However:

1. one more generalized force appear as a result of galilean invariance and the presence of a superfluid velocity which for slowly-varying condensate phase is related to the phase gradient: this force is the interdiffusion current, besides the normal-fluid velocity which again represents a potential vector able to drive transverse currents
2. four bulk (instead than one) and one shear viscosities appear, along with the usual heat conductivity, connected to corresponding longitudinal current-current, current-superfluid velocity, superfluid velocity-superfluid velocity, and transverse current-current response functions via generalized Kubo relations
3. two densities: total density (conserved via continuity equation) and superfluid density, that is an related to an appropriate limit of transverse response function since the normal fluid density measures how much the fluid responds to a rotation or twist (a transverse probe)
4. the superfluid density is different from the condensate density: at T=0, n_s can be different from the total density n only because of boundary conditions (due to its meaning as a response to a twist), while the condensate density n_c can be largely different from n because of interactions. A relation can be derived which connects n_s, n_c and the single-particle spectral function embodying the interactions
5. besides zero sound (collisionless sound mode corresponding to shape breathing of Fermi sphere) and first (ordinary, collision driven density wave) sound, a second sound mode appears which is associated to an entropy wave, its speed vanishing with the superfluid density as n_s / n_n

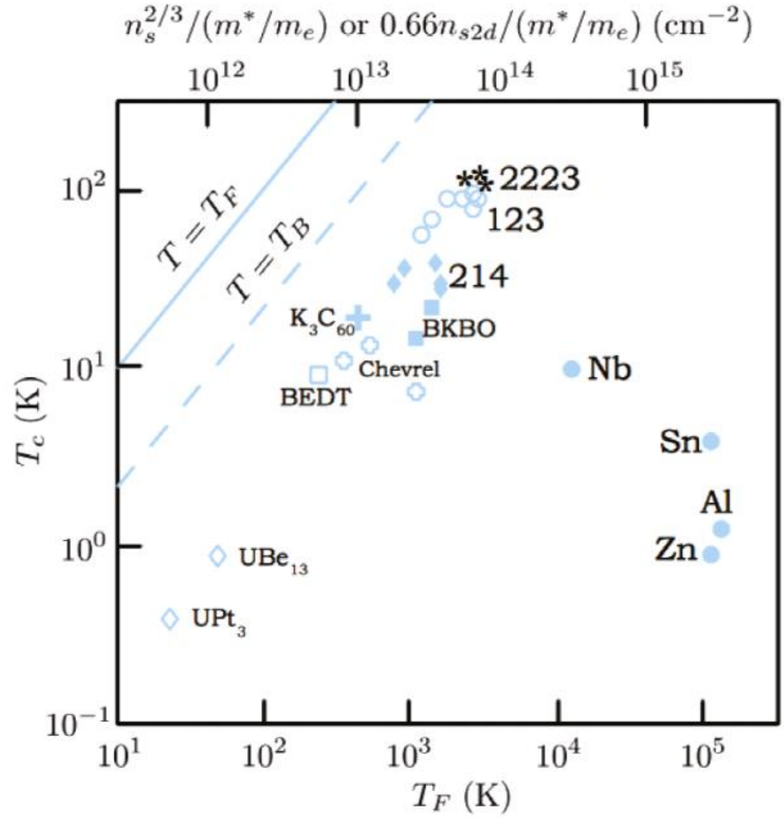

Fig. 2.45 Superconductivity and superfluidity: the universal Uemura plot. The critical temperatures T_c for a number of superconducting and superfluid materials vs. their Fermi temperature T_F (lower axis) or the temperature T_B corresponding to Bose-Einstein condensation of fermion pairs (upper axis) [34]

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Procedures

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- **Manage statistical-mechanics averages of moving systems via (linear or angular) velocity transformations**
- **Identify the superfluid order parameter for Bose and Fermi systems**
- **Express normal (or superfluid) density as a response function and identify the moment of inertia as a response function (in fact, the relation between moment of inertia and normal density)**
- **Express the relation between condensate and superfluid density, embodying the interactions via the single-particle spectral function**
- **Similarly to normal systems, write microscopic hydrodynamic two-fluid equations for the superfluid and make the connection with TD-DFT**
- **Similarly to normal systems, write equations for 1/2 and 1-body Green's functions and related self-energies**
- **Derive first-order perturbative expansions within conserving and gapless approximations**

Proposed exercises

domenica 14 giugno 2015 08:44

- **Study the papers**

1. **Wolfgang Ketterle, Ananth P. Chikkatur, and Chandra Raman, Collective enhancement and suppression in Bose-Einstein condensates. From <http://arxiv.org/pdf/cond-mat/0010375.pdf>**
2. **C. Raman, R. Onofrio, J. M. Vogels, J. R. Abo-Shaeer, and W. Ketterle, Dissipationless flow and superfluidity in gaseous Bose-Einstein condensates. From <http://arxiv.org/pdf/cond-mat/0008423.pdf>**
3. **Gordon Baym, D. H. Beck, C. J. Pethick, Low Temperature Transport Properties of Very Dilute Classical Solutions of 3He in Superfluid 4He. From <http://arxiv.org/pdf/1408.1619.pdf>**

- **Invent easy forms for the single- and two-particle spectral functions for a fictitious system and calculate the normal and superfluid density, and the shear and bulk viscosities**
- **Repeat explicitly the calculation of the approximated self-energies for both Phi-derivable and Gapless approximations in Hohenber and Martin paper [Annals of Physics 34, 291 (1965), Sec. E] and provide a diagrammatic graphical description**
- **See Notes, Problems and Solutions on these topics by Professor Phillip M. Duxbury, Michigan State University, Course PHY831: Graduate Statistical Mechanics From <http://www.pa.msu.edu/~duxbury/>
In particular:
http://www.pa.msu.edu/~duxbury/courses/phy831/Outline.html**
    1. **Complete Lecture Notes and Problems for Part 4**
    2. **Complete Solutions to Problems for Part 4**

Concepts

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- **The theory of Fermi liquids due to Landau is very powerful in higher dimensions. In essence, it allows to describe the even strongly correlated many-particle system in terms of quasi-particles, that are the single particles dressed by density fluctuation (particle-hole excitations in and out the Fermi sphere) induced by the interaction with the other particles: because of bare occupation-number arguments, these are very long-living excitations, the longer the closer to Fermi surface. Increasing temperature (i.e. by thermal effects) or interaction energy in spite of kinetic energy (i.e. by quantum effects), the momentum distribution appears to progressively dig in below the chemical potential and built up above it with a progressively reduced jump Z at the chemical potential. In other words, the spectral function A(ω), that is a lorentzian, gets preogressively sharper as k approaches the Fermi wave-vector, and the total weight of the lorentzian peak represents the fraction Z of the excitation that is in the quasiparticle state, whreas the rest 1-Z is in a continuous background with no well-defined structure: this is the most apparent manifestation of correlations, which all the other can be traced back to.**
- **The whole reasoning dramatically fails in 1D:**

1. **No individual motion in 1D is possible, thus "collectivization" of the excitations occurs**
2. **Because only collective excitations can exist, a single fermionic excitation necessarily has to split up into a collective excitation carrying charge (like a density or sound wave) and one carrying spin (like a spin wave), with in general different velocities**
3. **In higher dimensions, a divergence of the response function is a signature of a phase transition to a differently ordered state. Divergence is obtained whenever nesting of the Fermi surface occurs, that is exists a range of Q wavevectors such that $\xi(k+Q)=-\xi(k)$ so that $\xi(k)-\xi(k+Q)=2\xi(k)$ at the denominator of the response function. This is always the case in 1D at the Fermi wavevector, as linearization of $\xi(k)$ around k_F shows: $\xi(k) \sim v_F(\pm k-k_F)$ for $k\sim\pm k_F$. Moreover, if the divergence is in the particle-hole channel χ_{p-h}, this is a transition to a phase with either charge/density (Charge Density Wave) or spin ordering (Spin Density Wave, a kind of antiferromagnetic ordering). If the divergence is in the particle-particle χ_{p-p} channel, then the transition corresponds to a BCS-like pairing: in this case, the nesting is due to the pairing condition $\xi(k)=\xi(-k)$ itself or else time-reversal symmetry. In higher dimensions, either χ_{p-h} or χ_{p-p} diverge. In 1D, one is always in a nested condition**
4. **In higher dimensions, one may create a low-energy particle-hole excitation with infinitesimally small energy for q vectors wherever between 0 and $2k_F$. In 1D, the Fermi surface is a segment, and this operation is possible only at q=0 and $q=2k_F$**
5. **As a result, the average energy of a particle-hole excitation is linear in q and has a well-deined momentum. Also, the dispersion in energy is quadratic in q, going to zero faster than the average energy. Thus, in 1D particle-hole excitations are well-defined particles (not excitations dressing a particle as in Fermi liquids) with well-defined momentum and energy**

- **The essence of bosonization method is the following:**

1. **The original model of fermions with band curvature as in Fig. 2.1a is mapped into a model of fermions with the linear spectrum in Fig. 2.1b. A lower cutoff might be necessary to make the model well defined**
2. **The density fluctuations, which are a superposition of particle-hole excitations, are described by an operator which is - in fact - of bosonic nature. Due to the large number of occupied states, the density-fluctuation operators turn out to satisfy boson commutation relations (recovering an intuitive result)**
3. **Then, an effective single-particle operator is defined, one for each left and right linear branch. This can be expressed in terms of the density-fluctuation operator and turns out to be bosonic as well. Care is taken to globally conserve the number of particles. Then, new fields that are symmetric and antisymmetric combinations of left and right operators are defined**
4. **When the original Hamiltonian is re-written in terms of these bosonic operators after taking into account all possible processes allowed in 1D, it turns out to be quadratic (!) as a result of an exact construction within the limit of large number of occupied states and the low-energy behavior accessed. H is characterized by two parameters, the so-called Luttinger parameters, which can be determined after theoretical perturbative methods or - even better - simulational methods:**
   -- u representing the velocity of the excitations eventually renormalized by interaction processes with respect to its noninteracting v_F value, and
   -- K embodying the correlations with K=1 referring to the noninteracting system, K<1 to repulsive and K>1 to attractive interactions

- **As usual, thermodynamic properties, correlation properties, pairing properties and so on can be derived and expressed in terms of u and K. In particular, the discontinuity of n(k) at the Fermi wavevector disappears, and n(k) acquires a power-law singularity: a signature of Luttinger-liquid, 1D behavior. The DOS also goes to zero as a power law**
- **When spin is considered as well as charge/density, the number of fields doubles, while the charge/density and the spin channels remain separated (within this low-energy limiting behavior) and phase diagrams as complex as that in Fig. 2.9 are possible**

- **From T. Giamarchi, Quantum Physics in 1D, Clarendon**

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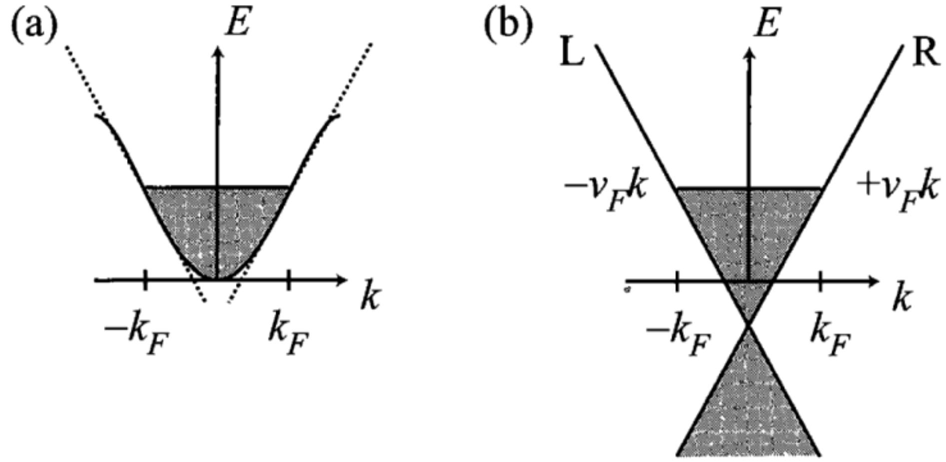

FIG. 2.1. The original model of fermions with band curvature (a) is replaced by a model of fermions with a linear spectrum (b). This forces to introduce two species of fermions (right (R) and left (L) going fermions). The spectrum is now extended to all values of k, leading to an infinite number of negative energy states. A cutoff on the momentum might be needed to make the model well-defined.

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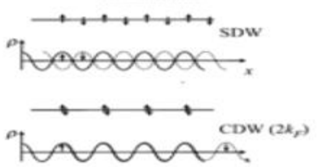
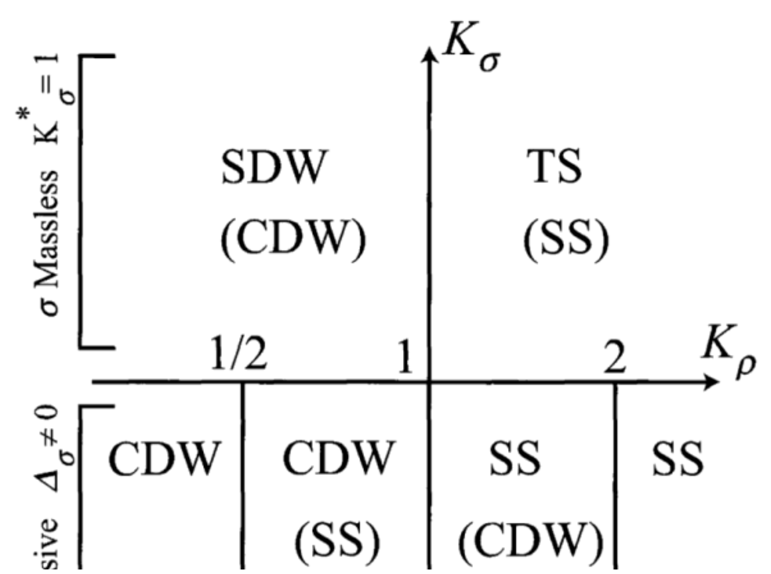


FIG. 2.7. Spin and charge density wave tendencies. In a spin density wave (antiferromagnetism) one has two waves of density for spin up and down with wavelength $2k_F$. The two waves are shifted relative to each other. The field ϕ_σ controls this dephasing (see text). The density is uniform and the spin modulation maximum. In a charge density wave, the two waves are in phase giving a density modulation and a zero spin modulation. Intuitively, one expects that repulsion between electrons favor the SDW order compared to the CDW one.

$$g_{1\perp} \int dx \cos(\sqrt{8}\phi_\sigma) \qquad (2.165)$$

The ordered value $\langle\phi_\sigma\rangle$ is thus different depending on the sign of $g_{1\perp}$



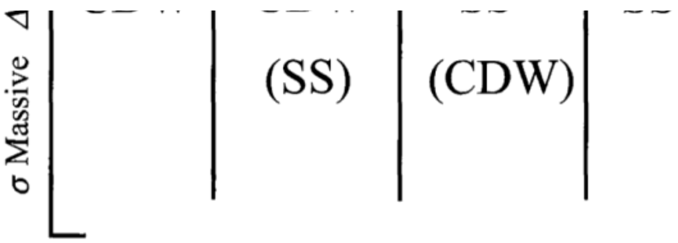


FIG. 2.9. Phase diagram of the system with spin for spin isotropic couplings. There are four sectors depending on the value of the parameters K_ρ and the sign of the backscattering term $g_{1\perp}$ (or alternatively the value of the bare parameter K_σ). The phases correspond to the most divergent susceptibility. I have indicated in parenthesis subdominant divergences. In the upper part ($K_\sigma > 1$) the spin sector is massless. In the lower part ($K_\sigma < 1$) the spin excitations are massive with a gap Δ_σ.

Procedures

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- **Express single-particle operator for left and right branch in terms of original fermionic operators**
- **Construct the conjugate Luttinger fields as symmetric and antysimmetric combinations of L and R fields**
- **Build up H in terms of conjugate Luttinger fields for different g-ologies**
- **Express relevant physical observables in terms of u and K Luttinger parameters**

Proposed exercises

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- **Study the paper**
  P. Pedri (Orsay), S. De Palo (Trieste), E. Orignac (ENS-Lyon), R. Citro (Salerno), M. L. Chiofalo (SNS Pisa),
  Collective excitations of trapped one-dimensional dipolar quantum gases. Journal-ref: Phys. Rev. A 77, 015601 (2008). From http://arxiv.org/pdf/0708.2789.pdf or

  Luttinger hydrodynamics of confined one-dimensional Bose gases with dipolar interactions

  This article has been downloaded from IOPscience. Please scroll down to see the full text article.

  2008 New J. Phys. 10 045011

  (http://iopscience.iop.org/1367-2630/10/4/045011)

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- **Choose from T. Giamarchi, Quantum Physics in 1D, Clarendon, one out of the following applications of bosonization method to physical systems, and perform the related calculations:**
  0. **Model with spin [Ch. 2.3] leading to the phase diagram**

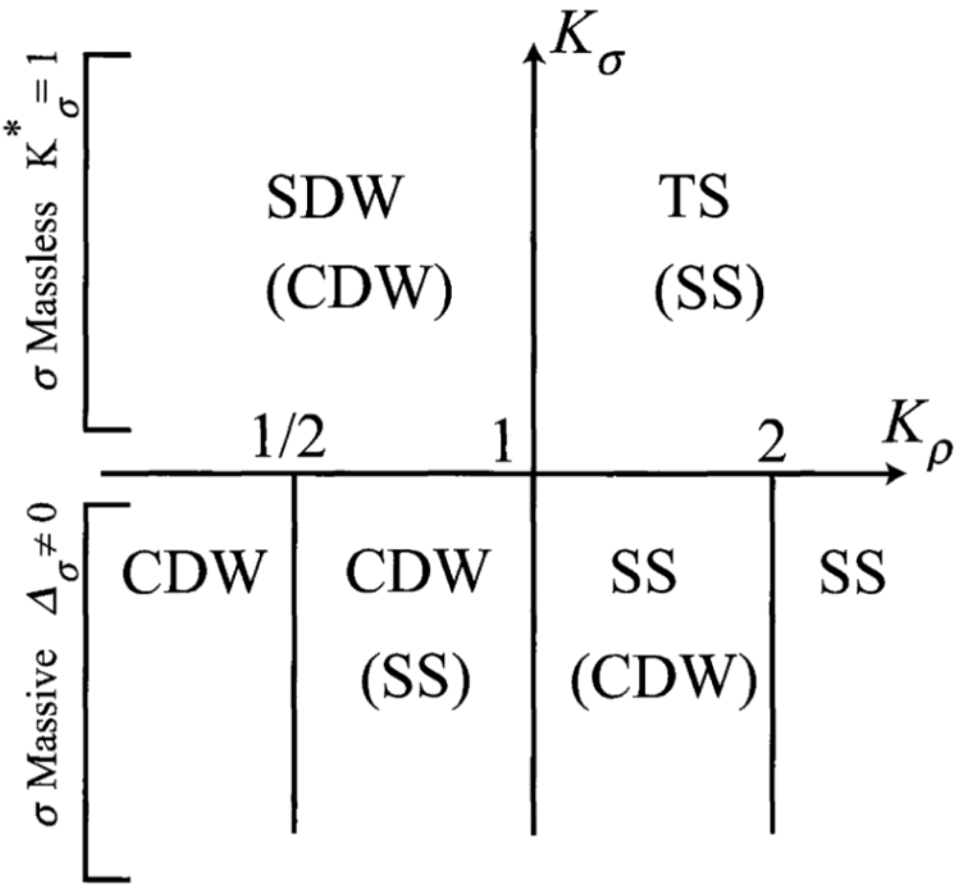

FIG. 2.9. Phase diagram of the system with spin for spin isotropic couplings. There are four sectors depending on the value of the parameters K_ρ and the sign of the backscattering term $g_{1\perp}$ (or alternatively the value of the bare parameter K_σ). The phases correspond to the most divergent susceptibility. I have indicated in parenthesis subdominant divergences. In the upper part ($K_\sigma > 1$) the spin sector is massless. In the lower part ($K_\sigma < 1$) the spin excitations are massive with a gap Δ_σ.

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1. **Spin 1/2 chains [Ch. 6]**
2. **Interacting fermions on a lattice [Ch.7]**
3. **Coupled fermionic chains [Ch.8]**
4. **Disordered systems [Ch. 9]**
5. **Interacting 1D bosons [Ch. 11.1]**
6. **Impurities in Fermi liquids [Ch. 11.2]**

Concepts

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Concepts_temp [will be replaced by dr. De Palo notes]

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- **From T. Giamarchi, Quantum Physics in 1D, Clarendon,**

$$\epsilon(q) = \frac{[\text{illegible}]}{2}[\cos(q_1) + \cos(q_2)]$$

The corresponding dispersion relation $\epsilon(q)$ is shown in Fig. 5.6. We just saw how two spinons get combined symmetrically to give a spin 1 solution (the magnon). They can also combine antisymmetrically to give a spin 0 bound state. This involves solutions with complex λs. These solutions are referred as 'string solutions' in the literature. Their study falls outside of this brief presentation and I refer the reader to the above-mentioned reviews for more material on this point.

This is a small tour of the information that one can directly extract form the Bethe-ansatz equations. Most of the thermodynamic properties can also be extracted analytically, using the so-called 'thermodynamic Bethe-ansatz' (Takahashi, 1999). Recently, progress was also made for the calculation of correlation functions in massive phases with the so-called form factors (Gogolin *et al.*, 1999). I refer the reader to the literature for more details on these points.

5.2 A zest of numerics

Let me now present very briefly some of the numerical methods that have proved very useful in one dimension. Indeed, the numerical methods have gained a considerable importance. In one dimension the finite size effects are quite small in themselves compared to higher dimensions, since the volume/surface ratio is optimal. In addition, in the same way that we used Bethe-ansatz to determine the Luttinger parameters one can of course use a numerical solution of the problem for this purpose. Combining the numerics with the Luttinger liquid concept has thus proved to be a very powerful tool.

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q.

5.2.1 *Exact diagonalizations*

This is the simplest numerical method in principle. One simply diagonalizes the full interacting Hamiltonian and determines the eigenvalues and the eigenvectors. Although the principle is simplicity itself, it is clear that the implementation of the method cannot be. To diagonalize an interacting Hamiltonian is indeed a formidable problem. The dimension of the Hilbert space is humongous. Let us consider, for example, the case of a spin Hamiltonian where on each site there is a spin 1/2. In that case the number of states per site is 2, which means that the size of the Hilbert space is 2^N. One has thus in principle to diagonalize a matrix $2^N \times 2^N$. Even for 15 sites this would represent if the matrix was full about 10^9 elements, something hard to store and manipulate on most computers. Fortunately the situation is slightly better. Since usually only neighbors are coupled by the interaction the Hamiltonian is a very sparse matrix. Keeping only the non-zero elements decreases a lot its size. One can also make a maximal use of the symmetries of the original system to further reduce the size of the matrix. Even with all these tricks the memory size to store and manipulate the elements of the Hamiltonian is the most severe limitation. Given the state of the art of the present computers it is very hard to exceed 36 sites for a spin system. For a system where there are more than two states per site the situation is of course much worse. The industry of exact diagonalization is thus a very strong encouragement to find Hamiltonians where the unnecessary states have been

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A ZEST OF NUMERICS 155

eradicated. This is, for example, the case of the t–J model that we will examine in much more details in Chapter 7. Even with all these tricks, diagonalizing such large Hamiltonians requires some special techniques, the method usually used being the Lanczos technique. I refer the reader to the literature for more details on the method itself (Lanczos, 1950; Bonner and Fisher, 1964; Oitmaa and Betts, 1978; Davidson, 1993).

The advantage of exact diagonalization is of course the exact and systematic character of it. Given a microscopic Hamiltonian one gets the lowest eigenstates and eigenvalues, without any approximation or intrinsic numerical limitation. The results are thus free of bias. Since both the eigenvalues and eigenvectors are known the correlation functions can be computed directly in real time or frequency without fudging. One can work directly at zero temperature (which can be also a drawback). Exact diagonalizations have been extremely useful to compute Luttinger parameters. One can directly compute numerically the compressibility and response to a twist in boundary conditions. Since the quantum numbers are known one can also extract the velocities directly from the spectrum. We will see examples of results based on exact diagonalization in Chapter 7.

The drawback is of course mainly the size limitation. Since the Hilbert space doubles every time one site is added, this is not a problem that will be solved in the future. This means that extracting the long-distance, low-energy behavior is a very tricky business. For the frequency dependence of the correlation functions, this limitation is very obvious. For a system with L sites one can expect that

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this limitation is very obvious. For a system with L sites one can expect that the lowest reachable frequency is of the order of W/L where W is the bandwidth of the system. Since $1K$ corresponds to 30 GHz, one is quite far from the low-frequency behavior in an experimental sense.

5.2.2 *Monte-Carlo*

Monte-Carlo is opposite in spirit to exact diagonalizations. It is a well-known technique at the classical level. One has a partition function

$$Z = \sum_{\text{config}} e^{-\beta H} \qquad (5.64)$$

The sum over all configurations is an N-dimensional integral, with N very large. The best way to evaluate such multiple integrals is a statistical method. A lucid exposition of the technique is given in Binder (1984) and Landau and Binder (2000). For classical systems the 'only' drawback of the Monte-Carlo method is the fact that the error in evaluating the integral decreases only as $1/\sqrt{t}$ where t is the computing time. It means that given enough time (and thus money) any problem can be in principle solved.

Unfortunately,[25] the situation is highly more complicated in the case of quantum problems. First, the equivalent of the partition function for a classical system is provided by the functional integral, which is a way to evaluate the partition

[25] Fortunately for us analytical guys ....

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function for a quantum problem. It means that the method can only compute the various quantities in imaginary time. Going back to the physically interesting (that is, the retarded) correlation function is a complicated business. There are various ways of doing the Monte-Carlo for fermions, too specialized and numerous to be examined here (see, e.g. Kalos, 1982; Ceperley, 1995; Grotendorst et al., 2002). The simplest is to compute directly the functional integral (C.3). This of course works only for bosons. For fermions the functional integral is not over numbers but over weird objects known as Grassmann variables. It is thus necessary to integrate over fermions. There are various ways to do this. Let me just mention the simplest method known as the Hirsh–Fye algorithm (Hirsch and Fye, 1986). Let us assume that one starts with the Hubbard model (see Chapter 7)

$$H = H_0 + U\sum_i (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2}) \qquad (5.65)$$

The partition function in a discrete path integral representation is

$$\begin{aligned} Z &= \mathrm{Tr}[\prod_{j=1}^{N_\tau} e^{-\Delta\tau H}] \\ &= \mathrm{Tr}[\prod_{j=1}^{N_\tau} e^{-\Delta\tau H_0 - \Delta\tau H_U}] \end{aligned} \qquad (5.66)$$

where $\Delta\tau N_\tau = \beta$ and terms of order $\Delta\tau^2$ have been discarded. The interaction term on each site can be decoupled by introducing an Ising variable $\sigma = \pm 1$ on each site (and at each time slice)

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$j=1$

where $\Delta\tau N_\tau = \beta$ and terms of order $\Delta\tau^2$ have been discarded. The interaction term on each site can be decoupled by introducing an Ising variable $\sigma = \pm 1$ on each site (and at each time slice)

$$e^{-\Delta\tau U(n_{i\uparrow}-1/2)(n_{i\downarrow}-1/2)} = \frac{e^{-(\Delta\tau U)/4}}{2}\mathrm{Tr}_\sigma[e^{\lambda\sigma(n_{i\uparrow}-n_{i\downarrow})}] \qquad (5.67)$$

where $\cosh(\lambda) = e^{\Delta\tau U/2}$. After the interaction has been decoupled using (5.67), the trace over the fermionic degrees of freedom can be done explicitly in (5.66). The evaluation of the partition function (and the various correlation functions) is thus reduced to the evaluation of the classical sum over the Ising variables σ. The weight of a given configuration of σ is given by the complicated determinant resulting from the integration over the fermionic degrees of freedom in (5.66). This integral over the σ can thus be done by a similar Monte-Carlo method than for a classical system.

The advantage of Monte-Carlo is its possibility to treat relatively large size systems. It is in principle also an unbiased method. The correlation functions are computed at finite temperatures that can either be viewed as an advantage or as a drawback.

Unfortunately, there are several drawbacks. The first problem is known as the sign problem. Since the weight of a given configuration is resulting (in our method) from the integrations over the fermionic degrees of freedom there is no

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guarantee that it is a positive number. In general, this is not the case, contrary to the classical case where the weights $e^{-\beta H}$ are intrinsically positive. It thus means that to compute the correlation function, one has now to add positive and negative numbers. Each individual term can thus be much larger than the final sum. It means that the statistical error that one can get in evaluating such a sum can (and in general will!) grow extremely fast. This contains some physics: we have reduced a fermionic problem for which only antisymmetric wave functions are allowed to a classical problem where one sums freely over the configurations. There should thus be something in the sum that cancels the unwanted configurations of the σ to keep only the good ones. The consequence of this problem is that, contrary to the classical case, the error can grow very fast in the calculation making any evaluation of the correlation function unfeasible. Spending more money on the calculation does not guarantee any more an increased accuracy in the results. This problem is yet unsolved. Various cures have been proposed, but they always require some knowledge of what should be the structure of the true fermionic wave function, which biases the method. In some fortunate cases, however, one can show that the weights are indeed positive. This is, for example, the case for spin systems on unfrustrated lattices, or for the Hubbard model at half-filling. In that case the sign problem does not occur and Monte-Carlo is an extremely efficient method.

The second problem comes from the fact that the method evaluates the corre-

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extremely efficient method.

The second problem comes from the fact that the method evaluates the corre-
lation functions in imaginary time. To make an 'analytical' continuation on a numerical result (with noise!) is black magic. Thus, it is not always easy to go from Monte-Carlo results to the physical correlation functions. Some 'voodoo' methods have been devised for that, known as Maximum Entropy methods. Monte-Carlo can also be used to determine Luttinger exponents. With this method the two easiest quantities are the compressibility and the response to a twist in boundary conditions. The parameter K can also in principle be extracted directly from the correlation functions since the systems that one can access are reasonably large.

5.2.3 *DMRG*

In one dimension there is a recent method that has allowed to make gigantic progress in our ability to obtain numerical solutions (White, 1993). It is at the moment the closest to an ultimate weapon as one can dream of. The idea is simple and directly inspired from the numerical renormalization group method used by Wilson for the Kondo problem. The idea is to diagonalize a problem but keeping only the low-energy states and then implement numerically a renormalization procedure. With such a method the drawbacks of the exact diagonalization due to the need to keep too many states are eliminated while in principle keeping an excellent accuracy for the low-energy physics.

However, the procedure is not so easy to do in practice. Let me illustrate the problem with free electrons. Let us assume that one has diagonalized a free electron system of size L. How can one obtain the low-energy physics for a segment of size $2L$ from the knowledge we have for the system of size L. If

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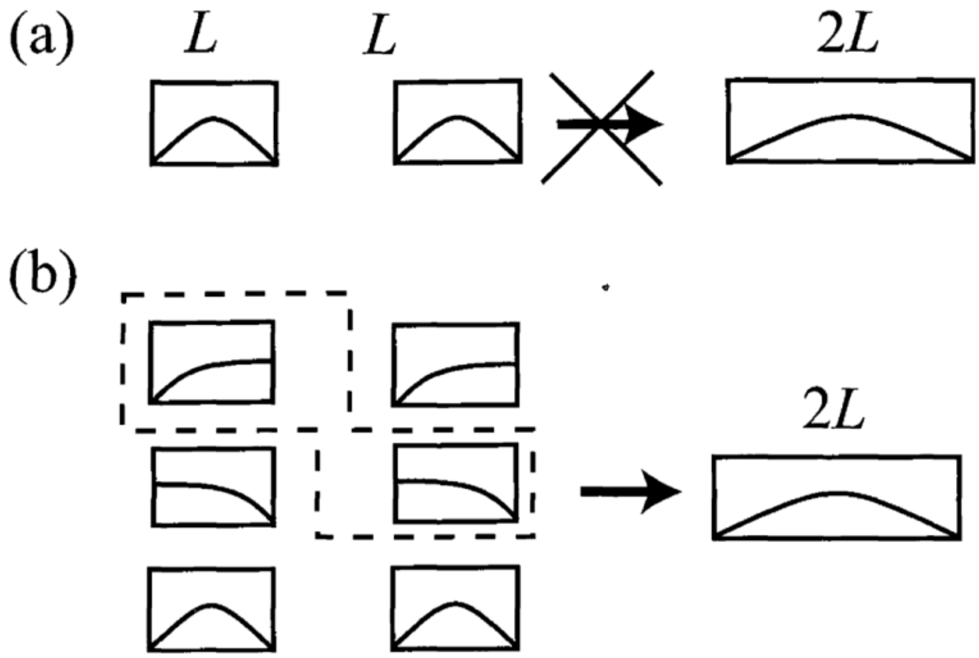

FIG. 5.7. To build a numerical renormalization group it is necessary to take into account various possible boundary conditions. (a) If one keeps only the low-energy of a system of size L with hard boundary condition then it is impossible to reproduce the low energy sector of a system of size $2L$ by coupling two such segments. (b) If all possible boundary conditions are allowed then it is possible to get a close approximate of a low-energy state in a segment of size $2L$ based on the low-energy properties of segments of size L. It is thus possible to build a numerical renormalization group.

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size $2L$ based on the low-energy properties of segments of size L. It is thus possible to build a numerical renormalization group.

one keeps all the states this is obviously easy, but let us assume that we have kept only the low-energy states of the segment of size L. In a renormalization group spirit we would only need the bottom of the spectrum to get the low-energy properties of the system and thus can throw away the states too far from the ground state since they will contribute little to the physical properties of the system. If there is a way to compute the low-energy of the segment of size $2L$, by reiterating the procedure one could in principle couple again two such segments and obtain ultimately the low-energy properties of a very long segment of material. In fact as noted by White, this method does not work very well if one does not pay special attention to the boundary conditions. Let us illustrate it by taking hard boundary conditions. In that case the ground state of the $2L$ segment has the form indicated in Fig. 5.7, with a maximum of density in the middle. On the other hand, the ground state of the L segments have a minimum of density at that point. It is thus practically impossible to reproduce the ground state of the $2L$ segment by combining low-energy states from L segments. The situation is quite different if one allows arbitrary boundary conditions as shown in Fig. 5.7. In that case it is very easy to reproduce the ground state of the $2L$ segment out of low-energy states of the L segment and the numerical RG can thus be constructed. The success of this procedure thus relies in the possibility to have the low-lying states for arbitrary boundary conditions without double

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counting. For the interacting system, the clever solution found by White was to compute the density matrix of the system. Part of the system is used to compute the density matrix, whereas part of the system acts as a bath to provide the various boundary conditions. The renormalization procedure can then be used. The method is too complex to be exposed in detail here and I refer the reader to Peschel *et al.* (1998) for more information.

Since this is in essence a method that retains only the low-energy properties of the system, and thus focus on the relevant quantities it can look at incredibly long systems. This allows to get rid of most of the size-effect and to look directly at the correlation functions. This is one of the main advantages of this DMRG technique. It allows a nearly direct calculation of all static quantities.

There are still some drawbacks. It is more difficult to extract from the method dynamical quantities, although the situation is rapidly improving. It is also not so easy to play with the boundary conditions. This can make it difficult to compute quantities that require such a change. This makes, for example, the calculation of the Luttinger parameters more complicated by this method since one cannot use the response to a twist easily, so quite often the parameter K is extracted from the static correlation functions. The method is also better suited to compute zero temperature quantities than finite temperature ones. But except for these few drawbacks it is clearly the method of choice to tackle one-dimensional problems. We will see various examples of phase diagrams that are computed using this method in the subsequent chapters.

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Procedures

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Proposed exercises

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- **See Notes, Problems and Solutions on these topics by Professor Phillip M. Duxbury, Michigan State University, Course PHY831: Graduate Statistical Mechanics From <http://www.pa.msu.edu/~duxbury/>**
  In particular:
  http://www.pa.msu.edu/~duxbury/courses/phy831/Outline.html
  1. **Complete Lecture Notes and Problems for Part 1**
  2. **Complete Solutions to Problems for Part 1**