

Acknowledgements

From a common book (Lipavský, Morawetz and Špička, 2001*b*) I could adapt parts into the chapters 3, 13, 14, 23 and appendix C, D for which copyright permission by EDP science is thanked for. I would have liked to convince Pavel Lipavský to be a coauthor, since he contributed main parts of sections 2.1, 2.2.2, 2.4, 2.5.1–2, 4, 5, 6.1, 6.3 and 16.1., 16.5–6. Especially the proof in appendix D has been composed in the book (Lipavský, Morawetz and Špička, 2001*b*) by him. The many enlightening discussions with Michael Männel are acknowledged who has worked out the Bose condensation of section 12.2 and 12.5 within his PhD thesis.

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It is important to note that the selfenergy contains exclusively the interaction of channel 1 with the surroundings and not with itself. Of course, the true selfenergy as defined above results after averaging over the impurity configuration if the impurity potential enters all parts of the Hamiltonian. Here we keep the non-averaged 'selfenergy' for the moment to obtain convenient and easy-to-interpret relations.

Due to the imaginary part of the selfenergy, the secular equation (6.42) does not result in eigen-states in the exact sense. We can introduce such eigen-states approximately neglecting the imaginary part,

$$[\varepsilon - E_1 - \text{Re}\Sigma_1(\varepsilon)] \Psi_1 = 0. \tag{6.44}$$

The eigen-energy obtained in this way is the quasiparticle energy ε .

6.6.1 Wave function renormalisation

Considering the norm

$$|\Psi_1|^2 + \sum_k |\Psi_k|^2 = 1 \tag{6.45}$$

we can introduce (6.41) which reads

$$\sum_k |\Psi_k|^2 = |\Psi_1|^2 \sum_k V_{1k} \left(\frac{1}{\omega - E_k} \right)^2 V_{k1} = -|\Psi_1|^2 \frac{\partial}{\partial \omega} \left(\frac{V_{1k} V_{k1}}{\omega - E_k} \right) = -|\Psi_1|^2 \frac{\partial}{\partial \omega} \Sigma_1 \tag{6.46}$$

such that the norm (6.45) of the wave function becomes normalised to

$$|\Psi_1|^2 = \frac{1}{1 - \frac{\partial}{\partial \omega} \Sigma} = z. \tag{6.47}$$

This function is the weight of the pole of the Green's function. Accordingly, the weight z is called wave-function renormalisation. With the probabilistic interpretation of the wave function, one can say that a particle spends the fraction of time z in its main state $|1\rangle$ and the fraction $1 - z$ in the environment.

6.6.2 Effective mass

The free energy of the Schrödinger equation $\omega = \epsilon_0 = k^2/2m$ becomes shifted by the real part of the selfenergy $\omega = \epsilon = \epsilon_0 + \text{Re}\Sigma(\epsilon)$. Therefore an effective mass appears as one can find from the definition of the velocity

$$v_{\text{quasi}} = \frac{k}{m^*} = \partial_k \epsilon = \partial_k \epsilon_0 + \frac{\partial \Sigma}{\partial \omega} \Big|_{\omega=\epsilon} \partial_k \epsilon = \frac{\partial_k \epsilon_0}{1 - \frac{\partial \Sigma}{\partial \omega} \Big|_{\omega=\epsilon}} = z \frac{k}{m}. \tag{6.48}$$

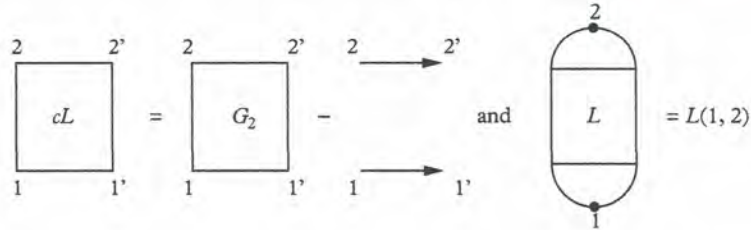


Figure 10.2: Correlated part of two-particle Green's function (10.23).

terms of Green's functions we introduce the correlated part of the two-particle Green's function including exchange by

$$cL(121'2') = G_2(121'2') - G^c(11')G^c(22') \tag{10.23}$$

illustrated by Figure 10.2. Here the factor c can be chosen as convenient. In the literature it ranges from $c = -i$ up to $c = 1$, which we will use in the variational approach in Chapter 11. In order to see how this factor appears or drops out in subsequent formulae, we will keep it here.

The density fluctuations (10.22) can be expressed with the help of two-particle Green's function as

$$\begin{aligned} \langle \delta\rho(11)\delta\rho(22) \rangle &= \langle \Psi_1^+ \Psi_2^+ \Psi_1 \Psi_2 \rangle - G^<(11)G^<(22) \\ &= i^2 \Theta(t_1 - t_2) G_{121+2+} + G^c(11^+)G^c(22^+) = icL^>(12) = icL^<(21) \\ \langle \delta\rho(22)\delta\rho(11) \rangle &= icL^<(12). \end{aligned} \tag{10.24}$$

As seen in Figure 10.2, it can be expressed together as a causal function

$$L^c(12) = \frac{1}{i} \Theta(t_1 - t_2) L^>(12) + \frac{1}{i} \Theta(t_2 - t_1) L^<(12) = L_{121+2+} \tag{10.25}$$

where we obey the Bose character of fluctuations in the definition (7.3).

With the help of the second equation of the Martin-Schwinger hierarchy (7.8), which couples the two-particle Green's function to the three-particle one, we get the following equation of motion for the correlator L defined in (10.23):

$$\begin{aligned} \left(i\hbar \frac{\partial}{\partial t_1} - \frac{\nabla_1^2}{2m} \right) L(121'2') &= \mp \frac{1}{c} \delta(1-2') G^c(21') \pm \frac{i}{c} G^c(11') G^c(22') \int d3V(13) G^c(33^+) \\ &\pm i G^c(22') \int d3V(13) L(131'3^+) \mp \frac{i}{c} \int d3V(13) G_3(1231'2'3^+). \end{aligned} \tag{10.26}$$

$$\Sigma_a^{\geq}(k, \omega) = \sum_b \int \frac{dq}{(2\pi\hbar)^2} V_{ab}(q)^2 f_{a,k-q}^{\geq} \int d\omega' \delta(\epsilon_{k-q} - \hbar\omega - \hbar\omega') \frac{\Pi_b^{\geq}(q, \omega')}{|\epsilon^R(q, \omega')|^2}. \quad (10.72)$$

In equilibrium the distributions are Fermi–Dirac ones and we can use $[1 - f(a) - f(b)] = g(a+b)$ with the Bose function $g(x) = 1/(\exp(x/T) - 1)$ and we rewrite the free-density fluctuation or polarisation function

$$\Pi_b^{\geq}(q, \omega) = \pm 2g_b(\pm\hbar\omega) \text{Im}\Pi_b(q, \omega) \quad (10.73)$$

where the imaginary part is

$$\text{Im}\Pi_b(q, \omega) = \pi \int \frac{dp}{(2\pi\hbar)^2} (f_{b,p} - f_{b,p+q}) \delta(\epsilon_p - \epsilon_{p+q} - \hbar\omega). \quad (10.74)$$

A final simplification of the selfenergy can be achieved in the limit of heavy masses of the scattering impurities. We are allowed to neglect quantum fluctuations of these impurities which are expressed by $g(\pm\hbar\omega)$ in (10.73) and replace $g(\pm\hbar\omega) \rightarrow \pm T/\hbar\omega$. Since $\epsilon^R = 1 - \sum_n V_{bb} \Pi_b^R$ we can split $V_{ab}^2 = V_{aa} V_{bb}$ to realise the $\text{Im}\epsilon^R$ part in (10.72) such that the selfenergy can be written

$$\begin{aligned} \Sigma_a^{\geq}(k, \omega) &= 2T \int \frac{dq}{(2\pi\hbar)^2} V_{aa}(q) f_{a,k-q}^{\geq} \int \frac{d\omega'}{\omega'} \delta(\epsilon_{k-q} - \hbar\omega - \hbar\omega') \text{Im} \frac{1}{\epsilon^R(q, \omega')} \\ &= -2\pi T \int \frac{dq}{(2\pi\hbar)^2} V_{aa}(q) \text{Re} \left(1 - \frac{1}{\epsilon^R(q, 0)} \right) f_{a,k-q}^{\geq} \delta(\epsilon_{k-q} - \hbar\omega). \end{aligned} \quad (10.75)$$

In the last step we used (10.67). The real part of the selfenergy (10.70) becomes

$$\Sigma_a(k, \omega) = T \int \frac{dq}{(2\pi\hbar)^2} V_{aa}(q) \text{Re} \left(1 - \frac{1}{\epsilon^R(q, 0)} \right) \frac{\wp}{\epsilon_{k-q} - \hbar\omega}. \quad (10.76)$$

In order to evaluate the effective mass according to (10.80), it remains to get an expression for the dielectric function. To this end we use the zero-temperature expansion (Hodges, Smith and Wilkins, 1971; Morawetz, 2003) of the dielectric function $\epsilon = 1 - V\Pi$ in quasi two-dimensions (10.66) since the leading temperature dependence is already in front of the integral. This means we consider the electrons as degenerated but the impurity particle–hole fluctuation as classical here. Changing the integration variables $z = q/2p_f$, we then obtain for the real part (10.76) of the dynamically screened selfenergy [$x = k/2p_f$, $x_0 = \hbar\omega/4\epsilon_f$]

10.5 Structure factor and pair-correlation function

The one-time pair-correlation function is defined as

$$n(1)n(2)g(1,2) = \langle \hat{\Psi}_1^+ \hat{\Psi}_2^+ \hat{\Psi}_2 \hat{\Psi}_1 \rangle |_{t_1=t_2} \quad (10.85)$$

and can be obtained if we consider only an infinitesimal propagation $t_2 = t_1 + 0 = t_{1+}$ of the fluctuation function (10.24)

$$\begin{aligned} -cL(x_1 t_1, x_2 t_{1+}) &= icL^<(12) = \langle \Psi_2^+ \Psi_2 \Psi_1^+ \Psi_1 \rangle - n(1)n(2) \\ &= \langle \Psi_1^+ \Psi_2^+ \Psi_2 \Psi_1 \rangle + \delta_{12}n(1) - n(1)n(2) \\ &= n(1)n(2)[g(12) - 1] + \delta_{12}n(1) \end{aligned} \quad (10.86)$$

which provides the pair-correlation function in terms of the time-diagonal of $L^<$. Changing to difference and centre-of-mass coordinates $r = x_1 - x_2$, $R = (x_1 + x_2)/2$ we can also introduce the structure function

$$[g(r, R) - 1]n(R + \frac{r}{2})n(R - \frac{r}{2}) + \delta(r)n(R) = n(R)(S(r, R) - \delta(r)) \quad (10.87)$$

Neglecting gradients in the density on the left side $n(R \pm r/2) \approx n(R)$ we obtain the known Fourier transform

$$S(R, q, t) - 1 = n(R, t) \int dr e^{-iqr} [g(R, r, t) - 1]. \quad (10.88)$$

The long-wavelength limit in equilibrium

$$\begin{aligned} S_{q=0} &= \int dr [S(r) - \delta(r)] = \frac{1}{n} \int dr \langle \delta \hat{n}(r) \delta \hat{n}(0) \rangle \\ &= \frac{1}{n} \frac{\langle N^2 \rangle - \langle N \rangle^2}{V} \equiv \frac{n}{\beta} \kappa = \frac{1}{m\beta v_t^2} \end{aligned} \quad (10.89)$$

determines the isothermal compressibility

$$\kappa = \frac{1}{n} \left(\frac{\partial n}{\partial p} \right)_\beta \quad (10.90)$$

and the isothermal sound velocity $mv_t^2 = (\partial p / \partial n)_\beta$.

Here we use the convenient coordinates (9.2) and its Fourier transform

$$\langle p | L(K) | p' \rangle = \int dr dr' ds e^{ipr - ip'r' - iKs} \langle r | L(s, R) | r' \rangle \quad (10.91)$$

where we will drop the centre-of-mass coordinate R . The pair-correlation function reads in these coordinates

$$\begin{aligned} [g(x_1, x_2) - 1]n(x_1)n(x_2) + \delta_{12}n(1) &= ic\langle x_1 - x_2 | L_u^<(0, \frac{x_1 + x_2}{2}) | x_1 - x_2 \rangle \\ &= ic \int \frac{dp dp' dK}{(2\pi)^9} e^{-i(p-p')(x_1-x_2)} \langle p | L_u^<(K) | p' \rangle. \end{aligned} \quad (10.92)$$

10.5.1 Fock approximation

In lowest-order perturbation theory we calculate the correlation function in Fock approximation which is the second diagram in Figure 10.1. The Hartree term obviously does not contribute to the pair-correlation function since it is diagonal in the spatial coordinates. Neglecting gradients in the centre-of-mass coordinate we obtain the causal function (10.29)

$$c\langle p | L_u^0(K) | p' \rangle = \mp (2\pi)^3 \delta(p + p') G_{u'} \left(\frac{K}{2} - p \right) \cdot G_{t'} \left(\frac{K}{2} + p \right). \quad (10.93)$$

Here we denote the product explicitly by a dot to distinguish from the operator product. From the causal expression (10.93) the correlation functions (10.44) follows

$$\langle p | L_u^{0\geq}(K) | p' \rangle = -\frac{i}{c} (2\pi)^3 \delta(p + p') G_{u'}^{\geq} \left(\frac{K}{2} - p \right) \cdot G_{u'}^{\leq} \left(\frac{K}{2} + p \right). \quad (10.94)$$

With the Wigner function $\rho(p, R, t) = G_u^<(p, R)$, the structure function (10.88) with the help of (10.92) is computed easily

$$S(q) = \frac{1}{n} \int \frac{dp}{(2\pi)^3} \rho_p (1 \mp \rho_{p-q}) \quad (10.95)$$

such that the isothermal compressibility (10.90) becomes

$$\frac{n}{\beta} \kappa = \frac{1}{n} \int \frac{dp}{(2\pi)^3} (1 \mp \rho_p) \rho_p \quad (10.96)$$

which is easily checked to be correct by

$$\kappa = \frac{1}{n^2} \frac{\partial n}{\partial \mu} = \frac{1}{n^2} \frac{\partial}{\partial \mu} \int \frac{dp}{(2\pi)^3} \frac{1}{e^{\beta(\epsilon_p - \mu)} \pm 1} = \frac{\beta}{n^2} \int \frac{dp}{(2\pi)^3} \rho_p (1 \mp \rho_p) \quad (10.97)$$

for Fermi/Bose distributions in equilibrium.

11.2.1 Screening for Coulomb systems

For Coulomb systems it is of advantage to consider the variation with respect to the external and mean field

$$\bar{U}_{11'} = U_{11'} \mp iV_{12}G_{22} + \delta_{11'}. \tag{11.25}$$

From (11.21) we see now that the screened selfenergy $\bar{\Sigma}$ which is the selfenergy diminished by the Hartree term $\Sigma + U = \bar{\Sigma} + \Sigma^H + U = \bar{\Sigma} + \bar{U}$ is written as

$$\bar{\Sigma}_{14}G_{41'} = iV_{12} \frac{\delta G_{11'}}{\delta U_{22}} = \mp i\Pi_{121'2}W_{12} \tag{11.26}$$

graphically seen in Figure 11.4.

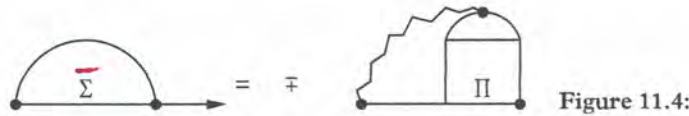


Figure 11.4:

To derive this, we have used the definition of the screened potential of Chapter 10.2.2

$$V_{12} \frac{\delta \bar{U}_{34}}{\delta U_{25}} = W_{12}\delta_{32}\delta_{45} \tag{11.27}$$

and the fact that the polarisation is given as the variation of the Green's functions with respect to the induced potential \bar{U}

$$\Pi_{13'1'3} = \mp \frac{\delta G_{11'}}{\delta \bar{U}_{33'}}. \tag{11.28}$$

Calculating the derivative in (11.27) explicitly with (11.25) one obtains

$$\frac{\delta \bar{U}_{33'}}{\delta U_{22'}} = \delta_{23}\delta_{2'3'} + iV_{36}\Pi_{656+4} \frac{\delta \bar{U}_{45}}{\delta U_{22}} \delta_{33'} \tag{11.29}$$

and the equation for the screened potential becomes

$$W_{13} = V_{13} + iW_{12}V_{34}\Pi_{424+2}. \tag{11.30}$$



11.6 Linear response

11.6.1 Basic relations

The response function χ describes the density change δn of the system when an external potential U^{ex} is applied. This disturbance creates an induced potential

$$V^{ind} = (V + f)\delta n + U^{ex} \quad (11.66)$$

where V is the interaction among the particles and f describes local correlations deviating from the mean field which are called local fields. The density response with respect to this induced potential is the polarisation function Π . Therefore we have the identities

$$\delta n = \chi U^{ex} = \Pi V^{ind} = \frac{\Pi}{1 - (V + f)\Pi} U^{ex} = \chi^s W \quad (11.67)$$

where we introduced the screened response $\chi^s = \Pi/(1 - f\Pi)$ and the screened potential

$$W = V\delta n + U^{ex}. \quad (11.68)$$

The external field is given by the external densities $U^{ex} = Vn^{ex}$ and its charges determine the electric displacement field $div D = en^{ex}$ while the sources of the electric field are the present internal charges, i.e. $div E = e(\delta n + n^{ex})$. Therefore one gets the dielectric function as

$$\epsilon = \frac{n^{ex}}{\delta n + n^{ex}} = \frac{U^{ex}}{e\delta n + U^{ex}} = \frac{U^{ex}}{W} = \frac{\chi^s}{\chi} = 1 - V \frac{\Pi}{1 - f\Pi} = 1 - V\chi^s. \quad (11.69)$$

The inverse dielectric function can be written as

$$\frac{1}{\epsilon} = \frac{V\delta n}{U^{ex}} + 1 = 1 + V\chi \quad (11.70)$$

11.6.2 Connection to diagrammatic expansions

With the help of (11.14), the density response to an external potential can be expressed in terms of the density-fluctuation function L of (11.16). Since the density is given by $\mp iG_{11+} = \langle a_1^\dagger a_1 \rangle = \langle \hat{n}_1 \rangle = n_1$ we have from (11.14) and (11.16) for the response function χ to an external potential

$$\chi_{12} = \frac{\delta n_1}{\delta U_{22}} = +iL_{121+2^+} = -i \langle (\hat{n}_1 - n_1)(\hat{n}_2 - n_2) \rangle. \quad (11.71)$$

The last identity follows from the definition of L and underlines the name-density fluctuation function. We see now that the linear-density variation due to an external potential can be written as

$$\delta n_1 = +iL_{121+2^+} U_2 = \chi_{12} U_{22}. \quad (11.72)$$

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For a macroscopic occupation of the ground state one can approximate the Bose function near its pole and solve the resulting equation

$$N_0 \approx \frac{2n_0 U_0 - \mu}{\beta((2n_0 U_0 - \mu)^2 - n_0^2 U_0^2)}$$

for μ

$$\mu = 2n_0 U_0 - \frac{1}{2\beta N_0} - \sqrt{n_0^2 U_0^2 + \frac{1}{(2\beta N_0)^2}} = n_0 U_0 + \mathcal{O}(N_0^{-1}) \quad (12.16)$$

which coincides with (12.6) in the noninteracting limit. The result is that, in the thermodynamic limit, $N_0 \rightarrow \infty$, $\mu = n_0 U_0$ (Shi and Griffin, 1998, p. 21). This relation will be used in \checkmark to eliminate μ .

For weak interaction it can be assumed that at $T = 0$ all particles are in the condensate, i.e. $N = N_0 + \mathcal{O}(U_0^2)$ and

$$E = \frac{N^2 U_0}{2\Omega} + \mathcal{O}(U_0^2).$$

From that ground-state energy one can obtain the pressure at $T = 0$

$$\mathcal{P} = - \left. \frac{\partial E}{\partial \Omega} \right|_{N=\text{const.}} = \frac{n^2 U_0}{2} + \mathcal{O}(U_0^2) = \frac{\rho^2 U_0}{2m^2} + \mathcal{O}(U_0^2) \quad (12.17)$$

where $\rho = mn$ is the mass density. This relation shows that $U_0 > 0$ guarantees also the stability of the system, i.e. a positive pressure. The pressure for $U_0 = 0$ vanishes at $T = 0$. According to the Nernst theorem (Landau and Lifschitz, 1984, p. 65) the entropy S is zero at $T = 0$. The sound velocity c follows from (Landau and Lifschitz, 1971, p. 284)

$$c^2 = \left. \frac{\partial \mathcal{P}}{\partial \rho} \right|_{S=\text{const.}} = \frac{n_0 U_0}{m} + \mathcal{O}(U_0^2).$$

Obviously the linear approach for small momenta of the Bogoliubov dispersion (12.1) is given by the macroscopic sound velocity at $T = 0$ (Bogoliubov, 1947). When approaching the phase transition from the normal phase, i.e. setting $n_0 = 0$ in (12.14), one finds that the critical temperature and density of the Bogoliubov approximation seem to be the same as for the ideal Bose gas obtained in Section 12.2.1.

Near the phase transition it is convenient to calculate the difference between the density of un-condensed particles and the ideal critical density n_{id} (Shi and Griffin, 1998, p. 33 f.)

in agreement with (12.32). The spectral function (Ambegaokar, 1969) shows consequently two parts, a particle and ‘antiparticle’ contribution¹

$$a = \pi \left(1 + \frac{\xi}{E}\right) \delta(\omega - \mu - E) + \pi \left(1 - \frac{\xi}{E}\right) \delta(\omega - \mu + E) \quad (12.49)$$

which fulfils the sum rule and collapses to the normal quasiparticle picture for $\Delta \rightarrow 0$. The consequent Green’s functions reads

$$g^<(p, \omega) = \pi \left(1 + \frac{\xi}{E}\right) \delta(\omega - \mu - E) f(E) + \pi \left(1 - \frac{\xi}{E}\right) \delta(\omega - \mu + E) f(-E). \quad (12.50)$$

The spectrum of available states is given by the first part and the spectrum of particles which can be removed are given by the second one. As illustrated in Figure 12.6 the gap for fermions changes the spectra in the characteristic way allowing the population of positive states below the Fermi energy. For a vanishing gap only the negative branch below Fermi energy and the positive branch above Fermi energy bears a non-vanishing weight; such that the normal quasiparticle spectrum $\xi = \epsilon - \epsilon_f$ is approached.

Introducing now one normal quasiparticle Green’s functions (9.17) and one anomaly one (12.50) in the two-particle propagator (12.39) we obtain from (12.41) just the correct finite-temperature gap equation

$$\begin{aligned} \Delta(p_1) &= \int \frac{dp_3}{(2\pi)^3} V(p_1 - p_3) \frac{f(E) - f(-E)}{2E} \Delta(p_3) \\ &= \mp \int \frac{dp_3}{(2\pi)^3} V(p_1 - p_3) \left(\frac{\tanh \frac{E}{2T}}{\coth \frac{E}{2T}} \right) \frac{\Delta(p_3)}{2E} \end{aligned} \quad (12.51)$$

with (12.48) for **F**ermions/Bosons respectively.

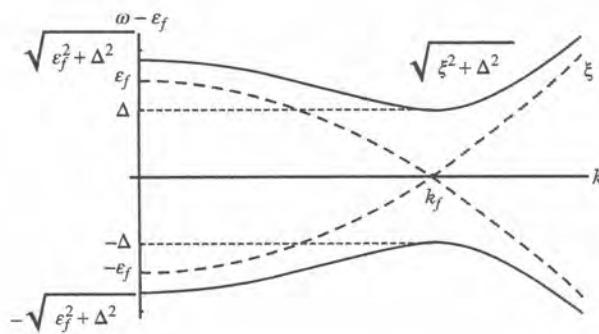


Figure 12.6: The quasiparticle spectrum for a finite-gap superconductor (fermions) with quadratic dispersion at $T = 0$.

¹ In fact it is the same as in relativistic mean-field models, see (22.32) and (22.33), which analogy is used as equivalent mass approach (Gulian and Zharkov, 1999).

and $f_B(\epsilon) = 1/(e^{\epsilon/T} - 1)$ is the Bose distribution function. In the normal phase, for $n_0 = 0$, the dispersion is (12.86)

$$\epsilon_q = \frac{\hbar^2 q^2}{2m} - \mu + 2n\mathcal{T}(0). \quad (12.92)$$

From (12.90) one sees that the chemical potential μ satisfies the Hugenholtz–Pines relation (Hugenholtz and Pines, 1959) $\mu = 2n\mathcal{T}(0) - n_0\mathcal{T}(0)$ in the condensed phase with the particle density (12.88).

$$\mu = \mathcal{T}(0) - \Delta(0)$$

12.6 Comparison of approximations

The expectation value of the total energy density can be calculated from the Green's function (Kadanoff and Baym, 1962), according to (7.38), as

$$\begin{aligned} \mathcal{E} &= \frac{\langle \hat{H} \rangle}{\Omega} = -\frac{T}{\Omega} \sum_{\mathbf{k}, \nu} \frac{1}{2} \left(z_\nu + \mu + \frac{\hbar^2 k^2}{2m} \right) G(\mathbf{k}, z_\nu) \\ &= \underbrace{\int \frac{d^3 k}{(2\pi)^3} E_{\mathbf{k}} f_B(E_{\mathbf{k}})}_{\mathcal{E}_{\text{qp}}} + \underbrace{\mathcal{T}(0) \left(n^2 - n n_0 + \frac{1}{2} n_0^2 \right)}_{\mathcal{E}_{\text{mf}}} \\ &\quad - \underbrace{\int \frac{d^3 k}{(2\pi)^3} E_{\mathbf{k}} v_{\mathbf{k}}^2}_{\mathcal{E}_{\text{cor}}} + \underbrace{\int \frac{d^3 k}{(2\pi)^3} \frac{n_0^2 \mathcal{T}^2(\mathbf{k})}{4E_{\mathbf{k}}}}_{\mathcal{E}_{2\text{p}}} (1 + 2f_B(E_{\mathbf{k}})). \end{aligned} \quad (12.93)$$

Different levels of approximation can now be distinguished in the way they treat the corresponding contributions to this energy density. The mean-field-like approximation $\mathcal{T}(\mathbf{q}) \approx U_0$ together with $E_{\mathbf{q}} = \epsilon_{\mathbf{q}} \approx \hbar^2 q^2/2m + n_0 U_0$ establishes the Hartree–Fock approximation as proposed by Huang et al. (Huang and Yang, 1957; Huang et al., 1957) and in (12.93) only the contribution of quasiparticles \mathcal{E}_{qp} and the mean field term \mathcal{E}_{mf} survive leading to

$$\mathcal{E} = \int \frac{d^3 k}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} f_B(\epsilon_{\mathbf{k}}) + U_0 \left(n^2 - \frac{1}{2} n_0^2 \right). \quad (12.94)$$

This energy density shows that, in addition to statistics, BEC is also energetically favoured, since a finite condensate density n_0 lowers the interaction energy. This phenomenon we called ‘attraction in momentum space’ (Huang, 1964; Leggett, 2001).

Approximating only $\mathcal{T}(\mathbf{q}) \approx U_0$ provides the Hartree–Fock–Bogoliubov or Popov approximation, with the typical Bogoliubov dispersion (12.13). Within this approximation a correlation term \mathcal{E}_{cor} of the energy density (12.93) remains besides the

$$G_{j,m} = t_{j+1} S_j^l G_{j+1,m}, \quad m \geq j+1. \quad (16.31)$$

The diagonal form is found from G_{11} of (16.25) easily to be

$$\langle k | G_{11} | k \rangle = \frac{S_k^l}{1 - t_{k+1}^2 S_{k+1}^r S_k^l} = \frac{1}{z - v_k - t_{k+1}^2 S_{k+1}^r - t_k^2 S_{k-1}^l} \quad (16.32)$$

where we used (16.22) once more. This completes the recursive construction of the Green's functions.

16.2.1 Summary of the method

For computational purposes let us collect the important steps and formulae.

1. Calculate the surface Green's functions of the left and right lead according to (16.24)

$$\begin{aligned} S_{N+1}^r &= \frac{1}{t_{N+1}} \left(\frac{z - v_{N+1}}{2t_{N+1}} + i \sqrt{1 - \left(\frac{z - v_{N+1}}{2t_{N+1}} \right)^2} \right) \\ S_0^l &= \frac{1}{t_0} \left(\frac{z - v_0}{2t_0} + i \sqrt{1 - \left(\frac{z - v_0}{2t_0} \right)^2} \right). \end{aligned} \quad (16.33)$$

2. Determine the surface Green's functions due to the recursive relations (16.22) and (16.23)

$$\begin{aligned} S_j^l &= \frac{1}{z - v_j - t_j^2 S_{j-1}^l} \\ S_{j+1}^r &= \frac{1}{z - v_{j+1} - t_{j+1}^2 S_{j+2}^r}. \end{aligned} \quad (16.34)$$

3. Compute the required elements of the Green's functions matrix according to (16.30), (16.31) and (16.32)

$$\begin{aligned} G_{kk} &= \frac{1}{z - v_k - t_{k+1}^2 S_{k+1}^r - t_k^2 S_{k-1}^l} \\ G_{j,m} &= t_{j+1} S_j^l G_{j+1,m}, \quad m \geq j+1 \\ G_{j+1,m} &= t_{j+1} S_{j+1}^r G_{j,m}, \quad m \leq j. \end{aligned} \quad (16.35)$$

and from (16.41) follows the transmission coefficient

$$\begin{aligned}
 t &= e^{-ikaN} (G_{N,1}\Omega_1 + G_{N,0}\Omega_0) \\
 &= -2it_1 e^{-ikaN} G_{N,0} \sin(ka) \\
 &= -2it_1 e^{-ika(N+1)} G_{N+1,0} \sin(ka)
 \end{aligned} \tag{16.43}$$

representing different equivalent forms. The reflection $R = |r|^2$ and transmission $T = |t|^2$ obey $T + R = 1$, of course.

16.3.1 Current and current fluctuations

For the tight-binding Hamiltonian (16.1) the velocity operator $\dot{x} = \frac{i}{\hbar}[H, x]$ is easily computed from the position operator $x = a \sum_j j |j\rangle \langle j|$ as

$$\dot{x} = \frac{ia}{\hbar} \sum_j t_{j+1} (|j\rangle \langle j+1| - |j+1\rangle \langle j|). \tag{16.44}$$

The mean current $j = \langle e\dot{x} \rangle$ is conserved. Therefore it is sufficient to calculate the current which runs from the atoms to the lead on the right side

$$j = \frac{iea}{\hbar} t_{N+1} (\langle \psi_N^* \psi_{N+1} \rangle - \langle \psi_{N+1}^* \psi_N \rangle) = \frac{iea}{\hbar} t_{N+1} (G_{N,N+1}^< - G_{N+1,N}^<) \tag{16.45}$$

H so far

where we introduced the definition of the correlated Green's functions $G^<$. The Green's functions provided ~~in the Appendix A~~ are causal functions. According to the Langreth-Wilkins rules (7.18), (7.17) and the recursion relation of the causal Green's functions (16.30) we can write

$$\begin{aligned}
 G_{N,N+1}^< &= t_{N+1} (G_{NN}^R S_{N+1}^< + G_{NN}^< S_{N+1}^A) \\
 G_{N+1,N}^< &= t_{N+1} (S_{N+1}^R G_{NN}^< + S_{N+1}^< G_{NN}^A)
 \end{aligned} \tag{16.46}$$

and repeatedly applying (16.22) the current (16.45) reads

$$j = \frac{ae}{\hbar} \prod_{j=1}^{N+1} t_j^2 \prod_{k=1}^{N-1} |S_k^<|^2 (S_{N+1}^{r<} S_0^{l>} - S_{N+1}^{r>} S_0^{l<}). \tag{16.47}$$

Further simplification can be achieved by rewriting the diagonal Green's functions G_{NN} in (16.47) into the Green's functions $G_{N+1,0}$ with the help of (16.31). We observe that the surface-correlated Green's function $S_0^{l<}$ is the one on the left lead. It can be expressed in terms of the spectral function $A_l = i(S_0^{lR} - S_0^{lA})$ and the Fermi-Dirac function f_l describing

If one denotes the unperturbed part as

$$G^{0<} = G^{0R} \Omega \Omega^\dagger G^{0A}, \quad (16.65)$$

the n -th order of (16.64) becomes identical to (6.5). The $G^<$ defined by (16.63) hence obeys the GKB equation,

$$G^< = G^R \Sigma^< G^A + (1 + G^R \Sigma^R) G^{0<} (1 + \Sigma^A G^A). \quad (16.66)$$

As in the general case discussed in Section 16.5, the GKB equation is consistent with any approximation of the selfenergy. 7. 2

Coherent diffraction Some electrons keep their initial parallel momentum, k_{\parallel} , i.e. they are diffracted coherently, as on the ideal barrier. These processes are covered by the second term of (16.66),

$$\hat{G}^< = (1 + G^R \Sigma^R) G^{0<} (1 + \Sigma^A G^A) = G^R \Omega \Omega^\dagger G^A. \quad (16.67)$$

With explicit site indices, the coherent part reads

$$\hat{G}_{jr, is}^< = \sum_{t, w \in \text{plane}} \sum_{l, m=0, -1} G_{jr, lt}^R \Omega_{lt} \Omega_{mw}^* G_{mw, is}^A. \quad (16.68)$$

After the averaging, the system is again a translational invariant so that it is advantageous to transform the in-plane site indexes into the momentum representation. From the Fourier transformation of the source term we find that the source is singular in momentum,

$$\sum_{t \in \text{plane}} \Omega_{lt} \Omega_{mw}^* e^{-ip_{\parallel}(r_t - r_w)} = |\Omega_{0, l}| (\Omega_{0, m}) (2\pi)^2 \delta(p_{\parallel} - k_{\parallel}). \quad (16.69)$$

Here, $|\Omega_{0, 1}|$ are from (16.91), and $(\Omega_{0, 1})$ are Hermitian conjugate to them. Since propagators, $G^{R, A}$ are regular in p_{\parallel} , the distribution of coherently diffracted particles $\hat{G}^<$ is singular, as one expects. We remind ourselves that the conservation of the parallel momentum applies only within the Brillouin zone. Processes with momentum transfer by multiples of the Brillouin vectors are included. The approximation of $G^<$ by $\hat{G}^<$ is called the non-vertex approximation. 16.7

16.5.2 Open system

One can take the barrier as a subsystem which is embedded into a reservoir formed by leads. If the barrier is very thick, its properties are dominated by the barrier region itself while the connection to the reservoir represents a perturbation. With the help of the diffraction we can thus formulate the contact between an open system and its reservoir.

To this end we make the Fourier transform of the GKB equation (16.66),

$$G_{ji}^<(p_{\parallel}) = \sum_{l,m=1}^N G_{jl}^R(p_{\parallel}) \Sigma_{lm}^<(p_{\parallel}) G_{mi}^A(p_{\parallel}) + (2\pi)^2 \delta(p_{\parallel} - k_{\parallel}) \sum_{l,m=-1,0} G_{jl}^R(k_{\parallel}) |\Omega_l\rangle \langle \Omega_m| G_{mi}^A(k_{\parallel}). \quad (16.70)$$

In the barrier region, $1 \leq j, i \leq N$, we express the off-diagonal elements in the source term from (16.36) and (16.37)

$$\sum_{l,m=-1,0} G_{jl}^R |\Omega_l\rangle \langle \Omega_m| G_{mi}^A = G_{j1}^R \times t S_0^{lR} (|\Omega_0\rangle + t S_{-1}^{lR} |\Omega_{-1}\rangle) ((\Omega_0| + (\Omega_{-1}| S_{-1}^{lA} t) S_0^{rA} t \times G_{1i}^A. \quad (16.71)$$

With respect to its effect on the barrier region, the source term can be replaced by a source acting exclusively on the 1-th layer,

$$\Sigma^{l<} = t S_0^{lR} (|\Omega_0\rangle + t S_{-1}^{lR} |\Omega_{-1}\rangle) ((\Omega_0| + (\Omega_{-1}| S_{-1}^{lA} t) S_0^{rA} t. \quad (16.72)$$

It is clear that if there would be electrons approaching the barrier from the right-hand side, a similar source, $\Sigma^{r<}$, results acting on the N -th layer. In the barrier region, the GKB equation with suppressed arguments reads

$$G^< = G^R (\Sigma^< + \Sigma^{l<}) G^A. \quad (16.73)$$

According to its position in the GKB equation (16.73), we have denoted the source, $\Sigma^{l<}$, by the symbol Σ reserved otherwise for the selfenergy. There are similarities and distinctions in their interpretations. Firstly, according to the Lippmann–Schwinger equation (4.23), the transport vertex $\Sigma^<$ describes ~~an~~ electrons sourced at a site where the crystal potential is perturbed by an impurity. Similarly, according to the Lippmann–Schwinger equation (16.6), the source term $\Sigma^{l<}$ describes electrons passing through the contact between the lead and barrier. Secondly, all electrons sourced by $\Sigma^<$ have been stolen from the system by the decay. The consistency between the transport vertex, $\Sigma^<$, and the decay rate $\propto -2\text{Im}\Sigma^R$, guarantees that all stolen electrons are re-emitted into the system, i.e. the number of particles conserves. In contrast, new electrons enter via the source $\Sigma^{l<}$. This arrival of electrons is compensated by the emission into leads, however, there is no consistency requirement between the two processes since emitted electrons never return into the barrier. The rate of emissions into leads reminds us that the decay is proportional to the imaginary part of the selfenergy-like surface terms,¹

¹ In equilibrium the number of emitted particles equals the number of entering particles,

$$-2f(E)\text{Im}\Sigma^{lR} = \Sigma^{l<}, \quad -2f(E)\text{Im}\Sigma^{rR} = \Sigma^{r0}.$$

This relation parallels the equilibrium relation between the selfenergy and the transport vertex, $-2f(E)\text{Im}\Sigma^R = \Sigma^<$.

phenomenon. If one ‘measures’ all states of the systems by their distance from equilibrium, instead of *formation* of correlations, one has to talk about their *decay*. Our presumption that the transient period is appreciably shorter than the local relaxation is thus just Bogoliubov’s principle of the decay of initial correlations. This decay of correlations is definitely a two-particle process.

The quantity which allows us to follow the two-particle and single-particle pictures in a unified manner is the energy of the system. It is composed from the kinetic energy E_{kin} and the correlation energy $E_{corr} = \langle V_D \rangle - \langle V_C \rangle$, where $\langle V_C \rangle$ subtracts the background. Of course, the total energy conserves,

$$E_{corr}(t) = E_{kin}^0 - E_{kin}(t), \tag{19.1}$$

where E_{kin}^0 is the initial value of the kinetic energy. We will monitor the time dependency of the transfer of the correlation energy into the kinetic one.

It is more convenient to calculate the kinetic energy than the correlation energy because the kinetic one is a single-particle observable. To this end we can use the kinetic equation, of course, which leads to the total energy conservation (19.1). It is immediately obvious that the ordinary Boltzmann equation cannot be appropriate for this purpose because the kinetic energy is an invariant of its collision integral and thus constant in time. It is possible to study this transient time regime within the Levinson equation for the Wigner function.

19.1 Formation of correlations

A first guess of the time-dependent formation of correlations can be found from the time-dependent Fermi golden rule

$$P_{nn'} = \frac{1}{\hbar^2} V_{nn'}^2 \left(\frac{\sin w_{nn'} \frac{t}{2}}{\omega_{nn'} \frac{1}{\hbar} \frac{t}{2}} \right)^2 = V(q)^2 \frac{1 - \cos \left(\frac{\Delta E t}{\hbar} \right)}{(\Delta E)^2} \tag{19.2}$$

expressing the transition probability between states n and n' which we consider as the state before and after the collision and $\Delta E = \epsilon_k + \epsilon_p - \epsilon'_{k+q} - \epsilon'_{p-q}$ denotes the energy difference between initial and final states. Taking the occupation factors into account, the time-dependent formation of kinetic energy is expected to have the form

$$E_{kin}(t) = \frac{1}{2} \int \frac{dk dp dq}{(2\pi \hbar)^9} V(q)^2 \frac{1 - \cos \left(\frac{\Delta E t}{\hbar} \right)}{\Delta E} \overset{\text{density}}{\rho_{k+q} \rho_{p-q} (1 - \rho_k) (1 - \rho_p)}. \tag{19.3}$$

Let us examine how this expected expression appears from kinetic theory.

19.1.1 Levinson equation

Though we have seen already how the Levinson equation (10.113) appears to let us shortly summarise the main steps, we substitute of the GKB ansatz (8.35) for $G^<$ into

the time diagonal part (9.76) of the Kadanoff and Baym equation (7.28). It is sufficient to restrict our attention to the Born approximation, $\mathcal{S}^{R,A} = V\delta(\tau)$ since over short times higher-order correlations have no time to build up as we will see later. The precursor of the Levinson equation for spatial homogeneous systems then reads

$$\frac{\partial}{\partial t}\rho(k, t) = \frac{2}{\hbar^2} \operatorname{Re} \int \frac{dpdq}{(2\pi\hbar)^6} V_q^2 \int_0^\infty d\tau S\left(t - \frac{\tau}{2}, \tau\right) D_{2p}(t - \tau). \quad (19.4)$$

All distributions are collected in

$$D_{2p}(t) = [1 - \rho_k(t)][1 - \rho_p(t)]\rho_{k-q}(t)\rho_{p+q}(t) - \rho_k(t)\rho_p(t)[1 - \rho_{k-q}(t)][1 - \rho_{p+q}(t)], \quad (19.5)$$

and all propagators are collected in

$$S(t, \tau) = g^R(k, t, \tau)g^R(p, t, \tau)g^A(k - q, t, -\tau)g^A(p + q, t, -\tau). \quad (19.6)$$

Within a simple approximation of the propagator, $[t_1 > t_3]$,

$$g^R(k, t_1, t_3) \approx -i \exp\left\{-i\frac{k^2}{2m\hbar}(t_1 - t_3) - \frac{t_1 - t_3}{2\tau}\right\}, \quad (19.7)$$

the final Levinson equation (Levinson, 1965, 1969) reads

$$\begin{aligned} \frac{\partial \rho_k(t)}{\partial t} = & \frac{2}{\hbar^2} \int_{t_0}^t d\bar{t} \int \frac{dpdq}{(2\pi\hbar)^6} |V(q)|^2 e^{\frac{i\bar{t}}{\tau}} \cos\left[\frac{\Delta E}{\hbar}(t - \bar{t})\right] \left\{ \rho_{k-q}(\bar{t})\rho_{p+q}(\bar{t}) [1 - \rho_k(\bar{t})] [1 - \rho_p(\bar{t})] \right. \\ & \left. - \rho_k(\bar{t})\rho_p(\bar{t}) [1 - \rho_{k-q}(\bar{t})] [1 - \rho_{p+q}(\bar{t})] \right\}, \end{aligned} \quad (19.8)$$

where t_0 denotes the time at which the interaction has been switched on and we abbreviate

$$\Delta E = \left(\frac{k^2}{2m} + \frac{p^2}{2m} - \frac{(k-q)^2}{2m} - \frac{(p+q)^2}{2m} \right). \quad (19.9)$$

The solution of the Levinson equation (19.8) in the short-time region $t \ll \tau$ can be written down analytically. In this time domain we can neglect the time evolution of distributions, $\bar{\rho}_a(\bar{t}) \approx \rho_a(0)$, and the life-time factor, $\exp\left\{-\frac{t-\bar{t}}{\tau}\right\} \approx 1$. Therefore the deviation of the Wigner distribution from its initial value, $\rho_a(t) = \rho_a(0) + \delta\rho_a(t)$, reads

$$\delta\rho_a(t) = 2 \sum_b \int \frac{dpdq}{(2\pi\hbar)^6} V_D^2(q) \frac{1 - \cos\{t\Delta E\}}{\Delta E^2} \left\{ \rho'_a \rho'_b (1 - \rho_a)(1 - \rho_b) - \rho_a \rho_b (1 - \rho'_a)(1 - \rho'_b) \right\}. \quad (19.10)$$

This formula shows how the two-particle and the single-particle concepts of the transient behaviour are combined in the kinetic equation. The right-hand side describes how two particles correlate their motion to avoid strong interaction regions. Since the process is very fast, the on-shell contribution to $\delta\rho_a$, proportional to t/τ , can be neglected in the assumed time domain and the $\delta\rho$ has the pure off-shell character as can be seen from the off-shell factor $(1 - \cos \{t\Delta E\})/\Delta E^2$. The off-shell character of mutual two-particle correlations is thus reflected in the single particle Wigner distribution. We refer to Eq. (19.10) as the *finite duration time* approximation. It carries the most important features of the build up of correlations after the interactions are switched on in the initially uncorrelated system. This we will demonstrate by some numerical examples.

Once formed, the off-shell contributions change in time with the characteristic time τ , i.e. following the relaxation (on-shell) processes in the system. Accordingly, the formation of the off-shell contribution signals that the system has reached the state where the further evolution can be described by the Boltzmann equation, i.e. the transient period has been accomplished. From the Wigner distribution (19.10) one can readily evaluate the increase of the kinetic energy,

$$E_{kin}(t) - E_{kin}^0 = \sum_a \int \frac{dk}{(2\pi\hbar)^3} \frac{k^2}{2m_a} \delta\rho_a(t). \quad (19.11)$$

After substitution $\delta\rho_a$ from (19.10) we symmetrize in k and p and anti-symmetrize in the initial and final states and obtain exactly the expected result (19.3), *compare also (A.16)*.

19.1.2 Formation of correlations in plasma

Starting with a sudden switching approximation, due to Coulomb interaction, the screening is formed during the first transient time period. This can be described by the non-Markovian Lenard–Balescu equation (Morawetz, 1994) instead of the static screened equation (19.8). With the same discussion as above but using the RPA approximation of Chapter 10.2.2 we end up instead of (19.3) with the dynamical expression of the correlation energy (for details, see (Morawetz, Špička and Lipavský, 1998),

$$E_{corr}^{dynam}(t) = - \sum_{ab} \int \frac{dkdpdq}{(2\pi\hbar)^9} \frac{V_C^2(q)}{|\epsilon^R(q, \frac{(p+q)^2}{2m_b} - \frac{p^2}{2m_b})|^2} \times \frac{1 - \cos \left\{ \frac{1}{\hbar} t \Delta E \right\}}{\Delta E^2} \left(\frac{(k-q)^2}{2m_a} - \frac{k^2}{2m_a} \right) \rho'_a \rho'_b (1 - \rho_a)(1 - \rho_b) \quad (19.12)$$

with the potential screened by the dielectric function ϵ^R . To demonstrate its results and limitations, we discuss (19.3) and (19.12) for equilibrium initial distributions. We assume a one-component plasma which possesses the Maxwellian velocity distribution during this formation time. From (19.12) we find analytically (Morawetz, Špička and Lipavský, 1998) the quantum result of the time derivative of the formation of the

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