Quasiclassical theory of electronic transport in mesoscopic systems: Luttinger liquids revisited

Ulrich Eckern[*] and **Peter Schwab**[**]

Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

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The method of the quasiclassical Green's function is used to determine the equilibrium properties of one-dimensional (1D) interacting Fermi systems, in particular, the bulk and the local (near a hard wall) density of states. While this is a novel approach to 1D systems, our findings do agree with standard results for Luttinger liquids obtained with the bosonization method. Analogies to the so-called $P(E)$ theory of tunneling through ultrasmall junctions are pointed out and are exploited. Further applications of the Green's function method for 1D systems are discussed.

1 Introduction

Quasiclassical methods, developed several years ago and used successfully to describe non-equilibrium states in superconductors and superfluids (see, e.g., [1–4]), have recently been extended to meso- and nanoscopic systems. This became possible after the formulation of boundary conditions, including hybrid structures and interface roughness [5–7]. In recent developments we focussed on spin-effects and spatial confinement, e.g., concerning the spin-Hall effect in a 2D electron gas [8], and spin relaxation in narrow wires in the presence of spin–orbit coupling [9]. Within the quasiclassical approach, it is also possible to study the influence of disorder and Coulomb interaction on the same footing [10, 11], which is manageable since the method works on an intermediate level: microscopic details of the wave-functions, on the scale of the interatomic distance, are integrated out, leaving equations of motion which can be solved with sufficient accuracy.

As an illustrative example, we apply in this paper the quasiclassical method to determine the equilibrium Green's function, and hence the density of states (DoS), of the (spinless) 1D model known as Luttinger liquid [12–14]. This model contains two fermionic branches, linearized near the Fermi points, with v_F and $N_0 = (\pi v_\mathrm{F})^{-1}$ the bare Fermi velocity and DoS. Only interaction processes with small ($\ll k_\mathrm{F}$) momentum transfer are considered: standard parameters are g_4 and g_2, for scattering processes involving only one or both branches, respectively. The dimensionless quantities $\gamma_4 = g_4/2\pi v_\mathrm{F}$ and $\gamma_2 = g_2/2\pi v_\mathrm{F}$ are useful. The spectrum of charge fluctuations is linear, $\omega(q) = v|q|$; the renormalized velocity, v, and the parameter K, given by

$$v = v_\mathrm{F}\left[(1+\gamma_4)^2 - \gamma_2^2\right]^{1/2}, \qquad K = \left[\frac{1+\gamma_4-\gamma_2}{1+\gamma_4+\gamma_2}\right]^{1/2}, \tag{1}$$

are often called Luttinger liquid parameters.

[*] Corresponding author: e-mail: ulrich.eckern@physik.uni-augsburg.de
[**] e-mail: peter.schwab@physik.uni-augsburg.de

In the following Section 2 we discuss the solution of the equation of motion for the quasiclassical Green's function in the presence of a fluctuating potential, the latter representing the fermion-fermion interaction. The Keldysh technique is employed throughout. Considering the average – with respect to the fluctuating field – of the Green's function and an analogy to the $P(E)$ theory, the field fluctuations are related to an effective impedance of the Luttinger liquid, and finally to the DoS (Section 3). In Section 4 we consider an insulating boundary, i.e. a reflecting wall, and determine the DoS boundary exponent. A concluding discussion is given in Section 5.

2 Quasiclassical equation of motion and its solution

In essence, the Keldysh technique [15, 16] differs from the zero-temperature and the Matsubara approach by employing time-ordering along a contour which runs from $-\infty$ to $+\infty$ and back to $-\infty$. Rewriting the theory in terms of standard $(-\infty \ldots +\infty)$ integrations, a 2×2 matrix structure results; e.g., the Green's function can be cast into the form

$$\check{G} = \begin{Bmatrix} G^{\mathrm{R}} & G^{\mathrm{K}} \\ 0 & G^{\mathrm{A}} \end{Bmatrix}. \tag{2}$$

Accordingly, considering some general 2-particle interaction V_0 and decoupling this interaction using the Hubbard–Stratonovich transformation within the path-integral formalism, two auxiliary fields are necessary. As a result, the Green's function can be expressed as an average of the free-particle Green's function in the presence of fluctuating potentials as follows (see, e.g., Ref. [10]):

$$\check{G} = \langle \check{G}_0[\Phi]\, \mathrm{e}^{\mathrm{Tr}\ln(\check{1}+\check{G}_0\check{\Phi})} \rangle_{0,\Phi} = \langle \check{G}_0[\Phi] \rangle_{\Phi} \,. \tag{3}$$

Here $\check{G}_0$ is the free-particle Green's function, and $\check{G}_0^{-1}[\Phi] = \check{G}_0^{-1} + \check{\Phi}$, where $\check{\Phi} = \phi_1 \check{\sigma}_1 + \phi_2 \check{\sigma}_1$; $\check{\sigma}_0$ and $\check{\sigma}_1$ denote the unit and the first Pauli matrix, and ϕ_1 and ϕ_2 correspond to the two potentials mentioned above. Furthermore, $\langle \ldots \rangle_{0,\Phi}$ denotes an average which is Gaussian by construction, and defined such that

$$\langle \phi_i(xt)\, \phi_j(x't') \rangle_{0,\Phi} = \frac{i}{2} \begin{Bmatrix} V_0^{\mathrm{K}} & V_0^{\mathrm{R}} \\ V_0^{\mathrm{K}} & 0 \end{Bmatrix}_{ij} (xt, x't') \,, \tag{4}$$

where for clarity space (x) and time (t) arguments are included. The average $\langle \ldots \rangle_{\Phi}$, defined through Eqs. (3) and (4), can be non-Gaussian. (The spin will be suppressed througout this paper.) Note that a "real" electrical potential can be included by the replacement $\phi_1 \to \phi_1 + e\phi_{\mathrm{ext}}$ in $\check{G}_0[\Phi]$ of Eq. (3); the particle's charge is $-e$. In the next step, we consider the quasiclassical approximation, i.e. we consider the difference $\check{G}_0^{-1}[\Phi]\,\check{G}_0[\Phi] - \check{G}_0[\Phi]\,\check{G}_0^{-1}[\Phi] = 0$, keeping only the leading terms in the gradients with respect to the (spatial) center-of-mass coordinate (which we again denote by x). The equation is then integrated with respect to the magnitude of the momentum. The result is

$$\left[\frac{\partial}{\partial t} + \frac{\partial}{\partial t'} + v_{\mathrm{F}} \hat{p} \cdot \nabla_x \right] \check{g}_{tt'}(\hat{p}x) = i[\check{\Phi}, \check{g}] \,, \tag{5}$$

where $\hat{p}$ is the direction of the center-of-mass momentum, and

$$[\check{\Phi}, \check{g}] \equiv \check{\Phi}(xt)\, \check{g}_{tt'}(\hat{p}x) - \check{g}_{tt'}(\hat{p}x)\, \check{\Phi}(xt') \,. \tag{6}$$

The quantity $\check{g}_{tt'}(\hat{p}x)$ is the so-called quasiclassical Green's function,

$$\check{g}_{tt'}(\hat{p}x) = \frac{i}{\pi} \int \mathrm{d}\xi \check{G}_{tt'}(\boldsymbol{p}, x) \,, \qquad \xi = p^2/2m - \mu \,, \tag{7}$$

a major advantage compared to the full Green's function is the normalization, $\check{g}\check{g} = \check{1}$. It should be noted that in the quasiclassical approximation, only long-wavelength contibutions of the fluctuating fields are taken into account – which is adequate for the problem addressed below. In the 1D case, $\nabla_x \to \partial_x$, and $\check{p} = \pm$. For the homogeneous equilibrium case, the solution is

$$\check{g}_0(\varepsilon) = \begin{Bmatrix} 1 & 2F(\varepsilon) \\ 0 & -1 \end{Bmatrix}, \tag{8}$$

where the Fourier transformed $(t - t' \to \varepsilon)$ quantity is given, and $F(\varepsilon) = \tanh(\beta\varepsilon/2)$, $\beta = 1/k_{\mathrm{B}}T$. A formal solution of Eq. (5) is found with the ansatz

$$\check{g}_{tt'}(\hat{p}x) = \mathrm{e}^{i\check{\varphi}(xt)}\, \check{g}_{0,t-t'}\, \mathrm{e}^{-i\check{\varphi}(xt')} \tag{9}$$

provided

$$(\partial_{\mathrm{t}} + v_{\mathrm{F}}\hat{p}\partial_x)\, \varphi(xt) \equiv D_{xt}\check{\varphi}\ (xt) = \check{\Phi}(xt)\,. \tag{10}$$

Apparently, $\check{\varphi}$ has the same matrix structure as $\check{\Phi}$, namely $\check{\varphi} = \varphi_1\check{\sigma}_0 + \varphi_2\check{\sigma}_1$. For example, we obtain explicitly from (9):

$$g^{\mathrm{R}}(tt') = \delta(t-t') - 2iF(tt')\cos\varphi_2 \sin\varphi_2'\, \mathrm{e}^{i(\varphi_1 - \varphi_1')}\,, \tag{11}$$

$$g^{\mathrm{K}}(tt') = 2F(tt')\cos\varphi_2 \cos\varphi_2'\, \mathrm{e}^{i(\varphi_1 - \varphi_1')}\,, \tag{12}$$

where $\varphi_j \equiv \varphi_j(xt)$ and $\varphi_j' \equiv \varphi_j(xt')$ for brevity. We will discuss below that, for the Luttinger model, it is sufficient to assume that the phases are Gaussian distributed. It is then straightforward to determine $\langle\check{g}\rangle_\phi$; for example, we obtain[1]

$$\langle\check{g}^{\mathrm{R}}\rangle_\Phi(tt') = \delta(t-t') + F(tt')\,\mathrm{e}^{-J_0(tt')}\,[\sinh(J_1(tt')) - \sinh(J_2(tt'))]\,, \tag{13}$$

$$= -\langle\check{g}^{\mathrm{A}}\rangle_\Phi(t't)\,, \tag{14}$$

where

$$J_0(tt') = \langle(\varphi_1 - \varphi_1')^2\rangle_\Phi/2 = J^{\mathrm{K}}(0) - J^{\mathrm{K}}(tt')\,, \tag{15}$$

$$J_1(tt') = \langle(\varphi_1 - \varphi_1')\,(\varphi_2 + \varphi_2')\rangle_\Phi = J^{\mathrm{R}}(tt') - J^{\mathrm{A}}(tt')\,, \tag{16}$$

$$J_2(tt') = \langle(\varphi_1 - \varphi_1')\,(\varphi_2 - \varphi_2')\rangle_\Phi = -J^{\mathrm{R}}(tt') - J^{\mathrm{A}}(tt')\,. \tag{17}$$

Note that J_0 and J_2 are even, and F and J_1 are odd under time reversal, $t - t' \to t' - t$. Then we define $J = -J_0 + J_1$, such that

$$J(t) = \int \frac{\mathrm{d}\omega}{2\pi}[J^{\mathrm{R}}(\omega) - J^{\mathrm{A}}(\omega)]\,[B(\omega) + 1]\,(\mathrm{e}^{-i\omega t} - 1)\,, \tag{18}$$

[1] The quantities discussed from here on depend on the time difference, $t - t'$, but we nevertheless use the notation tt' for brevity.

where $B(\omega) = \coth(\beta\omega/2)$, and we used $J^{\mathrm{K}}(\omega) = [J^{\mathrm{R}}(\omega) - J^{\mathrm{A}}(\omega)]\, B(\omega)$. From the relation $J^{\mathrm{R}}(tt') = J^{\mathrm{A}}(t't)$ we obtain $J^{\mathrm{A}}(\omega) = J^{\mathrm{R}}(-\omega)$, implying that $J^{\mathrm{R}}(\omega) - J^{\mathrm{A}}(\omega)$ is odd in frequency. Combining the above relations, the (normalized) DoS is given by

$$\begin{aligned} N(\varepsilon) = \mathrm{Re}\, g^{\mathrm{R}}(\varepsilon) &= 1 + \pi \int \mathrm{d}t\, \mathrm{e}^{i\varepsilon t}\, \{F(tt')\,[P(tt') - P(t't)]\}_{t'=0} \\ &= 1 + \tfrac{1}{2} \int \mathrm{d}\omega\, F(\varepsilon - \omega)\,[P(\omega) - P(-\omega)] \end{aligned} \tag{19}$$

with

$$P(\omega) = \frac{1}{2\pi} \int \mathrm{d}t\, \mathrm{e}^{J(t) + i\omega t}\,. \tag{20}$$

Note that $P(t=0) = 1/2\pi$, i.e. $\int \mathrm{d}\omega\, P(\omega) = 1$.

In order to complete the argument, the phase fluctuations are easily related to the potential fluctuations, according to the relation (compare Eq. (10))

$$J^{\mathrm{R}}(t) = \langle \varphi_1(xt)\, \varphi_2(x0) \rangle_\Phi = [D^{-1}_{xt} D^{-1}_{x't'} \langle \phi_1(xt)\, \phi_2(x't') \rangle_\Phi]_{x=x',t'=0}\,, \tag{21}$$

and the potential fluctuation can be related to the interaction. This last step, however, requires some discussion. First, note that expanding the exponent in Eq. (3) up to second order, neglecting higher order terms, corresponds to the random phase approximation (RPA). Given this (Gaussian) approximation, the procedure for performing the phase average, outlined above, is permitted. As an important point, however, *the RPA is known to be exact for calculating the density response of the Luttinger model*, and hence the effective interaction, which concludes the argument: the potential fluctuations are given by

$$\langle \phi_1(xt)\, \phi_2(x't') \rangle_\Phi = \frac{i}{2} V^{\mathrm{R}}(xt, x't')\,, \tag{22}$$

where $V^{\mathrm{R}}(xt, x't')$ is the screened (RPA) interaction. Thus $J^{\mathrm{R}} = (i/2)\, D^{-1} D^{-1} V^{\mathrm{R}}$ in an obvious short-hand notation.

3 Effective impedance and bulk DoS

The approach described in the preceding section is very similar to the theory of charge tunneling in ultrasmall junctions, as reviewed, e.g., in [17], which is also known as $P(E)$ theory. (See also [18] for related articles.) In this context, the quantity $P(E)$ characterizes the influence of the environment on the tunneling between the two electrodes. For example, the forward tunneling rate is found to be given by

$$\vec{\Gamma}(V) = (e^2 R_{\mathrm{T}})^{-1} \int \mathrm{d}E\, \mathrm{d}E'\, f(E)\,[1 - f(E' + eV)]\, P(E - E')\,, \tag{23}$$

where V is the voltage, R_{T} the tunneling resistance, and $f(E)$ the Fermi function. Note the detailed balance condition $P(-E) = \mathrm{e}^{-\beta E}\, P(E)$. Physically, $P(E)$ describes the probability of exchanging the energy E with the environment [17].

On the other hand, in the present context, consider the tunneling rate from the interacting one-dimensional wire into a non-interacting lead, which clearly is given by

$$\vec{\Gamma}(V) = (e^2 R_{\mathrm{T}})^{-1} \int \mathrm{d}\varepsilon\, f(\varepsilon)\, N(\varepsilon)\,[1 - f(\varepsilon + eV)]\,, \tag{24}$$

with $N(\varepsilon)$ the normalized DoS as given in Eq. (19). Using this equation as well as the properties of $P(\omega)$ as described in the previous section and the detailed balance condition, it is straightforward to confirm

that Eqs. (23) and (24) coincide, provided $P(E)$ from the tunneling theory is identified with $P(\omega)$. The reason for the complete correspondence between these two quantities is apparent on physical grounds, since the quantity $P(\omega)$ characterizing the Luttinger liquid arises from the auxiliary potential fluctuations due to the fermion–fermion interaction. In the zero-temperature limit, one finds easily

$$N(\varepsilon) = \int_0^{|\varepsilon|} \mathrm{d}\omega \, P(\omega) \qquad (T = 0) \,. \tag{25}$$

Exploiting the analogy further, we identify

$$J^{\mathrm{R}}(\omega) - J^{\mathrm{A}}(\omega) \equiv \frac{2\pi}{\omega} \frac{\mathrm{Re}\, Z(\omega)}{R_{\mathrm{K}}} \,, \tag{26}$$

where $R_{\mathrm{K}} = h/e^2 = 2\pi\hbar/e^2$ is the Klitzing constant, and we may call $Z(\omega)$ effective impedance of the Luttinger liquid. For the simple example of an ohmic impedance with a high-frequency cut-off

$$\frac{\mathrm{Re}\, Z(\omega)}{R_{\mathrm{K}}} = \frac{1}{g} \frac{1}{1 + (\omega/\omega_{\mathrm{R}})^2} \tag{27}$$

the result is [17]

$$P(\omega) = \frac{\mathrm{e}^{-2\gamma/g}}{\Gamma(2/g)} \frac{1}{\omega} \left[\frac{\omega}{\omega_{\mathrm{R}}} \right]^{2/g} \qquad (T = 0, 0 < \omega < \omega_{\mathrm{R}}) \,, \tag{28}$$

where γ is Euler's constant. Thus the DoS is found to vanish at the Fermi energy, $N(\varepsilon) \sim |\varepsilon|^{2/g}$, where the exponent is given by

$$\frac{2}{g} = 2 \left\{ \frac{\omega}{2\pi} [J^{\mathrm{R}}(\omega) - J^{\mathrm{A}}(\omega)] \right\}_{\omega \to 0} = -i \left\{ \frac{\omega}{\pi} \int \frac{\mathrm{d}q}{2\pi} \frac{V^{\mathrm{R}}(q\omega)}{(-i\omega + 0 + iqv_{\mathrm{F}})^2} \right\}_{\omega \to 0} \,, \tag{29}$$

where $V^{\mathrm{R}}(q\omega)$ is the screened retarded interaction. In order to determine this quantity, consider the 2×2 matrix structure of right- and left-moving particles, denoted by "+" and "−", the bare interaction and the non-interacting response function:

$$\hat{V}_0 = \begin{Bmatrix} g_4 & g_2 \\ g_2 & g_4 \end{Bmatrix}, \qquad \hat{\chi}_0 = \frac{1}{2\pi v_{\mathrm{F}}} \begin{Bmatrix} \dfrac{qv_{\mathrm{F}}}{-\omega - i0 + qv_{\mathrm{F}}} & 0 \\ 0 & \dfrac{qv_{\mathrm{F}}}{+\omega + i0 + qv_{\mathrm{F}}} \end{Bmatrix}, \tag{30}$$

as well as the RPA equation $\hat{V}^{\mathrm{R}} = (\hat{1} + \hat{V}_0 \hat{\chi}_0)^{-1} \hat{V}_0$. This matrix structure implies that we have to introduce a branch index for the fluctuating fields, which we suppressed up to now: $\breve{\varphi}, \breve{\Phi} \to \breve{\varphi}_{\pm}, \breve{\Phi}_{\pm}$. The density of states of the right-moving particles, for example, is determined from the $\breve{\varphi}_+ - \breve{\varphi}_+$ correlation functions. The relevant quantity, $\hat{V}^{\mathrm{R}}_{++}$, is straightforwardly determined and inserted into Eq. (29); the q-integral can be done by contour integration, and we obtain the standard [19] result:[2]

$$2/g = (K + K^{-1} - 2)/2 \,. \tag{31}$$

[2] See [20] for a recent summary. Note that often the parameter K is denoted by g, which we avoid here since we prefer to use the latter symbol for the dimensionless conductance, see Eq. (27), in accordance with the $P(E)$ theory [17].

4 DoS boundary exponent

Near a boundary or an interface the quasiclassical approximation is insufficient, and the quasiclassical propagators pointing into or out of the boundary (or interface) have to be connected by boundary conditions [5, 21]. The boundary condition is particularly simple for spinless fermions in one dimension at an impenetrable wall: obviously $\check{g}_{tt'}(\hat{p}x) = \check{g}_{tt'}(-\hat{p}x)$, to ensure that there is no current through the wall.

In the following we assume that the wall is located at $x = 0$, and that the particles move in the half-space $x < 0$. Instead of considering two branches of fermions in this half-space, we find it more convenient to mirror the left movers at the boundary and to consider only right movers in the full space, i.e.

$$\check{g}_{tt'}(+, x) = \begin{cases} \check{g}_{tt'}(+, x) & \text{for} \quad x < 0\,, \\ \check{g}_{tt'}(-, -x) & \text{for} \quad x > 0\,, \end{cases} \tag{32}$$

$$\check{\Phi}_{+}(x) = \begin{cases} \Phi_{+}(x) & \text{for} \quad x < 0\,, \\ \Phi_{-}(x) & \text{for} \quad x > 0\,. \end{cases} \tag{33}$$

This Green's function solves Eq. (5) both for $x \geq 0$ and $x \leq 0$. The bare interaction is now given in real space by

$$V_0(x, x') = g_4 \delta(x - x') + g_2 \delta(x + x')\,. \tag{34}$$

The Fourier transfrom of V_0 is thus off-diagonal in momentum space, since the g_2-term couples q with $-q$. Considering now the 2×2 matrix structure of particles with momentum q and $-q$, the bare interaction is

$$\begin{Bmatrix} V_{0,q,q} & V_{0,q,-q} \\ V_{0,-q,q} & V_{0,-q,-q} \end{Bmatrix} = \begin{Bmatrix} g_4 & g_2 \\ g_2 & g_4 \end{Bmatrix}, \tag{35}$$

i.e. identical to what was given in Eq. (30) above with just a different meaning of the matrix index. Also the non-interacting response function and the RPA equation for the screended interaction are the same as before. Due to the absence of translation symmetry the effective impedance depends on the distance from the boundary, and is given by

$$\frac{\mathrm{Re}\, Z(x, \omega)}{R_\mathrm{K}} = \frac{\omega}{2\pi}\, \mathrm{Im} \left[\int \frac{\mathrm{d}q}{2\pi}\, \frac{V^{\mathrm{R}}_{q,q}(\omega)}{(-i\omega + iqv_\mathrm{F})^2} + \mathrm{e}^{2iqx}\, \frac{V^{\mathrm{R}}_{q,-q}(\omega)}{(-i\omega + iqv_\mathrm{F})\,(-i\omega - iqv_\mathrm{F})} \right] \tag{36}$$

$$= \frac{1}{4} \left[K + K^{-1} - 2 + \cos\,(2\omega x/v)\,(K^{-1} - K) \right]. \tag{37}$$

Hence the density of states at the boundary is found to vanish as

$$N(\varepsilon) \sim |\,\varepsilon\,|^{(1-K)/K} \tag{38}$$

in agreement with the boundary exponent obtained in [22], and the impurity exponent given in [23]. In fact this result has been considerably debated [20, 23, 24]; compare also [25], as well as the detailed presentation by von Delft and Schoeller [26].[3]

[3] These authors emphasize the importance of a proper handling of Klein factors, i.e. fermionic anticommutation relations. For more recent studies of this aspect, see, for example, Ref. [27].

5 Summary

Quasiclassical theory is known to be a useful tool in the theoretical description of superconductors and superfluids, including non-equilibrium states and interfaces. For normal-conducting electrons the theory mainly serves for the microscopic foundation of a Boltzmann-like transport theory. However, when taking into account the Coulomb interaction in terms of a fluctuating Hubbard–Stratonovich field, the theory also captures important interaction effects, which are beyond the reach of the Boltzmann equation. In this article we illustrated this by considering the one-dimensional version of the theory, and demonstrated that it is possible to describe the non-Fermi liquid physics of Luttinger liquids. The mathematics involved is very similar to the $P(E)$ theory of tunneling, which we made use of in this article, and also to the functional bosonization approach to Luttinger liquids [28] (which we did not exploit here). We concentrated on the spinless case and on thermal equilibrium; the spin is straightforwardly included in the theory, and clearly – since we use the Keldysh formalism – non-equilibrium situations can be covered as well. We are confident that in the future the quasiclassical theory will become a useful, complementary approach to transport in interacting one-dimensional systems.

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