Chapter 25
Nonlocal Quantum Kinetic Theory and the Formation of Correlations

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Abstract The quantum version of the Boltzmann equation remains still the basis of modern transport theories. Extensions become necessary for transient-time effects like the femtosecond response and for strongly correlated systems. At short time scales higher correlations have no time to develop yet and femto-second laser excitation of collective modes in semiconductors as well as quenches of cold atoms in optical lattices can be described even analytically by fluctuations of the meanfield. For plasma systems exposed to a sudden switching, analytical results are available from the time-dependent Fermi's Golden Rule in good agreement with the results of two-time Green's functions solving the Kadanoff and Baym equation. At later times when correlations develop, a kinetic equation of nonlocal and non-instantaneous character unifies the achievements of the transport in dense quantum gases with the Landau theory of quasiclassical transport in Fermi systems. The numerical solution is not more expensive than solving the Boltzmann equation since large cancellations in the off-shell motion appear which are hidden usually in non-Markovian behaviors. The quasiparticle drift of Landau's equation is connected with a dissipation governed by a nonlocal and non-instant scattering integral in the spirit of Enskog corrections. These corrections are expressed in terms of shifts in space and time that characterize non-locality of the scattering process. In this way quantum transport is possible to recast into a quasi-classical picture. The balance equations for the density, momentum, energy and entropy include besides quasiparticle also the correlated two-particle contributions beyond the Landau theory. The medium effects on binary collisions are shown to mediate the latent heat, i.e., an energy conversion between correlation and thermal energy.

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G. G. N. Angilella and C. Amovilli (eds.), *Many-body Approaches at Different Scales*, https://doi.org/10.1007/978-3-319-72374-7_25

25.1 Introduction

Cold atoms in optical traps [1] and the femtosecond pump and probe experiments [2, 3] allow now to resolve the time-dependent formation of correlations. This has triggered an enormous theoretical activity [4]. Both different physical systems, the long-range Coulomb [5] as well as short-range Hubbard systems can be described by a common theoretical approach leading to a unique formula to describe the formation of correlations at short-time scale [6]. The basic observation here is that correlations need time to be formed such that the meanfield approximation is sufficient to describe the basic features of short-time formation of correlations. Calculating nonequilibrium Green's functions [7, 8] allows one to describe the formation of collective modes [3, 9], screening [7] and even exciton population inversions [10].

This becomes different at later times when essentially strong correlations are formed after a sudden quench. Here, the time-dependent description is covered by various kinetic equation approaches. It started with the foundation of Ludwig Boltzmann's famous equation [11] and has been rapidly developed, from important classical contributions [12–16] to quantum extensions, where the pioneering work along these lines was performed by [17, 18]. In the theory of condensed systems covered by the Landau concept of quasiparticles [19], the quantum Boltzmann-Uhling-Uhlenbeck (BUU) equation, differs from the classical one in the collision term, which takes into account that the final scattering states can be occupied and consequently blocked by the Pauli exclusion principle. Moreover, the quantum mechanical transition rate, rather than the classical one is used. The scattering integral of the Boltzmann equation remains still local in space and time. In other words, the Landau theory does not include a quantum mechanical analogy of virial corrections studied in the theory of gases.

To extend the validity of the Boltzmann equation to moderately dense gases, Clausius and Boltzmann included the space non-locality of binary collisions (cf. Chapter 16 in Ref. [20]). After one century, virial corrections won new interest as they can be incorporated into Monte Carlo simulation methods [21]. The microscopic theory of nonlocal corrections to the collision integral has been pioneered within the theory of gases by many authors [22–38].

In the limit of small scattering rates, the transport equation for the Green's function is converted into the kinetic equation of Boltzmann type by the extended quasiparticle approximation corresponding to the $\rho[f]$ functional. The resulting quantum kinetic theory unifies the achievements of transport in dense gases with the quantum transport of dense Fermi systems [39–43]. The quasiparticle drift of Landau's equation is connected with a dissipation governed by a nonlocal and non-instant scattering integral in the spirit of Enskog corrections. These corrections are expressed in terms of shifts in space and time that characterize the non-locality of the scattering process [44]. In this way quantum transport is possible to recast into a quasiclassical picture suited for simulations. The balance equations for the density, momentum, energy and entropy include quasiparticle contributions and the correlated two-particle contributions beyond the Landau theory as we will demonstrate in Sect. 25.3.2.

First we will discuss the transient time regime where the correlations are formed after a sudden quench with applications to femtosecond pumb and probe as well as cold atom experiments. Then we present the nonlocal kinetic theory in Sect. 25.3, which results from cancellation of off-shell parts by a proper extended quasiparticle picture. Two applications from nuclear and superconducting physics finally illustrate the usefullness of the concept in Sect. 25.4.

25.2 Formation of Correlations

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

$$P_{nn'} = \frac{1}{\hbar^2} V_{nn'}^2 \left(\frac{\sin \omega_{nn'} \frac{t}{2}}{\omega_{nn'} \frac{t}{2}} \right)^2 = 2V(q)^2 \frac{1 - \cos\left(\Delta E \frac{t}{\hbar}\right)}{(\Delta E t)^2} \tag{25.1}$$

expressing the transition probability between states n and n' which we consider as the state before and after the collision, and $\Delta E = \varepsilon_k + \varepsilon_p - \varepsilon'_{k+q} - \varepsilon'_{p-q}$ 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

$$E_{\rm kin}(t) = \int \frac{dkdpdq}{(2\pi\hbar)^9} V(q)^2 \frac{1 - \cos\left(\Delta E \frac{t}{\hbar}\right)}{\Delta E} \rho_{k+q} \rho_{p-q} (1 - \rho_k)(1 - \rho_p). \tag{25.2}$$

Exactly this expression is obtained if we use the Levinson equation [45] (with $\hbar = 1$)

$$\begin{aligned} \frac{\partial \rho_k(t)}{\partial t} &= 2 \int_0^{t-t_0} d\bar{t} \int \frac{dpdq}{(2\pi)^6} |V(q)|^2 e^{-\frac{\bar{t}}{\tau}} \cos\left[\Delta E \bar{t}\right] \\ &\times \left\{ \rho_{k-q} \rho_{p+q} \left[1 - \rho_k\right] \left[1 - \rho_p\right] - \rho_k \rho_p \left[1 - \rho_{k-q}\right] \left[1 - \rho_{p+q}\right] \right\}_{t-\bar{t}}, \end{aligned} \tag{25.3}$$

and neglect the memory in the distribution functions (finite duration approximation). This memory over-counts correlations [43] resulting into too much off-shell correlations [46].

The solution of the Levinson equation (25.3) in the short-time region $t \ll \tau$ can be written down analytically. It shows how the two-particle and the single-particle concept of the transient behavior is combined in the kinetic equation. The right-hand side of Eq. (25.3) describes how two particles correlate their motion to avoid strong interaction regions. Since the process is very fast, the on-shell contribution to $\delta\rho_k$, 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 $\sin(t\Delta E)/\Delta E$.

The off-shell character of mutual two-particle correlations is thus reflected in the single-particle Wigner distribution.

Starting with a sudden switching approximation, due to Coulomb interaction the screening is formed during the first transient time period and one finds analytically [47] the quantum result of the time derivative of the formation of correlation for statically as well as dynamically screened potentials

$$\frac{\partial}{\partial t}\frac{E^{\rm static}_{\rm corr}(t)}{n} = -\frac{e^2\kappa T}{2\hbar}\,{\rm Im}\left[(1+2z^2)e^{z^2}(1-{\rm erf}(z)) - \frac{2z}{\sqrt{\pi}}\right] \tag{25.4a}$$

$$\frac{\partial}{\partial t}\frac{E^{\rm dynam}_{\rm corr}(t)}{n} = -\frac{e^2\kappa T}{\hbar}\,{\rm Im}\left[e^{z_1^2}(1-{\rm erf}(z_1))\right], \tag{25.4b}$$

where $z = \omega_p\sqrt{t^2 - it\frac{\hbar}{T}}$ and $z_1 = \omega_p\sqrt{2t^2 - it\frac{\hbar}{T}}$. In Fig. 25.1 these formulas are compared with molecular dynamic simulations [48] in plasmas with $\Gamma = \frac{e^2}{a_e T} = 1$ and the Wigner-Seitz radius a_e.

The characteristic time of formation of correlations in the high temperature limit is the time of the inverse plasma frequency $\tau_c \approx \frac{1}{\omega_p} = \sqrt{2}/v_{\rm th}\kappa$, indicating that the dominant role is played by long range fluctuations. On the other hand, we also see that the correlation time is found to be given by the time a particle needs to travel through the range of the potential with a thermal velocity $v_{\rm th}$ and is not given by the time between successive collisions as one might have thought. For dense Fermi systems, like nuclear matter, one finds the build-up time where the correlation energy reaches its first maximum as the inverse Fermi energy $\tau_c = \hbar/\varepsilon_f$, in agreement with the quasiparticle formation time known as Landau's criterion. Indeed, the quasiparticle formation and the build up of correlations are two alternative views of the same phenomenon.

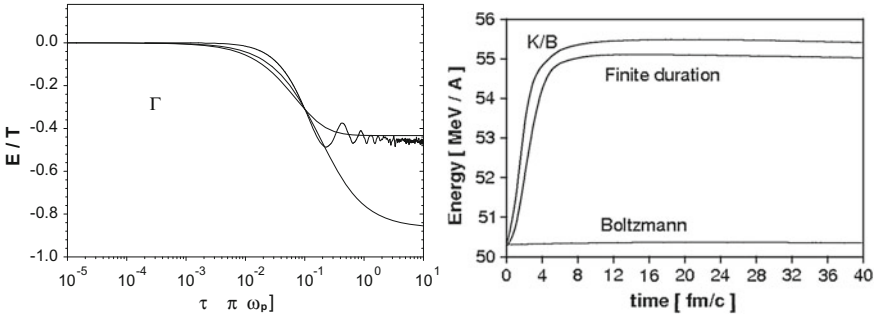

Fig. 25.1 (*Left*) The formation of correlation energy due to molecular dynamic simulations [48] together with the statically screened result of Eq. (25.4a) (curve below) and the dynamically screened result (curve above) of Eq. (25.4b) for a plasma, and (*Right*) a counter-flowing streams of nuclear matter [49] from a solution of the Kadanoff-Baym equation (KB) together with the results from the finite duration approximation and the Boltzmann equation

25.2.1 Quantum Quenches and Sudden Switching

Special preparation of cold atoms in optical lattices allows to study the local relaxation [1, 50] and to explore dissipation mechanisms [51]. We consider the time evolution of the reduced density matrix $\langle p+\frac{1}{2}q|\delta\rho|p-\frac{1}{2}q\rangle = \delta f(p,q,t)$ which is given by linearization $\delta[H,\rho] = [\delta H,\rho_0]+[H_0,\delta\rho]$ of the kinetic equation

$$\dot{\rho} + i[H,\rho] = \frac{\rho^{\text{l.e.}}-\rho}{\tau} \tag{25.5}$$

with respect to an external perturbation δV^{ext}. The effective Hamiltonian consists of the quasiparticle energy, the external and induced mean-field $\langle p+\frac{1}{2}q|\delta H|p-\frac{1}{2}q\rangle = \delta V^{\text{ext}} + V_q\delta n_q$ given by the interaction potential V_q and the density variation δn_q. As possible confining potential we assume a harmonic trap $V^{\text{trap}} = \frac{1}{2}Kx^2$, which leads to $\langle p+\frac{1}{2}q|\delta[V^{\text{trap}},\rho]|p-\frac{1}{2}q\rangle = -K\partial_p\partial_q\delta f(p,q,t)$.

The kinetic equation (25.5) is assumed to relax towards a local equilibrium of Fermi/Bose distribution with an allowed variation of the chemical potential

$$\begin{aligned}\left\langle p+\frac{q}{2}\right|\rho^{\text{l.e.}}-\rho\left|p-\frac{q}{2}\right\rangle &= \langle\rho^{\text{l.e.}}-\rho^0\rangle - \delta f(p,q,t)\\ &= -\frac{\Delta f}{\Delta\varepsilon}\delta\mu(q,t)-\delta f(p,q,t).\end{aligned} \tag{25.6}$$

Here, we use the short-hand notation $\Delta f = f_0(p+\frac{q}{2})-f_0(p-\frac{q}{2})$ and $\Delta\varepsilon = \varepsilon_{p+\frac{q}{2}}-\varepsilon_{p-\frac{q}{2}}$. This variation of the chemical potential allows to enforce the density conservation $n=\sum_p f=\sum_p f^{\text{l.e.}}$ [52–54] leading to the Mermin correction, i.e. a relation between density variation $\delta n(q,t)=\tilde{\Pi}(t,\omega=0)\delta\mu(q,t)$ and the polarization in random phase approximation (RPA)

$$\Pi(t,t') = i\sum_p [f_{p+\frac{q}{2}}(t')-f_{p-\frac{q}{2}}(t')]e^{\left(i\varepsilon_{p+\frac{q}{2}}-i\varepsilon_{p-\frac{q}{2}}+\frac{1}{\tau}\right)(t'-t)}, \tag{25.7a}$$

$$\tilde{\Pi}(t,\omega) = \int d(t-t')e^{i\omega(t-t')}\Pi(t,t'). \tag{25.7b}$$

The linearized kinetic equation (25.5) is solved considering the momentum derivatives of the last term as perturbation to obtain [6]

$$\begin{aligned}\delta f(p,q,t)-\delta f(p,q,0) = i\int_{t_0}^{t} dt' e^{\left[\left(i\Delta\varepsilon+\frac{1}{\tau}\right)(t'-t)\right]}\Big\{&\Delta f(t')\left[V_q\delta n(q,t')+V_q^{\text{ext}}(t')\right]\\ &+\frac{1}{i\tau\tilde{\Pi}(t',0)}\frac{\Delta f(t')}{\Delta\varepsilon}\delta n(q,t')+K\partial_p\partial_q\delta f(p,q,t')\Big\}.\end{aligned} \tag{25.8}$$

In case of a sudden quench the interaction is switched on suddenly and no external perturbation will be assumed $\delta V^{\rm ext} = 0$. Let us consider the time evolution of an empty place in the lattice if each second place was initially populated. The density $n_t = \frac{n}{2} + \delta n_t$ starts with $n_0 = 0$, which means $\delta n_0 = -n/2$ as initial condition. The solution without a confining trap ($K = 0$) reads

$$\delta n_s = -\frac{n}{2} \frac{(s+\frac{1}{\tau})^2 + b^2}{\sqrt{(s+\frac{1}{\tau})^2 + 4Jb(s^2 + \frac{s}{\tau} + nbV_q + b^2)}} \circ\!\!-\!\!\bullet \tag{25.9a}$$

$$\delta n_t = -\frac{n}{2} J_0(\sqrt{4Jbt}) e^{-\frac{t}{\tau}} - \frac{n}{4\gamma\tau^2} \int_0^t dx\, J_0(\sqrt{4Jbx}) e^{-\frac{t+x}{2\tau}} \times \left(2\gamma\tau \cos\gamma(t-x) + (1 - 2bnV_q\tau^2) \sin\gamma(t-x)\right), \tag{25.9b}$$

where $\gamma^2 = nbV + b^2 - 1/4\tau^2$, and J_0 the Bessel function. Besides the interaction-free result we obtain an additional contribution due to the interaction and dissipation presented by the relaxation time. Without interaction, $V = 0$, and damping $1/\tau \to 0$, we obtain the exact result of [50].

In Fig. 25.2 we compare Eq. (25.9) with the experimental data [1] where we plot the interaction free evolution together with the interaction one. The main effect of

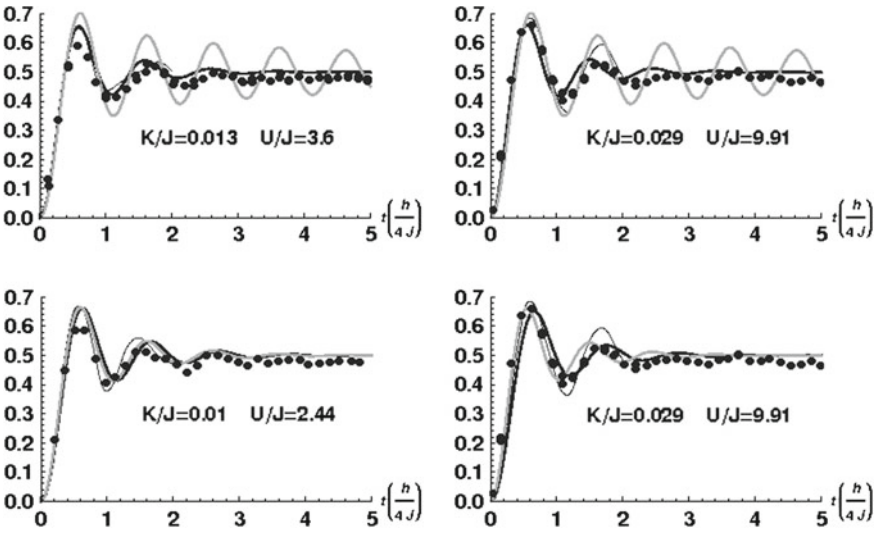

Fig. 25.2 Comparison of the experimental data of [1] (dots) with the RG calculation (thin line) [50] from [6]. Left: Mermin's correction of conserving relaxation time $\tau = 0.6\hbar/J$ approximation, Eq. (25.9), without (gray) and with interaction (black). Right: With (black) and without (gray) the influence of the trapping potential K/J

interaction is the damping which brings the curves nearer to the experimental data. Here, we use the parameter for the lattice constant given by half of the short laser wavelength $a = \lambda/2 = 765$ nm, which provides a wave vector of $q = \pi\hbar/a$, and an initial density $n = 1/2a$ with each second place filled. The relaxation time characterizes dissipative processes which we assume to arise due to polaron scattering. These lattice deformation processes are dominated by hopping transport at high temperatures and band regime transport at low temperature with the transition given by $\hbar/\tau = 2J \exp(-S)$, where S describes the ratio of polaron binding to optical phonon energy. This quantity is generally difficult to calculate [55] but in the order of one. We will use it as fit parameter and find a common value $\tau = 0.6\hbar/J$ for the results in the figures presented here. We see that the analytic result, Eq. (25.9), describes the data slightly better and we can give the time evolution up to more oscillations than it was possible by numerical renormalization group techniques.

25.2.2 Femtosecond Laser Response

Now we are interested in the short-time response of the system to an external perturbation V^{ext}. This is different from sudden quench since here we have initially $\delta f(p, q, 0) = 0$ and the system is driven out of equilibrium by V^{ext}. As the result we will obtain the dielectric response which gives microscopic access to optical properties. Integrating Eq. (25.8) over momentum one obtains the time-dependent density response

$$\delta n(q,t) = \int_{t_0}^{t} dt' \chi(t,t') V_q^{\text{ext}}(t') \tag{25.10}$$

describing the response of the system with respect to the external field in contrast to the polarization function, Eq. (25.7), which is the response to the induced field. One obtains the equation for $\chi(t,t')$ from Eq. (25.10) by interchanging integrations in Eq. (25.8)

$$\chi(t,t') = \Pi(t,t') + \int_{t'}^{t} d\bar{t} \left\{ \left[\Pi(t,\bar{t}) V_q + I(t,\bar{t}) \right] \chi(\bar{t},t') + R(t,\bar{t}) \right\}, \tag{25.11}$$

with the polarization Eq. (25.7) and Mermin's correction

$$I(t,t') = \sum_p \frac{f_{p+\frac{q}{2}}(t') - f_{p-\frac{q}{2}}(t')}{\varepsilon_{p+\frac{q}{2}} - \varepsilon_{p-\frac{q}{2}}} \frac{e^{\left(i\varepsilon_{p+\frac{q}{2}} - i\varepsilon_{p-\frac{q}{2}} + \frac{1}{\tau}\right)(t'-t)}}{\tau \tilde{\Pi}^{\text{RPA}}(t',0)}. \tag{25.12}$$

For cold atoms on the lattice we have obtained already the solution, Eq. (25.8), which we can use here with $\delta f(0) = 0$ and we have also

$$\Pi(t,t') = ne^{\frac{t'-t}{\tau}} \sin[b(t'-t)], \tag{25.13a}$$

$$I(t,t') = \frac{1}{\tau} e^{\frac{t'-t}{\tau}} \cos[b(t'-t)]. \tag{25.13b}$$

This will lead to the same response formula as a gas of particles with the thermal Fermi/Bose distribution for f_p. For the latter one we work in the limit of long wave lengths $q \to 0$ and the leading terms are $\Pi(t,t') \approx \frac{q^2 n(t')}{m}(t'-t)e^{(t'-t)/\tau}$ and $I(t,t') \approx \frac{1}{\tau} e^{(t'-t)/\tau}$, with the time-dependent density $n(t)$.

We introduce the collective mode of plasma/sound-velocity oscillations for Coulomb gas and for the Hubbard models respectively

$$\omega_p^2 = \begin{cases} \frac{ne^2}{m\varepsilon_0} & \text{for } V_q = \frac{e^2\hbar^2}{\varepsilon_0 q^2}, \varepsilon_p = \frac{p^2}{2m}, \\ bnaU & \text{for } V_q = Ua, \varepsilon_p = 2J(1-\cos\frac{pa}{\hbar}), \end{cases} \tag{25.14}$$

where we have used already $b = 4J\sin^2\frac{aq}{2\hbar}$. For Coulomb interactions one has an optical mode while for atoms on the lattice the mode is acoustic.

For the gas of particles it is convenient to transform Eq. (25.11) into a differential equation

$$\ddot{\chi}(tt') + \frac{1}{\tau}\dot{\chi}(tt') + \omega_p^2 \chi(tt') = 0 \tag{25.15a}$$

$$\chi(t,t) = 0, \quad \dot{\chi}(t,t')|_{t=t'} = -\omega_p^2/V_q, \tag{25.15b}$$

where the influence of the trap can be considered as well [6].

Interestingly, both solutions, the one for the Hubbard lattice and the one for the gas of particles, lead to the same result of the integral equation (25.11) via Eq. (25.15) for the two-time response function

$$V\chi(t,t') = -\frac{\omega_p^2}{\gamma} e^{-\frac{t-t'}{2\tau}} \sin\gamma(t-t'), \tag{25.16}$$

but with a different collective mode $\gamma = \sqrt{\omega_p^2 - \frac{1}{4\tau^2}}$ for the Coulomb gas, and $\gamma = \sqrt{\omega_p^2 + b^2 - \frac{1}{4\tau^2}}$ for cold atoms. In this sense, we consider Eq. (25.16) as universal short-time behavior.

The pump pulse is creating charge carriers in the conduction band and the probe pulse is testing the time evolution of this occupation [3]. The time delay after this probe pulse $T = t - t_0$ is Fourier transformed into frequency. The inverse dielectric function is then given by

$$\frac{1}{\varepsilon(\omega,t)} = 1 + \int_0^{t-t_0} dT e^{i\omega T} V\chi(t, t-T). \tag{25.17}$$

The integral in Eq. (25.17) with Eq. (25.16) describes the experimental time formation of plasma mode quite accurately [6]. The virtue of Eq. (25.17) is also that the long-time limit yields correctly the Drude formula

$$\lim_{t\to\infty}\frac{1}{\varepsilon}=1-\frac{\omega_p^2}{\gamma^2-\omega(\omega+\frac{i}{\tau})}, \tag{25.18}$$

leading to the Drude conductivity which is not easy to achieve within short-time expansions [56], and which had provided the wrong long-time limit $1-\omega_p^2/[\gamma^2-(\omega+i/\tau)^2]$ before.

25.3 Nonlocal Kinetic Theory

At later times, when correlations develop, the off-shell motion can be eliminated from the kinetic equation, which requires to introduce an effective distribution (the quasiparticle distribution f) from which the Wigner distribution ρ can be constructed

$$\rho[f]=f+\wp\int\frac{d\omega}{2\pi}\frac{1}{\omega-\varepsilon}\frac{\partial}{\partial\omega}\left((1-f)\sigma_\omega^<-f\sigma_\omega^>\right). \tag{25.19}$$

Here, $\sigma^>$ and $\sigma^<$ denote the self-energies describing all correlations and ε is the quasiparticle energy. This relation represents the extended quasiparticle picture derived for small scattering rates [41–43, 57]. The limit of small scattering rates has been first introduced by Craig [58]. An inverse relation $f[\rho]$ has been constructed [59]. For equilibrium non-ideal plasmas this approximation has been employed by [60, 61] and has been used under the name of the generalized Beth-Uhlenbeck approach by [62] in nuclear matter for studies of the correlated density. The authors in Ref. [63] have used this approximation with the name 'extended quasiparticle approximation' for the study of the mean removal energy and high-momenta tails of Wigner's distribution. The non-equilibrium form has been derived finally as the modified Kadanoff and Baym ansatz [64].

This extended quasiparticle picture leads to balance equations which include explicit correlation parts analogous to the virial corrections. The firmly established concept of the equilibrium virial expansion has been extended to nonequilibrium systems [42] although a number of attempts have been made to modify the Boltzmann equation so that its equilibrium limit would cover at least the second virial coefficient [24, 65, 66]. The corrections to the Boltzmann equation have the form of gradients or nonlocal contributions to the scattering integral. Please note that the nature of two-particle correlations induces gradients and therefore nonlocal kinetic and exchange energies [67, 68].

25.3.1 Nonlocal Kinetic Equation

The nonlocal quantum kinetic equation following from the extended quasiparticle approximation reads [42]

$$\frac{\partial f_1}{\partial t}+\frac{\partial \varepsilon_1}{\partial \mathbf{k}}\frac{\partial f_1}{\partial \mathbf{r}}-\frac{\partial \varepsilon_1}{\partial \mathbf{r}}\frac{\partial f_1}{\partial \mathbf{k}}=I_1^{\rm in}-I_1^{\rm out} \tag{25.20}$$

with the scattering-in

$$\begin{aligned} I_1^{\rm in}=\sum_b\int\frac{d^3p}{(2\pi)^3}\frac{d^3q}{(2\pi)^3}2\pi\delta\left(\varepsilon_1+\bar\varepsilon_2-\bar\varepsilon_3-\bar\varepsilon_4-2\Delta_E\right)\\ \times\left(1-\frac{1}{2}\frac{\partial\boldsymbol{\Delta}_2}{\partial\mathbf{r}}-\frac{\partial\bar\varepsilon_2}{\partial\mathbf{r}}\frac{\partial\boldsymbol{\Delta}_2}{\partial\omega}\right)_{\omega=\varepsilon_1+\bar\varepsilon_2}(1-f_1-\bar f_2)\bar f_3\bar f_4\\ \times\left|t_{\rm SC}\left(\varepsilon_1+\bar\varepsilon_2-\Delta_E,\mathbf{k}-\frac{\boldsymbol{\Delta}_K}{2},\mathbf{p}-\frac{\boldsymbol{\Delta}_K}{2},\mathbf{q},\mathbf{r}-\boldsymbol{\Delta}_r,t-\frac{\Delta_t}{2}\right)\right|^2, \end{aligned} \tag{25.21}$$

and the scattering-out by replacing $f\leftrightarrow 1-f$ and changing the sings of the shifts. All distribution functions and observables have the arguments

$$\varepsilon_1\equiv\varepsilon_a(\mathbf{k},\mathbf{r},t), \tag{25.22a}$$
$$\varepsilon_2\equiv\varepsilon_b(\mathbf{p},\mathbf{r}+\boldsymbol{\Delta}_2,t), \tag{25.22b}$$
$$\varepsilon_3\equiv\varepsilon_a(\mathbf{k}-\mathbf{q}+\boldsymbol{\Delta}_K,\mathbf{r}+\boldsymbol{\Delta}_3,t+\Delta_t), \tag{25.22c}$$
$$\varepsilon_4\equiv\varepsilon_b(\mathbf{p}+\mathbf{q}+\boldsymbol{\Delta}_K,\mathbf{r}+\boldsymbol{\Delta}_4,t+\Delta_t) \tag{25.22d}$$

and a bar indicates the reversed sign of the Δ's.

In the scattering-out (scattering-in is analogous) one can see the distributions of quasiparticles f_1f_2 describing the probability of a given initial state for the binary collision. The hole distributions giving the probability that the requested final states are empty and the particle distribution of stimulated collisions combine together in the final state occupation factors like $1-f_3-f_4=(1-f_3)(1-f_4)+f_3f_4$. The scattering rate covers the energy-conserving δ-function, and the differential cross section is given by the modulus of the T-matrix, $|t_{\rm SC}|$, reduced by the wave-function renormalizations $z_1\bar z_2\bar z_3\bar z_4$ [69]. We consider here the linear expansion in small scattering rates, therefore the wave-function renormalization in the collision integral is of higher order.

All Δ's are derivatives of the scattering phase shift ϕ,

$$t_{\rm SC}^R=|t_{\rm SC}|\,e^{i\phi}, \tag{25.23}$$

according to the following list

$$\boldsymbol{\Delta}_K = \frac{1}{2}\frac{\partial\phi}{\partial\mathbf{r}}, \tag{25.24a}$$

$$\Delta_E = -\frac{1}{2}\frac{\partial\phi}{\partial t}, \tag{25.24b}$$

$$\Delta_t = \frac{\partial\phi}{\partial\omega}, \tag{25.24c}$$

$$\boldsymbol{\Delta}_2 = \frac{\partial\phi}{\partial\mathbf{p}} - \frac{\partial\phi}{\partial\mathbf{q}} - \frac{\partial\phi}{\partial\mathbf{k}}, \tag{25.24d}$$

$$\boldsymbol{\Delta}_3 = -\frac{\partial\phi}{\partial\mathbf{k}}, \tag{25.24e}$$

$$\boldsymbol{\Delta}_4 = -\frac{\partial\phi}{\partial\mathbf{q}} - \frac{\partial\phi}{\partial\mathbf{k}}, \tag{25.24f}$$

$$\boldsymbol{\Delta}_r = \frac{1}{4}\left(\boldsymbol{\Delta}_2 + \boldsymbol{\Delta}_3 + \boldsymbol{\Delta}_4\right). \tag{25.24g}$$

As special limits, this kinetic theory includes the Landau theory as well as the Beth-Uhlenbeck equation of state [70, 71], which means correlated pairs. The medium effects on binary collisions are shown to mediate the latent heat which is the energy conversion between correlation and thermal energy [42, 72]. In this respect the seemingly contradiction between particle-hole symmetry and time reversal symmetry in the collision integral was solved [73]. Compared to the Boltzmann-equation, the presented form of virial corrections only slightly increases the numerical demands in implementations [74–77] since large cancellations in the off-shell motion appear which are hidden usually in non-Markovian behaviors. Details how to implement the nonlocal kinetic equation into existing Boltzmann codes can be found in [77].

25.3.2 Balance Equations

We multiply the kinetic equation (25.20) with a variable $\xi_1 = 1, \mathbf{k}, \varepsilon_1, -k_\mathrm{B}\ln[f_1/(1-f_1)]$ and integrate over momentum. It results in the equation of continuity, the Navier-Stokes equation, the energy balance and the evolution of the entropy, respectively. All these conservation laws or balance equations for the mean thermodynamic observables have the form

$$\frac{\partial\langle\xi^{\mathrm{qp}} + \xi^{\mathrm{mol}}\rangle}{\partial t} + \frac{\partial(\mathbf{j}_\xi^{\mathrm{qp}} + \mathbf{j}_\xi^{\mathrm{mol}})}{\partial\mathbf{r}} = \mathscr{I}_{\mathrm{gain}}, \tag{25.25}$$

consisting of a quasiparticle part

$$\xi^{\rm qp} = \int \frac{d^3k}{(2\pi)^3} \xi_1 f_1 \tag{25.26}$$

and the correlated or molecular contribution

$$\xi^{\rm mol} = \int \frac{d^3k d^3p d^3q}{(2\pi)^9} |t_{\rm SC}(\varepsilon_1+\varepsilon_2,k,p,q)|^2 \Delta \frac{\xi_1+\xi_2}{2} \times 2\pi\delta(\varepsilon_1+\varepsilon_2-\varepsilon_3-\varepsilon_4) f_1 f_2 (1-f_3-f_4). \tag{25.27}$$

The latter one has the statistical interpretation of the rate of binary processes $D = |t_{\rm SC}|^2\, 2\pi\delta(\varepsilon_1+\varepsilon_2-\varepsilon_3-\varepsilon_4)\,(1-f_3-f_4)\,f_1 f_2$ weighed with the lifetime of the molecule Δ_t, respectively. This has the form of a molecular contribution as if two particles form a molecule.

The quasiparticle currents of the observable reads

$$\mathbf{j}_\xi^{\rm qp} = \int \frac{d^3k}{(2\pi)^3} \xi_1 \frac{\partial \varepsilon_1}{\partial \mathbf{k}} f_1, \tag{25.28}$$

and the molecular currents we have obtained as [78]

$$\mathbf{j}_\xi^{\rm mol} = \frac{1}{2} \int \frac{d^3k d^3p d^3q}{(2\pi)^9} D(\xi_2 \boldsymbol{\Delta}_2 - \xi_3 \boldsymbol{\Delta}_3 - \xi_4 \boldsymbol{\Delta}_4). \tag{25.29}$$

It is the balance of observables carried by the different spatial off-sets.

The additional gain on the right side might be due to an energy or force feed from the outside or the entropy production by collisions.

Due to its intriguing vector character, let us give the Navier-Stokes equation explicitly. The inertial force density is given by the time derivative of the momentum density $\mathscr{Q}$. The deformation force density is given by the divergence of the stress tensor. The stress tensor we derived from the balance between the inertial and the deformation forces

$$\frac{\partial}{\partial t}\left(\mathscr{Q}_j^{\rm qp} + \mathscr{Q}_j^{\rm mol}\right) = -\sum_i \frac{\partial}{\partial r_i}\left(\mathscr{J}_{ij}^{\rm qp} + \mathscr{J}_{ij}^{\rm mol}\right) \tag{25.30}$$

with the momentum density consisting of the quasiparticle

$$\mathscr{Q}_j^{\rm qp} = \int \frac{d^3k}{(2\pi)^3} k_j f_1 \tag{25.31}$$

and molecular part

$$\mathscr{Q}_j^{\rm mol} = \frac{1}{2}\int \frac{d^3k d^3p d^3q}{(2\pi)^9}(k_j + p_j) D\Delta_t, \tag{25.32}$$

which gives the mean momentum carried by a molecule formed with the rate D and lifetime Δ_t.

The total stress tensor formed by the quasiparticles reads

$$\mathscr{J}_{ij}^{\rm qp} = \sum_a \int \frac{d^3k}{(2\pi)^3}\left(k_j \frac{\partial \varepsilon}{\partial k_i} + \delta_{ij}\varepsilon\right) f - \delta_{ij}\mathscr{E}^{\rm qp} \tag{25.33}$$

with quasiparticle energy functional [42]

$$\mathscr{E}^{\rm qp} = \sum_a \int \frac{d^3k}{(2\pi)^3} f_a(k)\frac{k^2}{2m} + \frac{1}{2}\sum_{ab}\int \frac{d^3k d^3p}{(2\pi)^6} f_a(k) f_b(p)\,{\rm Re}\, t_{\rm SC}(\varepsilon_1 + \varepsilon_2, k, p, 0) \tag{25.34}$$

instead of the Landau functional which is valid only in local approximation.

The collision-flux contribution, Eq. (25.29), reads

$$\mathscr{J}_{ij}^{\rm mol} = \frac{1}{2}\sum_{ab}\int \frac{d^3k\, d^3p\, d^3q}{(2\pi)^9} D\left[(k_j - q_j)\Delta_{3i} + (p_j + q_j)\Delta_{4i} - p_j\Delta_{2i}\right]. \tag{25.35}$$

It possesses a statistical interpretation as well. The two-particle state is characterized by the initial momenta $\mathbf{k}$ and $\mathbf{p}$ and the transferred momentum $\mathbf{q}$. The momentum tensor is the balance of the momenta carried by the corresponding spatial off-sets weighted with the rate to form a molecule D.

For the density $\xi = 1$ we do not have a gain. For momentum gain $\xi = k_j$ we get

$$\mathscr{F}_j^{\rm gain} = \sum_{ab}\int \frac{d^3k\, d^3p\, d^3q}{(2\pi)^9} D\Delta_{Kj}. \tag{25.36}$$

Dividing and multiplying by Δ_t under the integral, we see that the momentum gain is the probability $D\Delta_t$ to form a molecule multiplied by the force $\boldsymbol{\Delta}_K/\Delta_t$ exercised during the delay time Δ_t from the environment by all other particles. This momentum gain, Eq. (25.36), can be exactly recast together with the term of the drift into a spatial derivative [42]

$$\sum_a \int \frac{d^3k}{(2\pi)^3}\varepsilon\frac{\partial f}{\partial \mathbf{r}_j} + \mathscr{F}_j^{\rm gain} = \frac{\partial \mathscr{E}^{\rm qp}}{\partial \mathbf{r}_j} \tag{25.37}$$

of the quasiparticle energy functional, Eq. (25.34). Similarly, the energy gain combines with the drift into the total time derivative of the quasiparticle energy functional, Eq. (25.34)

$$\sum_a \int \frac{d^3k}{(2\pi)^3} \varepsilon \frac{\partial f}{\partial t} - \mathscr{I}^E_{\rm gain} = \frac{\partial \mathscr{E}^{\rm qp}}{\partial t}. \tag{25.38}$$

The only remaining explicit gain is the entropy gain

$$\mathscr{I}^S_{\rm gain} = -\frac{k_B}{2} \sum_{ab} \int \frac{d^3k\, d^3p\, d^3q}{(2\pi)^9} f_1 f_2 (1 - f_3 - f_4) \times 2\pi \delta(\varepsilon_1 + \varepsilon_2 - \varepsilon_3 - \varepsilon_4) |t_{\rm SC}|^2 \ln \frac{f_3 f_4 (1 - f_1)(1 - f_2)}{(1 - f_3)(1 - f_4) f_1 f_2}, \tag{25.39}$$

while the momentum gain and energy gain are transferring kinetic into correlation parts and do not appear explicitly. In Ref. [79] it is proved that this entropy gain is always positive establishing the H-theorem including single particle and two-particle quantum correlations.

25.4 Applications of Nonlocal Kinetic Theory

25.4.1 Low-Energy Heavy Ion Reactions

During a heavy ion collision we can access a state of matter which gives insight into special aspects of nonequilibrium processes. The dominant features are that we have strong short range interactions of typically 1 fm $= 10^{-15}$ m and the product of the range of interaction with Fermi momentum is in orders of one characteristic for a degenerate quantum system. Since the radius of typical nuclei is $R \approx 1.2A^{1/3}$ fm (where A is the nucleus baryon number) we see that the product of the radius with Fermi momentum is of few $\hbar$ indicating strong spatial inhomogeneity.

Numerical simulations extensively used to interpret experimental data from heavy ion reactions, are based either on the Boltzmann (BUU) equation or on the quantum molecular dynamics (QMD). Due to their quasiclassical character, they offer a transparent picture of the internal dynamics of reactions and allow one to link the spectrum of the detected particles with individual stages of reactions. They fail, however, to describe some energy and angular distributions of neutrons and protons in low and mid energy domain [80–82]. Appreciable values of the collision delay and space displacements show that the nonlocal collisions should be accounted for.

The nonlocal collisions have been implemented in Ref. [74] within the QMD and in Refs. [75, 76] within the BUU equation. Within the local approximation the distribution of high-energy protons is too low to meet the experimental values. The

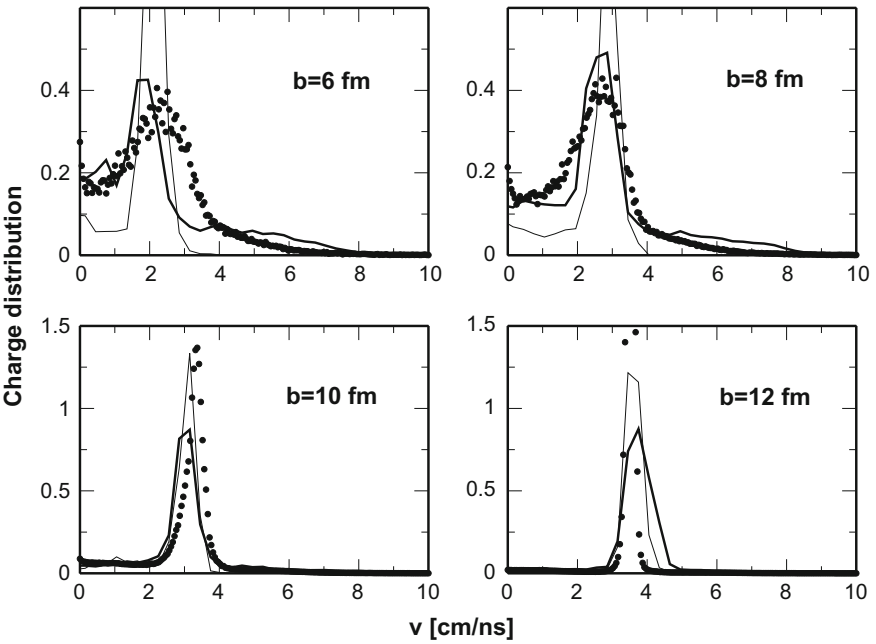

Fig. 25.3 The experimental charge distribution of matter (dotted line) versus velocity in comparison with in the BUU (thin solid line) and the nonlocal model with quasiparticle renormalization (thick line). Redrawn after Ref. [77]

influence of the nonlocal collisions on the reaction of heavy ions has been studied for the $^{181}_{73}\mathrm{Ta} + {}^{197}_{79}\mathrm{Au}$ reaction at 33 MeV [77]. Except for the nonlocal picture, a sufficiently large neck has been achieved by additional inclusion of fluctuations in the Boltzmann (BUU) equation [83, 84], resulting in Boltzmann-Langevin pictures [85–90]. The Boltzmann-Langevin equation has been derived assuming an additional coarse graining of phase-space [91, 92]. Fluctuations to the time-dependent Hartree-Fock (TDHF) equation have been analyzed before in Refs. [93, 94] and tested in Ref. [95].

INDRA observation shows the enhancement of emitted matter in the mid-rapidity region [96, 97]. The simulations can be compared to the experimental data of the Ta + Au collision [77]. In Fig. 25.3, the theoretical and experimental charge density distributions are compared. The experimental charge density distribution has been obtained using the procedure described in Ref. [98]. The data are represented by light gray points, the standard BUU calculation by the thin line and the nonlocal BUU with quasiparticle renormalization calculation by the thick line. A reasonable agreement is found for the nonlocal scenario including quasiparticle renormalization while simple BUU fails to reproduce mid-rapidity matter.

The comparison of the time evolutions of the transverse energy for 8 fm impact parameter can be seen in Fig. 25.4. We recognize that the nonlocal collision scenario

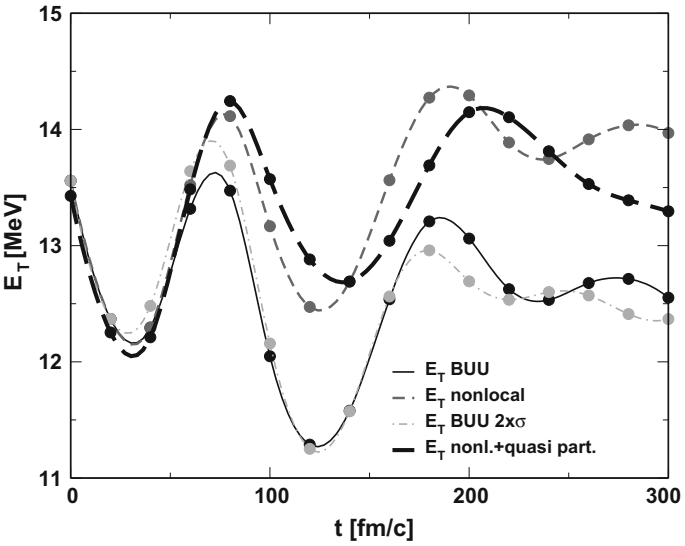

Fig. 25.4 The time evolution of the transverse energy including the Fermi motion for Ta + Au at $E_{\rm lab}/A = 33$ MeV and 8 fm impact parameter in the local BUU (black line), the nonlocal BUU (dashed line), the local BUU with doubled cross section (dashed dotted line) and the nonlocal scenario with the quasiparticle renormalization (long dashed line)

dissipates much more energy due to the inelastic character than by increasing the collision rate. The transverse energies including quasiparticle renormalization have a different period of oscillation which corresponds to a giant resonance. This period becomes longer for the case of quasiparticle renormalization which means that the compressibility decreases. In other words, the quasiparticle renormalization leads to a softer equation of state.

As documented by the improvement of the high-energy proton production and the midrapidity charge density distribution, the nonlocal treatment of the binary collisions brings a desirable contribution to the dynamics of heavy ion reactions. According to the experience from the theory of gases, one can also expect a vital role of non-localities in the search for the equation of state of the nuclear matter. It is encouraging that the nonlocal corrections are easily incorporated into the BUU and QMD simulation codes and do not increase the computational time.

25.4.2 Relation of Pairing Density to Correlated Density

In superconductors the correlated density which we found as the consequence of the time-nonlocality of the collision process, Eq. (25.27), becomes visible as the difference between the total and normal density $n_{\rm corr} = n - n_n$. The Wigner distribution

function has a two-part structure [99]

$$\rho = \frac{1}{2}\left(1+\frac{\xi}{E}\right) f(E) + \frac{1}{2}\left(1-\frac{\xi}{E}\right) f(-E) = \frac{1}{2} - \frac{\xi}{2E}\tanh\frac{1}{2}\beta E, \quad (25.40)$$

where $\xi = \varepsilon_p - \mu$ is the free-particle energy ε_p minus the chemical potential μ. The quasiparticle energy $E = \sqrt{\xi^2 + \Delta^2}$ describes the influence of the superconducting gap Δ on the excitation spectrum of the superconducting state. The Fermi-Dirac distribution is $f(x) = 1/(e^{\beta x}+1)$ with the inverse temperature $\beta = 1/k_{\mathrm{B}}T$. The density n is obtained by the momentum integral over Eq. (25.40) and introducing the density of states $h(\xi) = 2\sum_p 2\pi\delta(\xi - \varepsilon_p)$, one has

$$n = \int_{-\bar{\mu}}^{\infty} \frac{d\xi}{2\pi} h(\bar{\mu}+\xi)\left(\frac{1}{2} - \frac{\xi}{2E}\tanh\frac{1}{2}\beta E\right). \quad (25.41)$$

Here, we account for a possible electrostatic potential φ and the velocity v of superconducting electrons by $\bar{\mu} = \mu - e\varphi - mv^2/2$. For a vanishing gap we obtain the corresponding density n_n of normal electrons with the chemical potential $\bar{\mu}$ by $n_n = n(\Delta = 0)$. The difference

$$n_{\mathrm{corr}} = n - n_n \quad (25.42)$$

describes the correlated density. In the ground state the normal density turns into

$$n_n = 2\sum_p \Theta(\bar{\mu} - \varepsilon_p) \approx n_0 - \left(e\varphi + \frac{m}{2}v^2\right)\frac{h(\mu)}{2\pi} \quad (25.43)$$

where we have expanded $\bar{\mu}$ in first order around the Fermi energy, and n_0 describes the number of particles with no motion and no electrostatic potential. The correlated density Eq. (25.42) splits into two parts in the zero-temperature limit of Eq. (25.41)

$$n_{\mathrm{corr}} = \frac{1}{2}\int_0^{\infty} \frac{d\xi}{2\pi} h(\bar{\mu}+\xi)\frac{\sqrt{\xi^2+\Delta^2}-\xi}{\sqrt{\xi^2+\Delta^2}} - \frac{1}{2}\int_{-\bar{\mu}}^{0} \frac{d\xi}{2\pi} h(\bar{\mu}+\xi)\frac{\sqrt{\xi^2+\Delta^2}+\xi}{\sqrt{\xi^2+\Delta^2}}, \quad (25.44)$$

which vanishes for vanishing gap. Since the gap is only nonzero in the vicinity of the Fermi level given by the Debye frequency ω_D we can restrict the integration to the $\pm\omega_D$-range. Expanding the density of states for $\xi < \omega_D$ we obtain finally [100]

$$n_{\rm corr} = \frac{\partial h}{\partial \mu}\frac{\Delta^2}{4\pi}\left[\ln\left(\frac{\omega_D}{\Delta}+\sqrt{\frac{\omega_D^2}{\Delta^2}+1}\right)-\frac{1}{1+\sqrt{1+\frac{\Delta^2}{\omega_D^2}}}\right] \approx \frac{\partial h}{\partial \mu}\frac{\Delta^2}{4\pi}\ln\left(\frac{2\omega_D}{\sqrt{e}\Delta}\right) \tag{25.45}$$

for $\omega_D \gg \Delta$ in the last step.

Since the total system should stay neutral, we expect $n = n_0$ and the two contributions, $n_n - n_0$ according to Eq. (25.43) and $n_{\rm corr}$ of Eq. (25.45), should cancel. Therefore the required electrostatic potential must read

$$e\varphi = -\frac{m}{2}v^2 + \frac{\partial \ln h}{\partial \mu}\frac{\Delta^2}{2}\ln\left(\frac{2\omega_D}{\sqrt{e}\Delta}\right). \tag{25.46}$$

This resulting electrostatic potential has the form of a Bernoulli potential. Its purpose is to compensate the contribution due to diamagnetic currents and the associated inertial and Lorentz forces. It has a part directly linked to the gap.

The great hope was to measure the Bernoulli potential in order to access directly the gap parameter [101]. The experimental attempts to measure it, however, have yielded no result [102, 103]. Why no signal of thermodynamic corrections is seen remained a puzzle for nearly 30 years. The solution was found by a modification [104] of the Budd-Vannimenus theorem [105] which shows that the surface dipoles cancel the thermodynamical corrections exactly for homogeneous superconductors. The Budd-Vannimenus theorem has been applied also to finite Fermi systems within an exactly solved model to show the BEC-BCS transition in [106].

The electrostatic potential can leak out of a superconductor by three types of charges: (i) The bulk charge which describes the transfer of electrons from the inner to the outer regions of vortices creating a Coulomb force. This force has to balance the centrifugal force by the electrons rotating around the vortex center, the outward push of the magnetic field via the Lorentz force and the outward force coming from the fact that the energy of Cooper pairs is lower than the one of free electrons such that unpaired electrons in the vortex core are attracted towards the condensate around the core [107]. (ii) The surface charge [108] distributed on the scale of the Thomas-Fermi screening length. (iii) The surface dipole which cancels all contributions of pairing forces [109] resulting in an observable surface potential of

$$e\phi_0 = -\frac{f_{\rm el}}{n}. \tag{25.47}$$

The latter one gives rise to characteristic features predicted for experimental observations. The quadrupole resonance lines in the high-T_c material YBCO have been measured [110] and explained in [111, 112].

25.5 Summary

At short time scales after a sudden quench the correlations need time to be formed. This allows to describe the transient time scales by long-ranged time-dependent meanfield fluctuations. This transient time scale is essentially determined by the off-shell motion. At later times when strong correlations are formed there is a cancellation of off-shell processes in the kinetic equation using a proper extended quasiparticle picture. The remaining modifications of the quantum Boltzmann equation consist in the nonlocal collision scenario where the off-sets are uniquely determined by the phase shift of the T-matrix and the quasiparticle energies modifying the drift. The resulting balance equations show besides the quasiparticle parts of the Landau theory also explicit two-particle contributions of short living molecules. The energy and momentum conservation is ensured due to an internal transfer of energy and momentum analogously to a latent heat. Only for the entropy an explicit gain remains.

The entropy as a measure of complexity, or inversely as the loss of information [113], plays a central role in processes like nuclear or cluster reactions [114], where the kinetic and correlation energy of projectile and target particles transform into heat. In nuclear matter, mainly the single-particle entropy [115–119] is discussed as in ultra-cold atoms [120]. The equilibrium entropy has been given in a form of cluster expansion where the two-particle part is given by the two-particle correlation function [121] which has been calculated numerically for different systems [122, 123]. The majority of approaches calculate the classical entropy in various approximations [124, 125]. Here we have obtained the quantum two-particle entropy explicitly in terms of phase shifts of the scattering T-matrix in nonequilibrium. The second law of thermodynamics holds also in nonlocal kinetic theory. The single-particle entropy can decrease on cost of the molecular part of entropy describing the two-particles in a molecular state. Overall, the H-theorem is maintained [79].

The numerical solution of the nonlocal kinetic equation requires no more time than solving the usual Boltzmann equation. Two distinct examples from nuclear collision and from superconductivity have been shortly discussed as illustrative examples.

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