Ann. Phys. (Leipzig) **8** (1999) Spec. Issue, 65 – 68

Local fields in non–linear quantum transport

A. Fechner[1], **G. Cuniberti**[2], **M. Sassetti**[3], **and B. Kramer**[1]

[1] I. Inst. für Theor. Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg
[2] Max–Planck–Inst. für Physik komplexer Systeme, Nöthnitzerstraße 38, D-01187 Dresden
[3] Dipartimento di Fisica, INFM, Università di Genova, Via Dodecaneso 33, I-16146 Genova
`fechner@physnet.uni-hamburg.de`

Received 30 July 1999, accepted 1 August 1999 by M. Schreiber

Abstract. We investigate the dynamical interplay between currents and electromagnetic fields in frequency-dependent transport through a single-channel quantum wire with an impurity potential in the presence of electron-electron interactions. We introduce and discuss a formalism which allows a self-consistent treatment of currents and electromagnetic fields.

Keywords: strongly correlated systems, non–linear effects, fermions in reduced dimensions
PACS: 71.10Pm, 72.20Ht, 42.65Ky

1 Introduction

In order to describe frequency-dependent quantum transport properties, it is necessary to take into account local fields. However, since the microscopic charge and current distributions are rapidly varying functions of space and time the solution of Maxwell's equations is a complex task. Especially in the presence of non–linear effects, a self-consistent theory of frequency and time dependent transport is very challenging [1].

Here, we address this question for a simple but nonetheless non-trivial system, namely a single-channel quantum wire of interacting electrons with one potential barrier embedded in three dimensions (3D). The interaction is taken into account using the Luttinger model [2, 3]. The system has a non–linear dc-current-voltage characteristic due to the simultaneous presence of both, the electron-electron interaction and the tunnel barrier [4, 5]. We demonstrate explicitly the essential features of self–consistency for an infinite barrier. The connection between local and external field is worked out and generalized to the situation of a finite barrier. The results of the present considerations are the starting point for the more general case, namely the non-linear, frequency dependent transport effects in (1D) disordered systems containing many impurities.

2 Local fields

For a discussion of local-field effects one has to distinguish between longitudinal electric fields, $\nabla \times \boldsymbol{E}_L(\boldsymbol{r},\omega) = 0$, and transverse electric fields, $\nabla \cdot \boldsymbol{E}_T(\boldsymbol{r},\omega) = 0$. Using the microscopic Maxwell equations and the continuity equation, they are connected with each other and with the currents as well as in general an external field [1],

$$\boldsymbol{E}_{\rm L}(\boldsymbol{q},\omega) = \boldsymbol{E}_{\rm L,ext}(\boldsymbol{q},\omega) + \frac{1}{{\rm i}\epsilon_0\omega}\boldsymbol{J}_{\rm L}(\boldsymbol{q},\omega) \tag{1}$$

$$\boldsymbol{E}_{\rm T}(\boldsymbol{q},\omega) = \boldsymbol{E}_{\rm T,ext}(\boldsymbol{q},\omega) + {\rm i}\mu_0\omega g_0(\boldsymbol{q},\omega)\boldsymbol{J}_{\rm T}(\boldsymbol{q},\omega), \tag{2}$$

where $g_0(\boldsymbol{q},\omega) = [|\boldsymbol{q}|^2 - (\omega/c)^2]^{-1}$. The longitudinal and transverse currents are related to the total current $\boldsymbol{J}$ by $\boldsymbol{J}_{\rm L}(\boldsymbol{q},\omega) = \boldsymbol{q}\,[\boldsymbol{q}\cdot\boldsymbol{J}(\boldsymbol{q},\omega)]/q^2$ and $\boldsymbol{J}_{\rm T}(\boldsymbol{q},\omega) = \boldsymbol{J}(\boldsymbol{q},\omega) - \boldsymbol{J}_{\rm L}(\boldsymbol{q},\omega)$. In order to evaluate the local fields one has to close eqs. (1) and (2) by a transport equation which connects currents and local fields in terms of a microscopic theory. In a linear system, this would be the Kubo theory. In the general case, the non-linear relation between the current and the local field has to be used.

3 The model

In order to apply Maxwell's equations, which incorporate naturally Coulomb interaction, the quantum wire has to be considered as embedded in 3D. This is achieved by assuming a confinement perpendicular to the, say, x-direction and projecting the relevant operators onto the eigenfunctions of the confinement Hamiltonian. We use $\Phi_{nk}(\boldsymbol{r}) = e^{{\rm i}kx}\varphi_n(\boldsymbol{R})/\sqrt{L}$ as a complete set of functions where k is the wavenumber along the direction of the wire, L the system length along x, $\varphi_n(\boldsymbol{R})$ the confinement wave function ($\boldsymbol{R} = (y,z)$), and n the corresponding quantum numbers.

The Hamiltonian consists of the kinetic energy, the electron-electron interaction, the confinement energy, the coupling to the scalar electric potential $V(\boldsymbol{r},t)$, and the potential barrier of height $U_{\rm b}$ at $x_{\rm b}$, $H = H_{\rm kin} + H_{\rm conf} + H_{\rm int} + H_{\rm em} + H_{\rm b}$, with

$$H_{\rm int} = \sum_{n,l,s,p}\int\int {\rm d}x{\rm d}x'\,\Psi_n^\dagger(x)\Psi_l(x)U_{nlsp}(x-x')\Psi_s^\dagger(x')\Psi_p(x') \tag{3}$$

$$H_{\rm em} = e\int {\rm d}\boldsymbol{r}\rho(\boldsymbol{r})V(\boldsymbol{r},t), \tag{4}$$

$$H_{\rm b} = \int {\rm d}\boldsymbol{r}\rho(\boldsymbol{r})U_{\rm b}(\boldsymbol{r}), \tag{5}$$

where,

$$U_{nlsp}(x-x') = \int_S\int_{S'} {\rm d}^2R\,{\rm d}^2R'\,\varphi_n^*(\boldsymbol{R})\varphi_l(\boldsymbol{R})U_{\rm ee}(\boldsymbol{r}-\boldsymbol{r}')\varphi_s^*(\boldsymbol{R}')\varphi_p(\boldsymbol{R}') \tag{6}$$

is the projected interaction potential, $\Psi_n(x)$ the fermion field of the n-th band,

$$\rho(\boldsymbol{r}) = \sum_{n,l}\varphi_n^*(\boldsymbol{R})\varphi_l(\boldsymbol{R})\Psi_n^\dagger(x)\Psi_l(x), \tag{7}$$

the charge density. The current is related to $\rho(\boldsymbol{r})$ via the 3D continuity equation.

The scalar electric potential in eq. (4) is the local potential. In general, the local vector potential should also be included because even for a longitudinal external source, a transverse field is generated. However, the amplitude of the induced transverse field is of the order $(v_{\rm F}/c)^2$, thus negligible [6], and eq. (2) does not contribute.

The above general expressions are needed in order to treat especially quantum wires with more than one subband. Here, we restrict to only one subband, thus $n = l = s = p = 0$.

The dispersion relation of the collective excitations obtained by using the Luttinger model [2, 3] is $\omega(q) = |q|v_{\rm F}[1 + U(q)/\pi\hbar v_{\rm F}]^{1/2}$, where $q \equiv q_x$. It reflects the Fourier transform of the interaction potential, $U(q) \equiv U_{0000}(q)$ [7].

4 Some simple examples

Neglecting currents and induced fields perpendicular to the wire, eq. (1) can be rewritten in terms of the local field projected onto the lowest subband,

$$E(q,\omega) = E_{\rm ext}(q,\omega) - \frac{iq^2}{e^2\omega}U(q)J(q), \tag{8}$$

where $J(q)$ is the x component of the current.

The clean Luttinger wire was already discussed in [7]. The frequency–dependent conductivity is in this case

$$\sigma(q,\omega) = \frac{{\rm i}e^2 v_{\rm F}}{\pi\hbar}\frac{\omega}{\omega^2 - \omega^2(q)}. \tag{9}$$

One can show that the current of the non–interacting system driven by the local field is equivalent to the current through the interacting system in response to the external field, $E(q,\omega)\sigma_0(q,\omega) = E_{\rm ext}(q,\omega)\sigma(q,\omega)$, where $\sigma_0(q,\omega)$ corresponds to the conductivity of the non–interacting wire. In the following we will see that this remains true in the presence of a tunnel barrier of infinite strength where the non–linearity does not play any role.

In the presence of a single potential barrier, assumed to be uniform over the cross–section of the wire, $U_{\rm b}(\boldsymbol{r}) = U_{\rm b}\delta(x - x_{\rm b})$, a relation can be derived which links the current at different positions [8]. In wave number space,

$$I(q,\omega) = I_0(q,\omega) + r(q,\omega)[I_{\rm b}(\omega) - I_{0,{\rm b}}(\omega)] \tag{10}$$

where $I_0(q,\omega)$ represents the current in the clean system, $I_{\rm b}(\omega)$ is the current at the barrier, and the ratio of conductivities without barrier at the two positions considered is $r(x,\omega) = \sigma(x - x_{\rm b},\omega)/\sigma(x = 0,\omega)$. The total current is non–linear due to the presence of $I_{\rm b}$ [9].

In order to demonstrate how self–consistency affects the electric field inside the wire, we start with an infinite barrier, $I_b = 0$, decoupling the system into two separate wires. In this case, dc–transport is forbidden but the displacement contribution to the current is finite.

We evaluate the linear current in eq. (10) in terms of the local field by using the conductivity of the non–interacting system. Inserting this into eq. (8), gives a self–consistent equation for the local field. The solution is

$$E(q,\omega) = \frac{\sigma(q,\omega)}{\sigma_0(q,\omega)}E_{\rm ext}(q,\omega) - \frac{\sigma(q,\omega)}{\sigma_0(q,\omega)}\,e^{{\rm i}qx_{\rm b}}\frac{\int dq\,\sigma(-q,\omega)e^{-{\rm i}qx_{\rm b}}E_{\rm ext}(q,\omega)}{\sigma(x=0,\omega)}. \tag{11}$$

It is important to note that an equivalent result would have been obtained by driving the current with the external field using the conductivity of the interacting system in complete analogy with the single clean wire mentioned above. This is consistent with the common textbook knowledge [10] that without a non–linearity the Coulomb interaction is automatically taken into account self–consistently in the Luttinger model.

The second term in eq. (11) represents the contribution due to the barrier. In order to show its influence on the local field we consider $\omega \to 0$. For zero–range interactions it generates a delta peak at the position of the barrier which is broadened when increasing the range of the interaction.

For a finite barrier, I_b is highly non–linear due to the presence of the interaction [4]. It is then easy to show from eq. (10) that the two cases, (i) interacting system driven by external field and (ii) non–interacting system driven by local field are no longer equivalent. In order to take properly into account the combined effect of the interaction, the non–linearity as well as the local fields, the current at the barrier has to be driven by the local field but here incorporating also the interaction.

5 Summary

We investigated self-consistency in time-dependent transport through a non–linear system, in particular through a quantum wire with a tunnel barrier. For an infinite barrier, we obtained that by renormalising the electric field the current is given by the conductivity of the non-interacting system. In the non-linear case, one has to consider both, the renormalized field and the interaction.

This work was supported by the EU within the TMR program, INFM via PRA(QTMD)97, Cofinanziamento (MURST)98 and the Deutsche Forschungsgemeinschaft via the SFB 508 of the Universität Hamburg

References

[1] O. Keller, Phys. Rep. **268** (1996) 85
[2] F. D. M. Haldane, J. Phys. C **14** (1981) 2585
[3] J. Voit, Rep. Prog. Phys. **58** (1995) 977
[4] C. L. Kane and M. P. A. Fisher, Phys. Rev. B **46** (1992) 15233
[5] G. Cuniberti, M. Sassetti, and B. Kramer, Europhys. Lett. **37** (1997) 421
[6] A. Fechner, M. Sassetti, and B. Kramer, unpublished
[7] G. Cuniberti, M. Sassetti, and B. Kramer, Phys. Rev. B **57** (1998) 1515
[8] M. Sassetti and B. Kramer, Phys. Rev. B **54** (1996) R5203
[9] A. Fechner, M. Sassetti, and B. Kramer, Europhys. Lett. **45** (1999) 693
[10] G. D. Mahan, *Many–Particle Physics*, Plenum Press, New York 1981